



**Technical Report Series on Global Modeling and Data Assimilation,
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Randal D. Koster, Editor

**Soil Moisture Active Passive (SMAP) Project Assessment Report
for Version 4 of the L4_SM Data Product**

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EXECUTIVE SUMMARY

This report provides an assessment of Version 4 of the SMAP Level 4 Surface and Root Zone Soil Moisture (L4_SM) product, released on 14 June 2018. The assessment includes comparisons of L4_SM soil moisture and temperature estimates with in situ measurements from core validation sites and sparse networks. The assessment further includes a global evaluation of the internal diagnostics from the ensemble-based data assimilation system that is used to generate the L4_SM product, including observation-minus-forecast (O-F) brightness temperature residuals and soil moisture analysis increments. Together, the core validation site comparisons and the statistics of the assimilation diagnostics are considered primary validation methodologies for the L4_SM product. Comparisons against in situ measurements from regional-scale sparse networks are considered a secondary validation methodology because such in situ measurements are subject to upscaling errors from the point-scale to the grid-cell scale of the data product.

The Version 4 L4_SM product benefits from an improved land surface modeling system and from retrospective surface meteorological forcing data that are as consistent as possible with the present-day data in terms of their climatology. Specifically, the model changes include revised parameters and parameterizations for (i) the surface energy balance, (ii) recharge from below of the model's surface excess reservoir, and (iii) the snow depletion curve. Updated ancillary inputs include improved datasets for land cover, topography, and vegetation height. The Version 4 algorithm further includes a revised approach to precipitation corrections that improves the precipitation climatology in Africa and the high-latitudes. Moreover, for system calibration the model is forced retrospectively with MERRA-2 reanalysis data, which are more consistent with the near-real time GEOS forward processing (FP) data used during the SMAP period than the retrospective GEOS data that were available for previous L4_SM versions.

An analysis of the time-average surface and root zone soil moisture shows that the global pattern of arid and humid regions is captured by the Version 4 L4_SM estimates. Owing to the changes in the land surface modeling system, surface soil moisture is typically drier by several volumetric percent in Version 4 compared to Version 3, whereas root zone soil moisture is wetter in Version 4 in some regions and drier in others. Because of these climatological differences, the Version 3 and Version 4 products should *not* be combined into a single dataset for use in applications.

Results from the core validation site comparisons indicate that Version 4 of the L4_SM data product meets the self-imposed L4_SM accuracy requirement, which is formulated in terms of the RMSE after removal of the long-term mean difference (ubRMSE). The overall ubRMSE of the 3-hourly L4_SM data at the 9 km scale is $0.039 \text{ m}^3 \text{ m}^{-3}$ for surface soil moisture and $0.029 \text{ m}^3 \text{ m}^{-3}$ for root zone soil moisture, below the $0.04 \text{ m}^3 \text{ m}^{-3}$ requirement. The L4_SM estimates are an improvement over estimates from a model-only Nature Run version 7.2 (NRv7.2), which demonstrates the beneficial impact of the SMAP brightness temperature data. Overall, L4_SM surface and root zone soil moisture estimates are more skillful than NRv7.2 estimates, with statistically significant improvements at the 5% level for surface soil moisture R and anomaly R values. Results from comparisons of the L4_SM product to in situ measurements from more than 400 sparse network sites corroborate the core validation site results.

The instantaneous soil moisture analysis increments lie within a reasonable range and result in spatially smooth soil moisture analyses. The long-term mean soil moisture analysis increments make up a small but non-negligible fraction of the water balance. The O-F residuals exhibit only small regional biases on the order of 1-3 K between the (rescaled) SMAP brightness temperature observations and the L4_SM model forecast, which indicates that the assimilation system is reasonably unbiased. The spatially averaged time series standard deviation of the O-F residuals is 5.1 K, which reduces to 3.7 K for the observation-minus-analysis (O-A) residuals, reflecting the impact of the SMAP observations on the L4_SM system. Regionally, the time series standard deviation of the normalized O-F residuals deviates considerably from

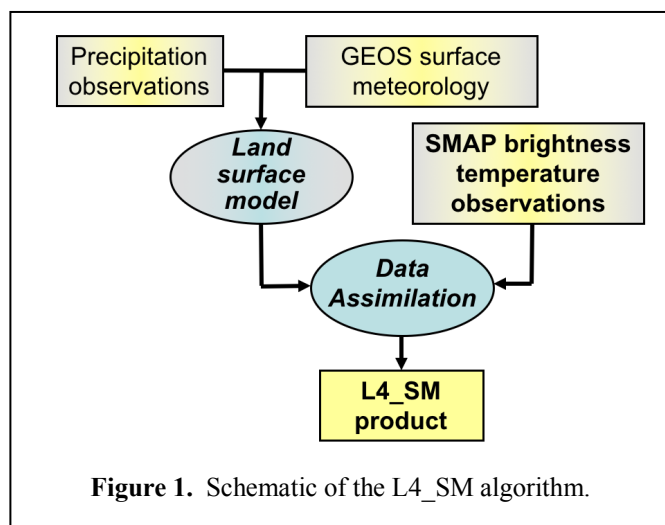
unity, which indicates that the L4_SM assimilation algorithm either over- or underestimates the actual errors that are present in the system.

In future versions, the assimilation of enhanced-resolution and/or water-corrected brightness temperatures from the Level 1 product will be explored. Planned improvements further include additional refinements of the precipitation corrections using a regional product for Australia. Moreover, a refined analysis of the impact of the assimilated SMAP observations and the ensemble perturbations will be facilitated by the construction of ensemble-based model-only reference data. Nevertheless, Version 4 of the L4_SM product is sufficiently mature and of adequate quality for distribution to and use by the larger science and application communities.

1 INTRODUCTION

The NASA Soil Moisture Active Passive (SMAP) mission provides global measurements of L-band (1.4 GHz) brightness temperature from a 685-km, near-polar, sun-synchronous orbit. These observations are primarily sensitive to soil moisture and temperature in the top few centimeters of the soil. SMAP data can therefore be used to enhance understanding of processes that link the water, energy, and carbon cycles, and to extend the capabilities of weather and climate prediction models (Entekhabi et al. 2014).

The suite of SMAP data products includes the Level 4 Surface and Root Zone Soil Moisture (L4_SM) product, which provides deeper-layer soil moisture estimates that are not available in the Level 2-3 retrieval products. The L4_SM product is based on the assimilation of SMAP brightness temperatures into the NASA Catchment land surface model (Koster et al. 2000) using a customized version of the Goddard Earth Observing System (GEOS) land data assimilation system (Figure 1; Reichle et al. 2014a, 2017a,b). This system propagates the surface information from the SMAP instrument to the deeper soil and provides global, 3-hourly estimates of soil moisture and other land surface fields without gaps in coverage. The publication latency of the L4_SM product is about 2.5 days. This latency is driven by the availability of the gauge-based precipitation product used to force the land surface model (Reichle et al. 2014b, 2017a,b; Reichle and Liu 2014).



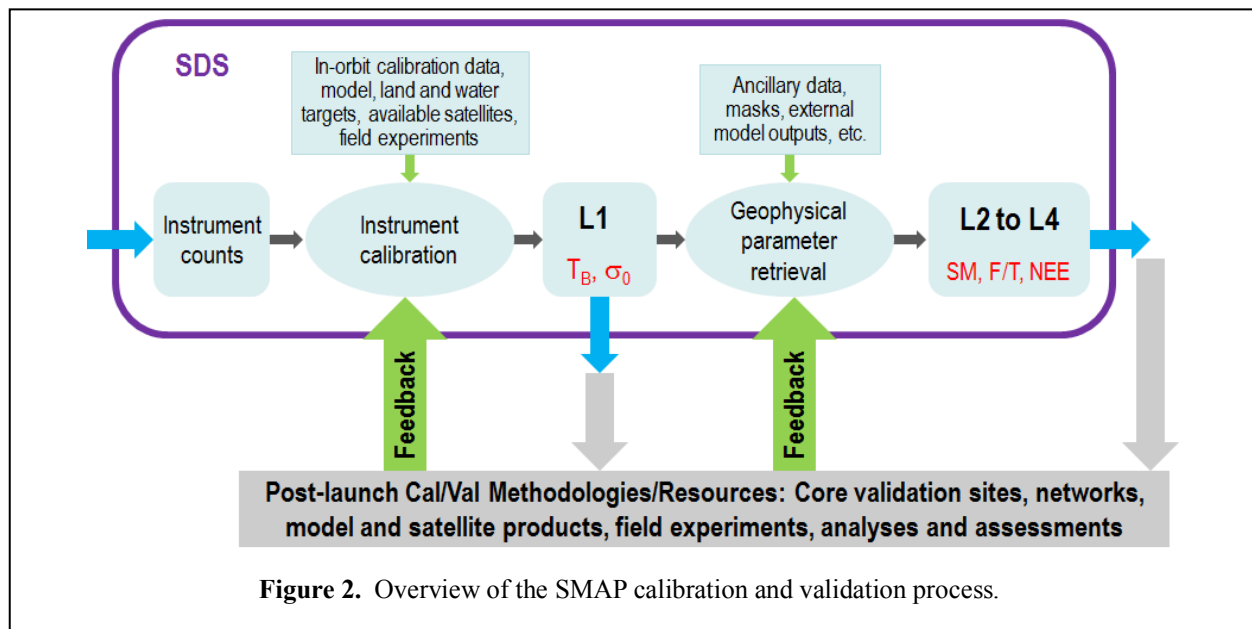
The L4_SM product provides surface and root zone soil moisture (along with other geophysical fields) as 3-hourly, time-average fields on the global, cylindrical, 9 km Equal-Area Scalable Earth, version 2 (EASEv2) grid in the “geophysical” (or “gph”) output Collection (Reichle et al. 2018a). Moreover, instantaneous soil moisture and soil temperature fields before and after the assimilation update are provided every three hours on the same grid in the “analysis update” (or “aup”) output Collection, along with other assimilation diagnostics and error estimates. Time-invariant land model parameters, such as soil porosity, wilting point, and microwave radiative transfer parameters, are provided in the “land-model-constants” (or “lmc”) Collection (Reichle et al. 2018a).

For geophysical data products that are based on the assimilation of satellite observations into numerical process models, validation is critical and must be based on quantitative estimates of uncertainty. Direct comparison with independent observations, including ground-based measurements, is a key part of the validation. This assessment report provides a detailed description of the status of the L4_SM data quality for the Version 4 release of the L4_SM data product. The L4_SM validation process and data quality of previous versions are discussed in (Reichle et al. 2015, 2016, 2017a,b).

2 SMAP CALIBRATION AND VALIDATION OBJECTIVES

During the post-launch SMAP calibration and validation (Cal/Val) phase each science product team pursues two objectives:

1. Calibrate, verify, and improve the performance of the science algorithm.
2. Validate the accuracy of the science data product as specified in the science requirements and according to the Cal/Val schedule.



The overall SMAP Cal/Val process is illustrated in Figure 2. This assessment report describes how the L4_SM team addressed the above objectives prior to the Version 4 release. The validation approach and procedures follow those described in the SMAP Science Data Cal/Val Plan (Jackson et al. 2014), the SMAP L2-L4 Data Products Cal/Val Plan (Colliander et al. 2014), and the Algorithm Theoretical Basis Document for the L4_SM data product (Reichle et al. 2014b).

SMAP established unified definitions to address the mission requirements. These are documented in the SMAP Handbook (Entekhabi et al. 2014), where calibration and validation are defined as follows:

- *Calibration*: The set of operations that establish, under specified conditions, the relationship between sets of values or quantities indicated by a measuring instrument or measuring system and the corresponding values realized by standards.
- *Validation*: The process of assessing by independent means the quality of the data products derived from the system outputs.

In order to ensure the public's timely access to SMAP data, the mission is required to release validated data products within one year of the beginning of mission science operations. The objectives and maturity of the SMAP validated release products follow the guidance provided by the Committee on Earth Observation Satellites (CEOS) Working Group on Calibration and Validation (CEOS 2015):

- Stage 1: Product accuracy is assessed from a small (typically < 30) set of locations and time periods by comparison with in situ or other suitable reference data.

- Stage 2: Product accuracy is estimated over a significant set of locations and time periods by comparison with reference in situ or other suitable reference data. Spatial and temporal consistency of the product and with similar products has been evaluated over globally representative locations and time periods. Results are published in the peer-reviewed literature.
- Stage 3: Uncertainties in the product and its associated structure are well quantified through comparison with reference in situ or other suitable reference data. Uncertainties are characterized in a statistically robust way over multiple locations and time periods representing global conditions. Spatial and temporal consistency of the product and with similar products has been evaluated over globally representative locations and periods. Results are published in the peer-reviewed literature.
- Stage 4: Validation results for Stage 3 are systematically updated when new product versions are released and as the time-series expands.

For the Version 4 release the L4_SM team has completed Stages 1-3. (Publication of the Version 4 results in a peer-reviewed journal is pending. Version 2 results were published in the peer-reviewed literature (Reichle et al. 2017a,b).) The Cal/Val program will continue through the above stages over the SMAP mission life span. Incremental improvements are ongoing as more measurements become available from the SMAP observatory. Version 4 data will be replaced in the archive when upgraded product versions become available.

3 L4_SM CALIBRATION AND VALIDATION APPROACH

During the mission definition and development phase, the SMAP Science Team and Cal/Val Working Group identified the metrics and methodologies that would be used for L2-L4 product assessment. These metrics and methodologies were vetted in community Cal/Val Workshops and tested in SMAP pre-launch Cal/Val rehearsal campaigns. The following validation methodologies and their general roles in the SMAP Cal/Val process were identified:

- *Core Validation Sites*: Accurate estimates at matching scales for a limited set of conditions.
- *Sparse Networks*: One point in the grid cell for a wide range of conditions.
- *Satellite Products*: Estimates over a very wide range of conditions at matching scales.
- *Model Products*: Estimates over a very wide range of conditions at matching scales.
- *Field Campaigns*: Detailed estimates for a very limited set of conditions.

With regard to the CEOS Cal/Val stages (section 2), core validation sites address Stage 1, and satellite and model products are used for Stage 2 and beyond. Sparse networks fall between these two stages.

For the L4_SM data product, all of the above methodologies can contribute to product assessment and refinement, but there are differences in terms of the importance of each approach for the validation of the L4_SM product.

The assessment of the L4_SM data product includes comparisons of SMAP L4_SM soil moisture estimates with in situ soil moisture observations from core validation sites and sparse networks. The assessment further includes a global evaluation of the internal diagnostics from the ensemble-based data assimilation system that is used to generate the L4_SM product. This evaluation focuses on the statistics of the observation-minus-forecast (O-F) residuals and the analysis increments. Together, the core site comparisons and the statistics of the assimilation diagnostics are considered primary validation methodologies for the L4_SM product.

Comparisons against in situ measurements from regional-scale sparse networks are considered a secondary validation methodology because such in situ measurements are subject to upscaling errors from the point-scale to the grid-cell scale of the data product.

Due to their very limited spatial and temporal extent, data from field campaigns play only a tertiary role in the validation of the L4_SM data product. Note, however, that field campaigns are instrumental tools in the provision of high-quality, automated observations from the core validation sites and thus play an important indirect role in the validation of the L4_SM data product.

4 L4_SM ACCURACY REQUIREMENT

There is no formal Level 1 mission requirement for the validation of the L4_SM product, but the L4_SM team self-imposed an accuracy requirement mirroring the one that applies to the L2_SM_AP product. Specifically, the L4_SM surface and root zone soil moisture estimates are required to meet the following criterion:

$ubRMSE \leq 0.04 \text{ m}^3 \text{ m}^{-3}$ within the data masks specified in the *SMAP Level 2 Science Requirements* (that is, excluding regions of snow and ice, frozen ground, mountainous topography, open water, urban areas, and vegetation with water content greater than 5 kg m^{-2}),

where ubRMSE is the RMSE computed after removing long-term mean bias from the data (Entekhabi et al. 2010; Reichle et al. 2015, their Appendix A). (The ubRMSE is also referred to as the standard deviation of the error.) This criterion applies to the L4_SM instantaneous surface and root zone soil moisture estimates at the 9 km grid-cell scale from the “aup” Collection. It is verified by comparing the L4_SM product to the grid-cell scale in situ measurements from the core validation sites (section 6.2). The criterion applies to the site-average ubRMSE, which is obtained by averaging across the ubRMSE values for all 9 km core site reference pixels that provide suitable in situ measurements (Reichle et al. 2015).

L4_SM output fields other than instantaneous surface and root zone soil moisture are provided as research products (including surface meteorological forcing variables, soil temperature, evaporative fraction, net radiation, etc.) and will be evaluated against in situ observations to the extent possible given available resources.

As part of the validation process, additional metrics (including bias, RMSE, time series correlation coefficient R, and anomaly R values) are computed for the L4_SM output fields to the fullest extent possible. This includes computation of the metrics outside of the limited geographic area for which the $0.04 \text{ m}^3 \text{ m}^{-3}$ validation criterion is applied.

For the computation of the *anomaly* R metric, climatological values of soil moisture from a given dataset (i.e., the L4_SM product or the in situ measurements) at a given location are computed for each day of the year, thereby generating a local climatological seasonal cycle for that dataset. Anomaly time series are then computed by subtracting this climatological seasonal cycle from the corresponding raw data. The anomaly R metric is derived by computing the correlation coefficient between the L4_SM and the in situ anomaly time series.

The validation includes additional metrics that are based on the statistics of the O-F residuals and other data assimilation diagnostics (section 6.4). Reichle et al. (2015) provide detailed definitions of all the validation metrics and confidence intervals used here.

5 L4_SM VERSION 4 RELEASE

5.1 Process and Criteria

Since the beginning of the SMAP science data flow on 31 March 2015, the L4_SM team has been conducting frequent assessments of the L4_SM data product and will continue to evaluate the product throughout the life of the SMAP mission. The assessments are based on core validation sites, sparse networks, and assimilation diagnostics, and they already capture a wide range of geophysical conditions. The current status of this process is summarized in the present assessment.

The validation against in situ measurements includes metrics for a model-only “Nature Run,” version 7.2 (NRv7.2). The NRv7.2 estimates are based on the same land surface model and forcing data as the Version 4 L4_SM estimates; the NRv7.2 estimates, however, do not benefit from the assimilation of the SMAP brightness temperature observations. Specifically, the NRv7.2 estimates are the result of a single-member land model integration within the L4_SM system but without the ensemble perturbations and without the assimilation of the SMAP L1C_TB observations; any accuracy in the NRv7.2 estimates is thus derived from the imposed meteorological forcing and land model structure and parameter information. The NRv7.2 estimates were generated for the period 1 January 1990 to present. In addition to serving as a reference for the model-only skill in the L4_SM assessment, the NRv7.2 estimates also provide the model climatological information required by the L4_SM assimilation algorithm (Reichle et al. 2014b).

5.2 Processing Options and Science ID Version

The L4_SM product version used to prepare this assessment report has Science Version ID **Tv4000**. The Tv4000 data were generated between February and May 2018 using the L4 Operations System in its “test” (T) configuration (ECS Version ID 777) and are not publicly available. The L4_SM algorithm released on 14 June 2018 and the associated (publicly available) Version 4 L4_SM data product (ECS Version ID 4; Reichle et al. 2018b,c,d) are expected to have only very minor differences from the Tv4000 algorithm and data product.

The L4_SM Tv4000 algorithm assimilated test data of the Version 4 SMAP L1C_TB brightness temperatures (CRID T15160 for 2015-16 and CRID T15570 for 2017-18) that were likewise generated between October 2017 and April 2018 in preparation for the Version 4 release of the Level 1 products on 6 June 2016.

The assessment period for this report is defined as the 3-year period from **1 April 2015, 0z to 1 April 2018, 0z**. The start date matches the first full day when the radiometer was operating under reasonably stable conditions following instrument start-up operations. The end date was selected to allow sufficient time for analysis and preparation of this assessment report as well as other documents (such as the NSIDC User Guide) required for the Version 4 release on 14 June 2018.

For illustrating select changes from the previous L4_SM product versions, this report also used published Version 3 L4_SM data (Science Version ID Vv3030; Reichle et al. 2017e,f,g), along with the corresponding model-only Nature Run version 4.1 (NRv4.1; section 5.3.1).

As in previous versions, Version 4 of the L4_SM algorithm ingests only the SMAP L1C_TB radiometer brightness temperatures, contrary to the originally planned use of downscaled brightness temperatures from the L2_SM_AP product and landscape freeze-thaw state retrievals from the L2_SM_A product. The latter two products are based on SMAP radar observations and are only available for the 10-week period from 13 April to 7 July 2015 because of the failure of the SMAP radar instrument. The decision

to use only radiometer (L1C_TB) inputs for the Version 4 release was made to ensure homogeneity in the longer-term L4_SM data record.

5.3 Summary of Changes from Previous Versions

This section provides a summary of algorithm changes between previous L4_SM versions and the Version 4 algorithm and product assessed here. The point of reference is Version 2 of the L4_SM algorithm, which used the Catchment model version associated with Nature Run v4 (NRv4) and brightness temperature scaling parameters derived solely from Soil Moisture Ocean Salinity (SMOS) version 5 observations (Reichle et al. 2017a, their section 2).

5.3.1 Changes from Version 2 to Version 3

Version 3 of the L4_SM algorithm used the Catchment model version associated with NRv4.1, which is identical to NRv4 except for the following two changes:

- 1.) For the pre-SMAP period (2000-2014), NRv4.1 is driven with surface meteorological forcing data from a newer version of the GEOS FP-IT product (based on GEOS-5.12.4, as opposed to GEOS-5.9.1 for NRv4; Lucchesi et al. 2015). For the SMAP period (2015-present), the NRv4.1 and NRv4 forcing data are identical.
- 2.) In NRv4.1 the albedo is calculated directly from the boundary condition data and no longer backed out from the GEOS-5 net shortwave radiation forcing as in NRv4, which results in differences between NRv4.1 and NRv4 only at times and locations for which there is a difference in snow cover between the Nature Run and the GEOS system that provides the Nature Run forcing data.

These model changes result in slightly different brightness temperature scaling parameters, model soil moisture initial conditions, and soil moisture climatology estimates between L4_SM Versions 2 and 3.

The brightness temperature scaling parameters in the Version 3 L4_SM algorithm were based on more and newer SMOS data (6 years of SMOS version 620, compared to 4 years of SMOS version 5 in the Version 2 L4_SM algorithm). More importantly, Version 3 of the L4_SM algorithm assimilated SMAP observations in Eastern Europe, the Middle East, and East Asia due to expanded coverage of the brightness temperature scaling parameters. Specifically, in Version 3 the latter were based on two years of SMAP Version 3 brightness temperature observations where the SMOS brightness temperature climatology is unavailable due to radio-frequency interference. In these regions of expanded SMAP assimilation coverage, the Version 3 L4_SM product differs significantly from the Version 2 data. Elsewhere, including at all in situ measurement sites used in the validation, the differences between the Version 2 and Version 3 data are minimal.

5.3.2 Changes from Version 3 to Version 4

Version 4 of the L4_SM algorithm used the Catchment model version associated with NRv7.2, which constitutes a relatively major revision of the modeling system. Specifically:

- 1.) NRv7.2 uses land cover, topography, and vegetation height parameter values that are based on more recent and improved datasets (Mahanama et al. 2015). Land cover inputs were updated to the GlobCover2009 product, which results in a slightly different land mask between the Version 3 and Version 4 L4_SM products. Topographic statistics in NRv7.2 rely on observations from the

Shuttle Radar Topography Mission where available. Finally, vegetation height inputs are derived from space-borne Lidar measurements (Simard et al. 2011).

- 2.) In situ soil moisture measurements from the Soil Climate Analysis Network and U.S. Climate Reference Network were used to calibrate a particular Catchment model parameter (α) that governs the recharge of soil moisture from the model's root-zone excess reservoir into the surface excess reservoir. Specifically, the replenishment of soil moisture near the surface from below under non-equilibrium conditions was substantially reduced in NRv7.2 compared to NRv4 and NRv4.1, which brings the revised model's surface soil moisture more in line with the in situ measurements and also with SMAP Level 2 soil moisture retrievals. This approach was motivated by Koster et al. (2018), who used the SMAP Level 2 soil moisture retrievals to calibrate α locally for a domain that includes the Contiguous U.S. and parts of Canada and Mexico (their Figure 2). In contrast, the Version 4 L4_SM system uses a spatially constant value of $\alpha=0.04$ based on calibration vs. the above-mentioned sparse network in situ measurements. Note that core site in situ measurements were not used in the model calibration.
- 3.) The heat capacity associated with the model's prognostic land surface temperatures was increased to $70,000 \text{ J m}^{-2} \text{ K}^{-1}$ in NRv7.2 for all land cover classes to improve the numerical stability of the surface energy balance calculations. Across all GEOS systems since MERRA (Rienecker et al. 2011), including those used for SMAP L4_SM Versions 1-3 (i.e., NRv4 and NRv4.1), this heat capacity was set to $200 \text{ J m}^{-2} \text{ K}^{-1}$ for all land cover classes except broadleaf evergreen forest, for which it was set to $70,000 \text{ J m}^{-2} \text{ K}^{-1}$. The change to $70,000 \text{ J m}^{-2} \text{ K}^{-1}$ in NRv7.2 for all land cover classes implies that the thickness of the surface soil layer (`clsm_dztsurf`) associated with the diagnosed area-averaged land surface temperature (`surface_temp`) extends from 0 to 5 cm below the surface everywhere. Consequently, the top layer of the soil heat diffusion sub-model (with temperature `soil_temp_layer1`) extends from 5 to 15 cm below the surface everywhere. In NRv4 and NRv4.1, for all land cover classes except broadleaf evergreen forests, the modeled land surface temperature was for a negligibly thin soil layer, and therefore `soil_temp_layer1` described the soil temperature from 0 to 10 cm below the surface.
- 4.) NRv7.2 uses a revised formulation to compute the surface aerodynamic roughness as a function of leaf area index.
- 5.) The model parameter that governs the model's snow accumulation and depletion curve (i.e., the minimum snow water equivalent in snow-covered area fraction, or WEMIN) was reduced to 13 kg m^{-2} in NRv7.2. from 26 kg m^{-2} in NRv4 and NRv4.1. This change improves the model's snow cover fraction estimates vs. satellite observations (Reichle et al. 2017d).
- 6.) For the broadleaf evergreen vegetation class, the physical temperature used in the microwave radiative transfer model was changed to the temperature of the top layer of the soil heat diffusion sub-model (`soil_temp_layer1`). In Versions 1-3, this input was given by the average of `soil_temp_layer1` and the surface temperature (`surface_temp`). For all other vegetation classes this input remains `soil_temp_layer1`.
- 7.) The microwave radiative transfer parameters are calibrated following De Lannoy et al. (2013, 2014). The specific parameters used in the initial Version 4 algorithm were calibrated using a modeling system that fell between NRv4.1 and NRv7.2 and includes only some of the changes discussed above (new vegetation height, precipitation and heat capacity). As a result, the long-term mean and variance of the modeled brightness temperatures do not match those of the (unscaled) observations as closely as in the Version 3 system. Any residual biases in the modeled brightness temperatures, however, are in any case addressed through the brightness temperature scaling parameters (Reichle et al. 2014b, 2017a,b). A new calibration of microwave radiative

transfer parameters using NRv7.2 is underway. The newly calibrated parameters will be used in a future L4_SM release.

- 8.) For all versions of the SMAP L4_SM system, the precipitation forcing is based on merging model-generated background precipitation with observation-based precipitation products (Reichle and Liu 2014; Reichle et al. 2017a,c). For the pre-SMAP period (1990-2014), the model-based precipitation forcing in NRv7.2 is from the MERRA-2 reanalysis (Gelaro et al. 2017) rather than the GEOS FP-IT system (Lucchesi et al. 2015). Specifically, the precipitation generated by the atmospheric general circulation model within the MERRA-2 system (Reichle et al. 2017c) is corrected to the gauge-based Climate Prediction Center Unified (CPCU) precipitation product except in Africa and the high latitudes. See Reichle et al. (2017a) for details about the SMAP L4_SM precipitation correction approach.
- 9.) For NRv7.2, the model background precipitation is rescaled prior to applying the CPCU-based corrections so that its *climatology* matches that of the Global Precipitation Climatology Project (GPCPv2.2) data. This is done separately for MERRA-2 (1990-2014) and GEOS FP (2015-present; Lucchesi et al. 2013). (In NRv4 and NRv4.1, only the CPCU data are rescaled to the GPCPv2.2 climatology.) Where the CPCU data are not used to correct the model background precipitation, including in Africa and the high latitudes, the L4_SM precipitation forcing during the SMAP period is therefore substantially different in NRv7.2 compared to NRv4 and NRv4.1.

Moreover, the following changes impact the L4_SM brightness temperature analysis.

- 10.) In Version 4 of the L4_SM algorithm, the “*catchment deficit*” model prognostic variable is no longer included in the state vector of the Ensemble Kalman filter analysis, and analysis increments are no longer computed for this variable.
- 11.) The calibration of the assimilated SMAP brightness temperatures changed substantially from Version 3 to Version 4. Over land, L1C_TB brightness temperatures are warmer by 3-4 Kelvin on average in Version 4 compared to earlier versions (Peng et al. 2017, 2018).
- 12.) The Version 4 reprocessing scheduled for summer 2018 will use brightness temperature scaling parameters based on 8 years of SMOS (version 620) observations and 3 years of SMAP Version 4 L1C_TB observations where the SMOS climatology is unavailable due to radio-frequency interference. (The Tv4000 test data assessed here were generated using brightness temperature scaling parameters based on 7 years of SMOS (version 620) data and 2.5 years of SMAP L1C_TB test data (T15160, T15570)). Moreover, where the scaling parameters are derived from SMOS observations, they are further corrected for long-term mean differences between SMOS and SMAP observations. (SMOS and SMAP are independently calibrated and have somewhat different brightness temperature climatologies (Peng et al. 2018).)
- 13.) The Version 4 algorithm ensures that fore- and aft-looking brightness temperatures for the same location (i.e., 36 km EASEv2 grid cell) and from the same half-orbit are assimilated at the same L4_SM analysis time. Such observations are separated in time by less than one minute and should therefore be assimilated together. In previous versions, however, fore- and aft-looking brightness temperatures for the same location and half-orbit were assimilated at different analysis times if their exact observation times happened to fall into different analysis time windows.

Finally, the Version 4 data are more compliant with the Climate and Forecast (CF) Metadata Convention.

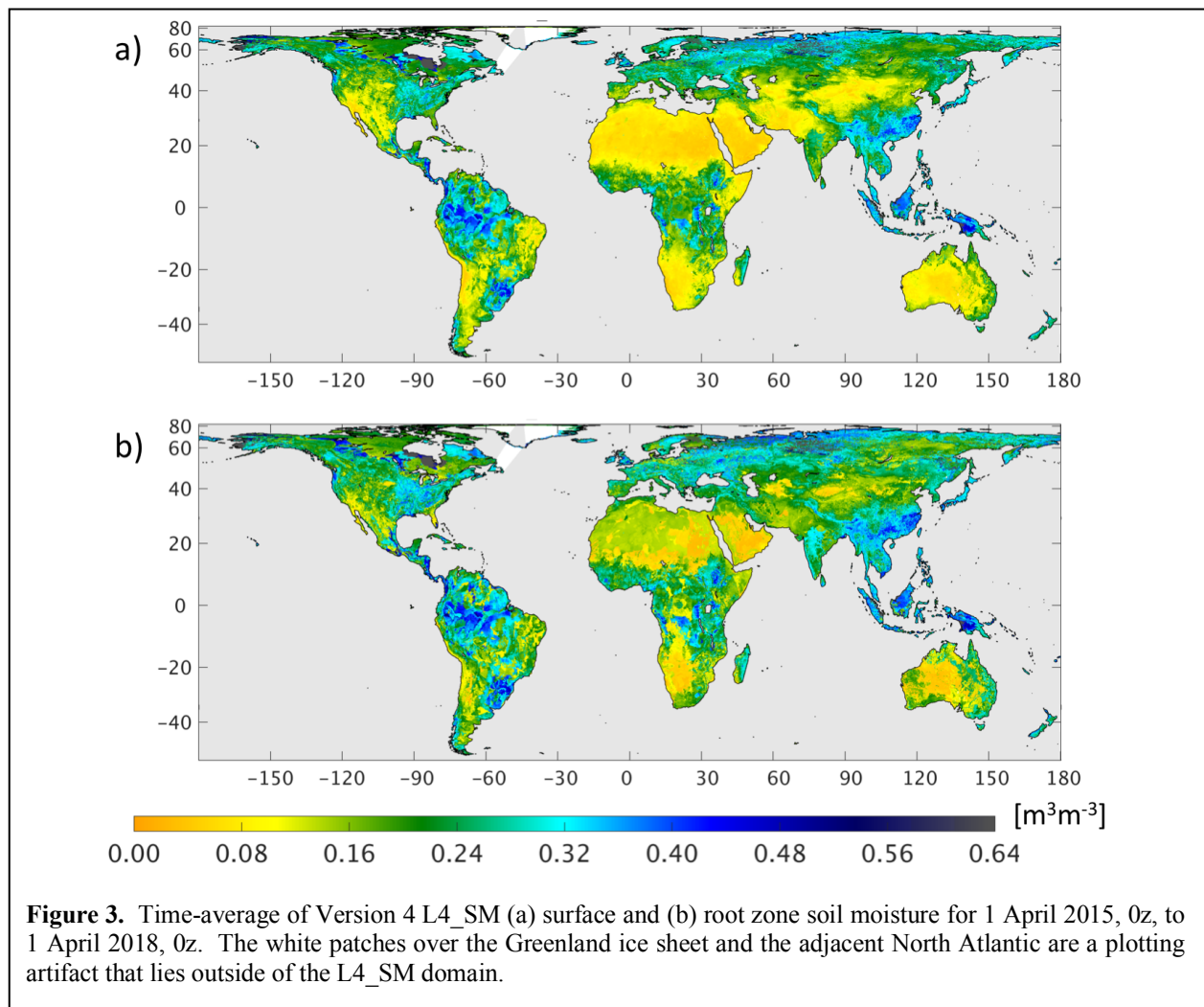
- 14.) Specifically, in addition to latitude and longitude coordinates and EASEv2 grid cell indices, the L4_SM data now include x and y projection coordinate variables as well as an EASE Grid 2.0 projection mapping variable, which improves interoperability with ArcGIS, QGIS, OPeNDAP, and programmatic access.

6 L4_SM DATA PRODUCT ASSESSMENT

This section provides a detailed assessment of the Version 4 L4_SM data product. First, global patterns and features are discussed briefly (section 6.1). Next, we present comparisons and metrics versus in situ measurements from core validation sites (section 6.2) and sparse networks (section 6.3). Thereafter, we evaluate the assimilation diagnostics (section 6.4) through an analysis of the O-F brightness temperature residuals, the soil moisture increments, and the data product uncertainty estimates.

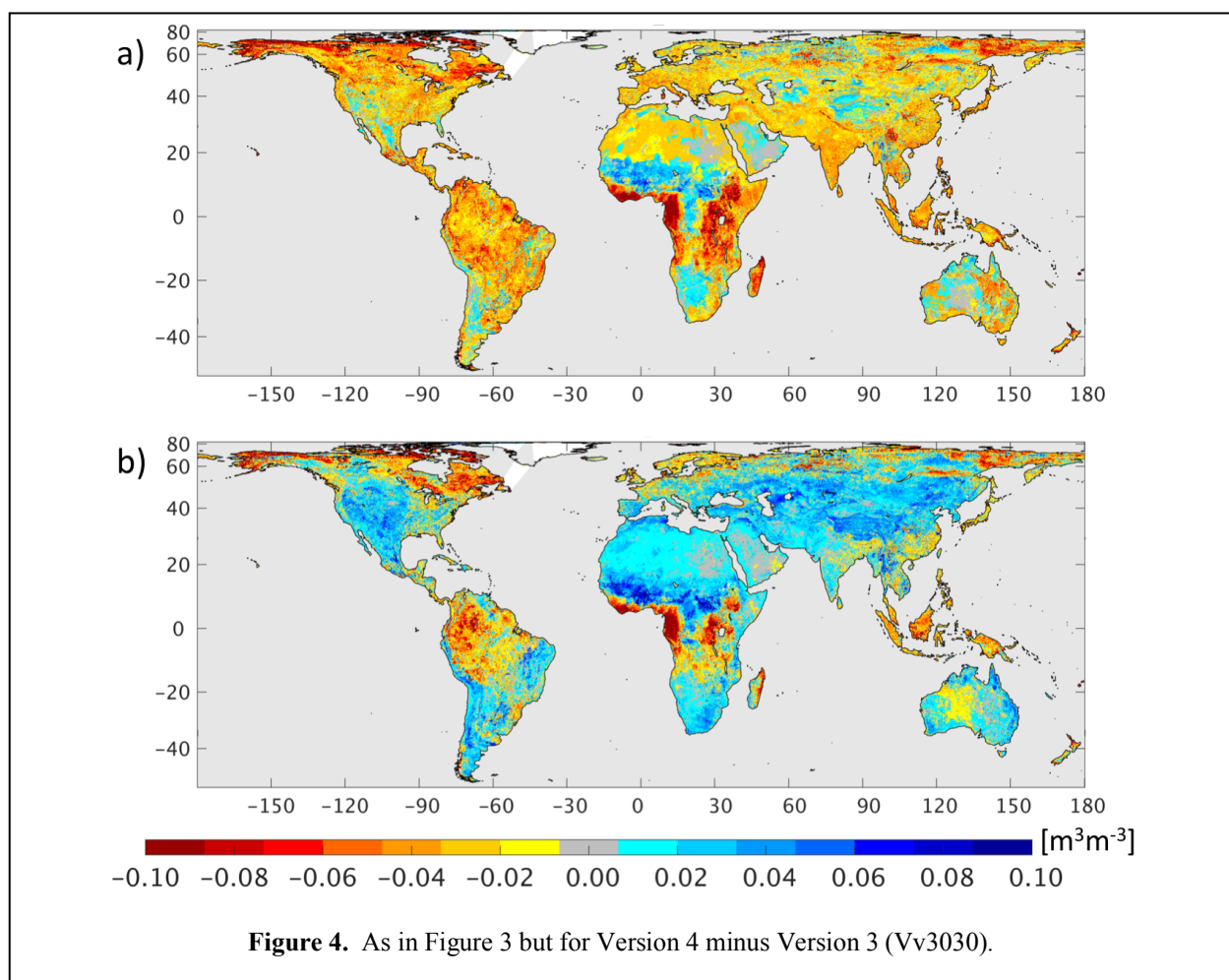
6.1 Global Patterns and Features

Figure 3 shows global maps of time-averaged Version 4 L4_SM surface and root zone soil moisture for the validation period (1 April 2015, 0z to 1 April 2018, 0z). The global patterns are as expected – arid regions such as the southwestern US, the Sahara Desert, the Arabian Peninsula, the Middle East, southern Africa, and central Australia exhibit generally dry surface and root zone soil moisture conditions, whereas the tropics (Amazon, central Africa, and Indonesia) and high-latitude regions show wetter conditions.



Generally, the global patterns of absolute soil moisture values are dominated by soil parameters and climatological factors. The influence of soil texture is noticeable in the coarse-scale patterns in the Sahara Desert, where little is in fact known about the spatial distribution of mineral soil fractions. Areas with peat soil include, for example, the region along the southern edge of Hudson Bay and portions of Alaska. In the land model, the soils in this region are assigned a high porosity value and show persistently wetter conditions than seen in other areas.

Figure 4 shows global maps of the change in time-averaged soil moisture fields between Versions 3 and 4. Generally, the long-term mean surface soil moisture in Version 4 is drier than in Version 3, in many regions by several volumetric percent, and by $0.02 \text{ m}^3 \text{ m}^{-3}$ in the global average. In contrast, root zone soil moisture is generally wetter in Version 4 than in Version 3 by a few volumetric percent, except in most of the tropics and high latitudes, where Version 4 is drier than Version 3 by several volumetric percent. In the global average, there is no change in the long-term mean root zone soil moisture.



The differences in soil moisture between the two versions stem mostly from two changes in the underlying modeling system (section 5.3.2). First, the reduced replenishment of soil moisture near the surface from below under non-equilibrium conditions in NRv7.2 is largely responsible for the drier surface soil moisture conditions in Version 4 compared to Version 3 outside of Africa and the high latitudes. Second, the rescaling of the background model precipitation to the GPCPv2.2 climatology resulted in

substantial changes in the soil moisture climatology in Africa and the high latitudes. Generally, this rescaling reduced the precipitation and thus the soil moisture compared to Version 3 in the high latitudes and portions of Africa. In the Sahel and parts of central Africa, however, the Version 4 precipitation and soil moisture are increased compared to Version 3, thus reducing a known dry bias in GEOS FP precipitation in these regions. (Because there were only minor changes to the modeling system between Version 2 and Version 3, the time-average soil moisture values for Versions 2 and 3 are similar.)

Because of the climatological differences in soil moisture (Figure 4), the Version 3 and Version 4 products should *not* be combined into a single dataset for use in applications.

The L4_SM product also includes a large number of output fields that are not subject to formal validation requirements. Such “research” output includes the surface meteorological forcing fields, land surface fluxes, soil temperature and snow conditions, runoff, and error estimates (derived from the ensemble). See Reichle et al. (2015, their section 6.1) for more discussion of the global patterns and features found in the L4_SM product.

6.2 Core Validation Sites

6.2.1 Method

This section addresses validation using SMAP core validation sites, which provide in situ measurements of soil moisture and soil temperature conditions at the scale of 9 km and 33 km grid cells. Details about the processing of the data and the validation methodology can be found in Reichle et al. (2015, their section 6.2.1). The status of the core validation sites is reviewed periodically. In a change from previous L4_SM assessments, this report uses reference pixel data on the 33 km EASEv2 grid (defined through suitable aggregation of the 3 km EASEv2 grid), instead of the 36 km reference pixels used in Reichle et al. (2015, 2016, 2017a). The change ensures consistency with the validation approach of the SMAP Level 2 soil moisture calibration and validation team, who switched to 33 km reference pixels following the release of the enhanced-resolution Level 2 passive soil moisture retrieval products (Jackson et al. 2017).

The set of core sites that provide data for this assessment of the L4_SM product are listed in Table 1, along with the details of the 9 km and 33 km reference pixels that are used. The table shows that the present L4_SM validation is based on a total of 49 reference pixels from 19 different core validation sites, representing a ~50% increase in number relative to the 33 reference pixels from 13 different core validation sites used in the Version 2 assessment report (Reichle et al. 2016). Surface soil moisture measurements are available for all 49 reference pixels, which include 18 reference pixels at the 33 km scale from 18 different sites and 31 reference pixels at the 9 km scale from 18 different sites. For root zone soil moisture, measurements are available for only 19 reference pixels from 7 different core sites, including 7 reference pixels at the 33 km scale from 7 different sites and 12 reference pixels at the 9 km scale from 6 different sites. The 9 km reference pixels for root zone soil moisture belong to the core validation sites of Little Washita (Oklahoma), Fort Cobb (Oklahoma), South Fork (Iowa), Kenaston (Saskatchewan), TxSON (Texas), and Yanco (Australia), which is the same set of sites that was available for the Version 2 assessment report (Reichle et al. 2016). This very limited set obviously lacks the diversity to be fully representative of global conditions.

The metrics are computed from 3-hourly data, provided at least 480 measurements, or about 2 months of data, are available after quality control. The computation of the anomaly R value (section 4) further requires estimates of the 3-year mean seasonal cycle, for which we required a minimum of at least 80 measurements for a given month across the 3-year validation period. This requirement implies that the anomaly R metric is available for surface soil moisture at only 11 (13) reference pixels at the 9 km (33 km) scale and for root zone soil moisture at only 6 reference pixels (at both scales).

Table 1 also lists the depths of the deepest sensors that contribute to the in situ root zone soil moisture measurements. The measurements from the individual sensors are vertically averaged with weights that are proportional to the spacing of the depth of the sensors within the 0-100 cm layer depth of the L4_SM root zone soil moisture estimates. At all reference pixels except Little River and Yanco, the deepest sensors are at 45 cm or 50 cm depth. At Little River and Yanco, the deepest sensors are at 30 cm and 75 cm, respectively, with Yanco's second-deepest sensors being installed at 45 cm depth. In all cases, the deepest sensors are therefore weighted most strongly in the computation of the vertical average. To compute the vertically averaged root zone soil moisture at a given time from a given sensor profile, all sensors within the profile must provide measurements that passed the automated quality control.

Table 1. Core validation sites and reference pixels for L4_SM validation. 33 km reference pixels shown in bold.

Site Name	Country	Climate Regime	Land Cover	Reference Pixel										
				ID	Latitude [degree]	Longitude [degree]	Horizontal Scale [km]	Depth of Deepest Sensor [m]	Number of Sensors (Surface Soil Moisture)			Number of Sensors (Root Zone Profiles)		
									Min.	Mean	Max.	Min.	Mean	Max.
REMEDHUS	Spain	Temperate	Croplands	03013302	41.29	-5.46	33	0.05	8	12.5	15	n/a	n/a	n/a
				03010903	41.42	-5.37	9	0.05	4	4.0	4	n/a	n/a	n/a
				03010908	41.32	-5.27	9	0.05	4	4.0	4	n/a	n/a	n/a
Reynolds Creek	USA (Idaho)	Arid	Grasslands	04013302	43.19	-116.75	33	0.05	7	7.0	7	n/a	n/a	n/a
				04010907	43.19	-116.72	9	0.05	4	4.0	4	n/a	n/a	n/a
				04010910	43.09	-116.81	9	0.05	4	4.0	4	n/a	n/a	n/a
Yanco	Australia (New South Wales)	Arid	Cropland / natural mosaic	07013301	-34.86	146.16	33	0.75	8	20.0	23	7	7.0	7
				07010902	-34.72	146.13	9	0.05	8	8.6	9	n/a	n/a	n/a
				07010916	-34.98	146.31	9	0.05	8	10.2	11	n/a	n/a	n/a
Carman	Canada (Manitoba)	Cold	Croplands	09013301	49.60	-97.98	33	0.05	8	18.0	20	n/a	n/a	n/a
				09010906	49.67	-97.98	9	0.05	8	10.1	11	n/a	n/a	n/a
Ngari	Tibet	Cold	Barren / sparse	12033301	32.50	79.96	33	0.05	6	6.0	6	n/a	n/a	n/a
Walnut Gulch	USA (Arizona)	Arid	Shrub open	16013302	31.75	-110.03	33	0.05	8	15.8	18	n/a	n/a	n/a
				16010906	31.72	-110.09	9	0.05	8	9.4	11	n/a	n/a	n/a
				16010907	31.72	-109.99	9	0.05	8	10.1	11	n/a	n/a	n/a
				16010913	31.83	-110.90	9	0.05	6	6.0	6	n/a	n/a	n/a
Little Washita	USA (Oklahoma)	Temperate	Grasslands	16023302	34.86	-98.08	33	0.45	8	11.0	12	8	9.0	11
				16020905	34.92	-98.23	9	0.05	4	4.0	4	n/a	n/a	n/a
				16020906	34.92	-98.14	9	0.45	4	4.0	4	4	4.0	4
				16020907	34.92	-98.04	9	0.45	4	4.0	4	4	4.0	4
Fort Cobb	USA (Oklahoma)	Temperate	Grasslands	16033302	35.38	-98.64	33	0.45	8	10.5	11	8	9.6	11
				16030911	35.38	-98.57	9	0.45	4	4.0	4	4	4.0	4
				16030916	35.29	-98.48	9	0.45	4	4.0	4	4	4.0	4
Little River	USA (Georgia)	Temperate	Cropland / natural mosaic	16043302	31.67	-83.60	33	0.30	8	17.7	19	8	16.2	18
				16040901	31.72	-83.73	9	0.30	8	8.0	8	6	6.0	6
				16040906	31.64	-83.64	9	0.30	5	5.0	5	5	5.0	5
St Josephs	USA (Indiana)	Temperate	Croplands	16063302	41.39	-85.01	33	0.05	8	8.3	9	n/a	n/a	n/a
				16060907	41.45	-84.97	9	0.05	7	7.0	7	n/a	n/a	n/a
South Fork	USA (Iowa)	Cold	Croplands	16073302	42.42	-93.41	33	0.50	8	17.6	19	8	12.5	14
				16070909	42.42	-93.53	9	0.50	4	4.0	4	4	4.0	4
				16070910	42.42	-93.44	9	0.50	4	4.0	4	4	4.0	4
				16070911	42.42	-93.35	9	0.50	4	4.0	4	4	4.0	4
Monte Buey	Argentina	Temperate	Croplands	19023301	-32.91	-62.51	33	0.05	8	10.0	12	n/a	n/a	n/a
				19020902	-33.01	-62.49	9	0.05	5	5.0	5	n/a	n/a	n/a
Tonzi Ranch	USA (California)	Temperate	Savannas woody	25013301	38.45	-120.95	33	0.05	8	14.5	20	n/a	n/a	n/a
				25010911	38.43	-120.95	9	0.05	8	17.0	26	n/a	n/a	n/a
Kenaston	Canada (Saskatchewan)	Cold	Croplands	27013301	51.47	-106.48	33	0.50	8	26.7	30	8	24.4	30
				27010910	51.39	-106.51	9	0.05	8	8.0	8	8	8.0	8
				27010911	51.39	-106.42	9	0.50	8	12.7	14	8	11.6	14
Valencia	Spain	Cold	Savannas	41010906	39.57	-1.26	9	0.05	7	7.0	7	n/a	n/a	n/a
Niger	Niger	Arid	Grassland	45013301	13.57	2.66	33	0.05	6	6.0	6	n/a	n/a	n/a
				45010902	13.57	2.66	9	0.05	4	4.0	4	n/a	n/a	n/a
Benin	Benin	Tropical	Savannas	45023301	9.83	1.73	33	0.05	7	7.0	7	n/a	n/a	n/a
				45020902	9.77	1.68	9	0.05	5	5.0	5	n/a	n/a	n/a
TxSON	USA (Texas)	Temperate	Grasslands	48013301	30.35	-98.73	33	0.50	8	26.9	28	8	23.0	24
				48010902	30.43	-98.81	9	0.50	8	9.5	10	8	8.3	9
				48010911	30.28	-98.73	9	0.50	8	14.2	15	8	13.7	14
HOBE	Denmark	Temperate	Croplands	67013301	55.97	9.10	33	0.05	8	12.4	15	n/a	n/a	n/a
				67010901	55.97	9.10	9	0.05	5	5.0	5	n/a	n/a	n/a

Across the reference pixels listed in Table 1, the average number of individual surface soil moisture sensors that contribute to a given 33 km reference pixel ranges between 6.0 and 26.9, with a mean value of 13.8. The corresponding number of sensor profiles for root zone soil moisture ranges between 7.0 and 24.4, with a mean value of 14.5. At the 9 km scale, 13 of the 31 reference pixels are based on just 4 individual sensor profiles, while most of the rest of the 9 km reference pixels consist of about 10 sensor profiles each. The mean value of surface soil moisture sensors per 9 km reference pixel is 6.8, and the corresponding number of root zone profiles is 6.2. The sampling density (sensors per area) is therefore higher for the 9 km reference pixels than for the 33 km reference pixels. For most reference pixels, individual sensor profiles tend to drop out temporarily. This leads to undesirable discontinuities in the reference pixel average soil moisture. To mitigate this effect, for reference pixels with 8 or fewer individual sensor profiles, quality-controlled in situ measurements from all contributing sensor profiles were required for the computation of the reference pixel average.

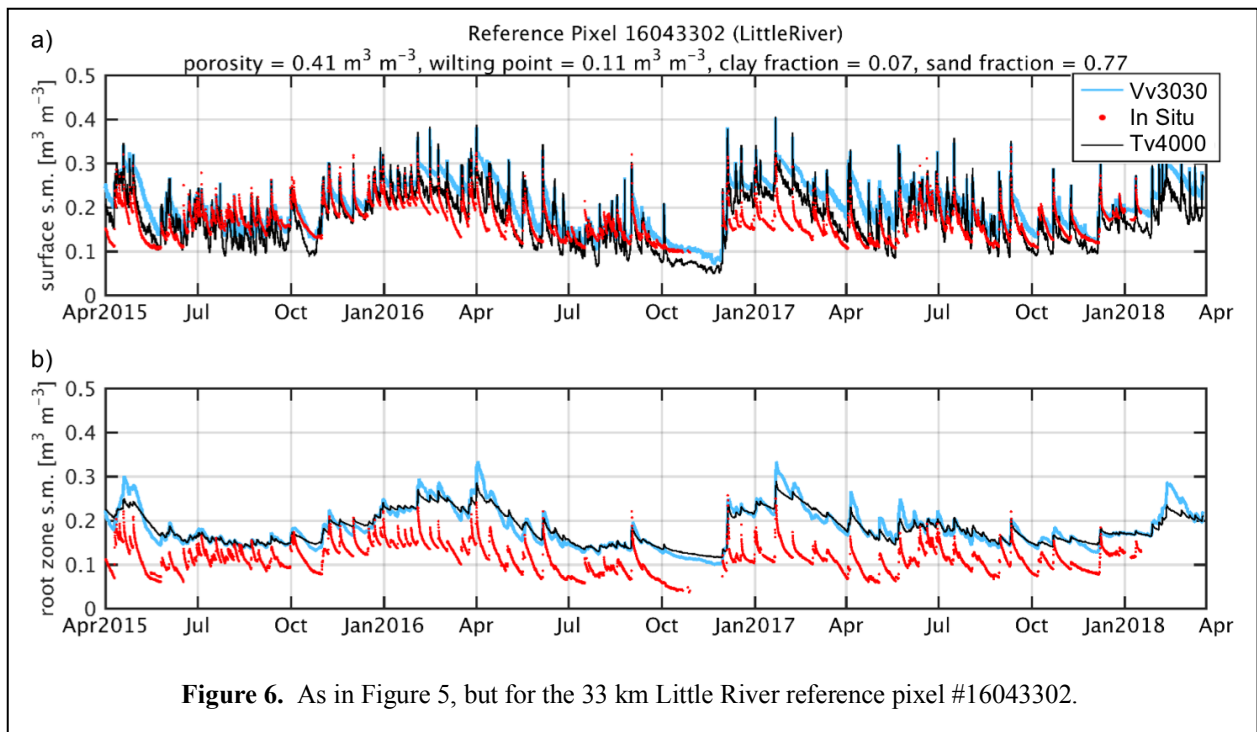
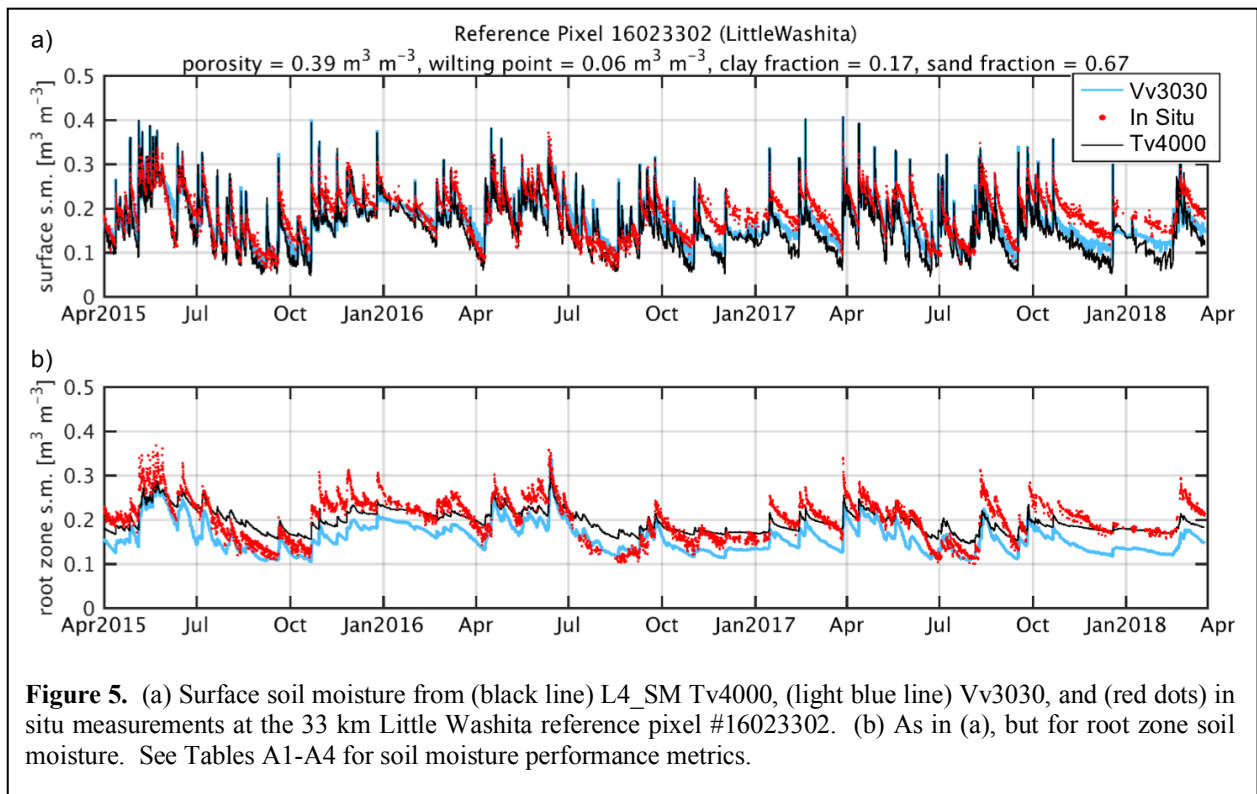
Core site metrics are provided separately for the 9 km and 33 km reference pixels. Summary metrics are obtained by averaging across the metrics from all individual reference pixels at the given scale (Table 1). For the 9 km metrics, we first average each metric across the 9 km reference pixels within each of the 18 sites that have more than one 9 km reference pixel. This first average is weighted by the number of measurements that contribute to the metric at a given 9 km reference pixel. Second, we average the resulting metrics across sites. This approach gives equal weight to each site and differs from the straight average over all 9 km reference pixels that was used in previous assessments (Reichle et al. 2015, 2016, 2017a), which somewhat arbitrarily gave more weight to sites that had more 9 km reference pixels. (We computed summary metrics using both methods and found the results to be very close. That is, the conclusions remain the same regardless of how exactly the average is computed.)

Finally, in situ measurements are used for validation only if the model (or assimilation) estimates indicate non-frozen and snow-free conditions (Reichle et al. 2015, their section 6.2.1). Because the soil temperature and snow states differ between the four L4_SM and Nature Run products examined here (Tv4000, Vv3030, NRv7.2, and NRv4.1), in situ measurements were used only if all four products indicate favorable validation conditions. This cross-masking ensures that the metrics are directly comparable across all four products.

6.2.2 Results

In this section, we first revisit the three sites – Little Washita, Little River, and South Fork – that were discussed in detail in previous L4_SM assessments. We refer the reader to Reichle et al. (2015, 2016, 2017a) for brief discussions of the general site characteristics and further references. Next, we discuss the summary metrics across all sites, which are used to determine whether the L4_SM product accuracy requirement (section 4) has been met. For reference, Tables A1-A8 in the Appendix provide a complete listing of the various skill metrics for all reference pixels, including both versions of the L4_SM product and the corresponding Nature Run estimates.

Figures 5-7 illustrate the soil moisture time series for the Version 4 product (black lines), in situ measurements (red dots), and Version 3 estimates (blue lines). Overall, the estimates from both L4_SM product versions track the in situ measurements reasonably well. At the 33 km Little Washita reference pixel (#16023602) (Figure 5), the differences in surface soil moisture between the two versions are generally small. Root zone soil moisture is nearly unbiased in Version 4 ($-0.006 \text{ m}^3 \text{ m}^{-3}$) compared to the considerably larger dry bias in Version 3 ($-0.041 \text{ m}^3 \text{ m}^{-3}$). There is, however, also a somewhat larger ubRMSE in Version 4 ($0.029 \text{ m}^3 \text{ m}^{-3}$) than in Version 3 ($0.025 \text{ m}^3 \text{ m}^{-3}$) (Table A3).



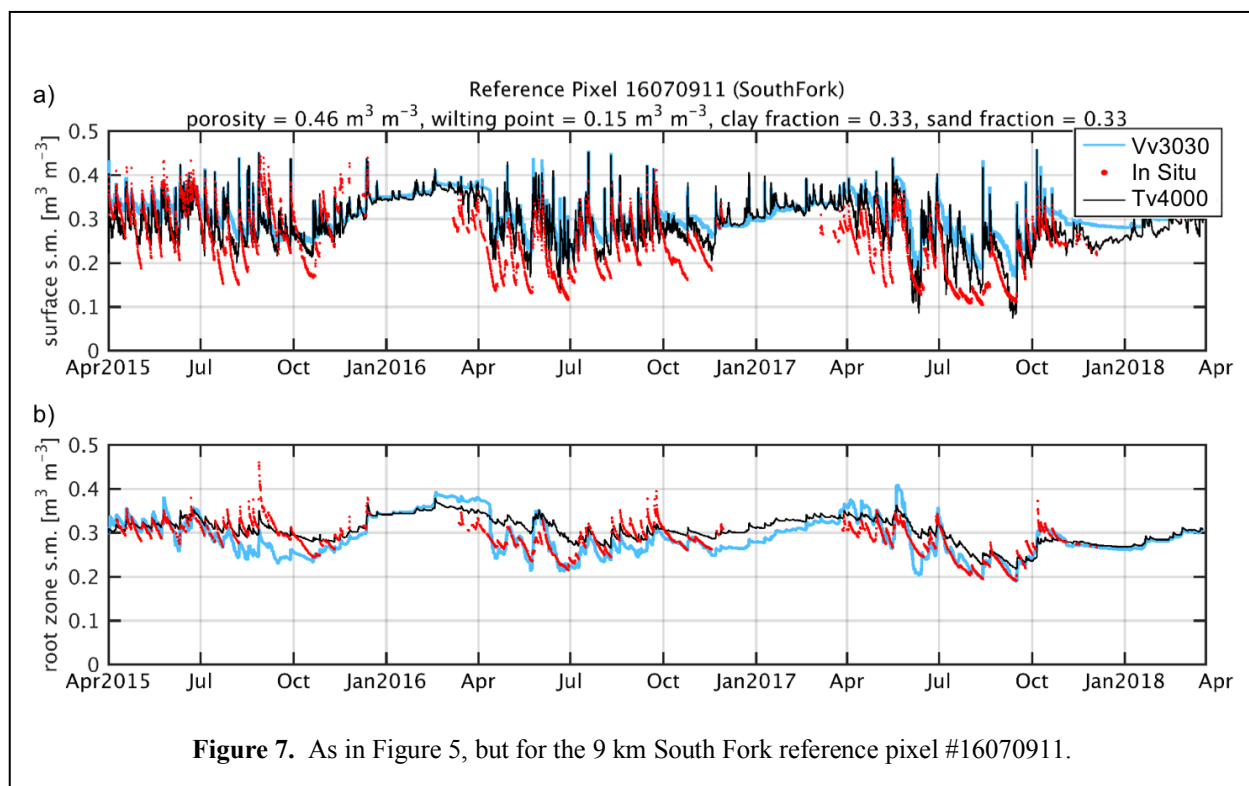


Figure 7. As in Figure 5, but for the 9 km South Fork reference pixel #16070911.

At the 33 km Little River reference pixel (#16043302), surface soil moisture estimates are considerably improved in Version 4 compared to Version 3 (Figure 6). This improvement is primarily because of the reduction in upward recharge from the root zone to the surface excess reservoir (section 5.3.2), which results in improvements in the surface soil moisture mean and dynamic range. Quantitatively, the ubRMSE is $0.037 \text{ m}^3 \text{ m}^{-3}$ in Version 4, down from $0.041 \text{ m}^3 \text{ m}^{-3}$ in Version 3 (Table A1), and the R value is 0.74 in Version 4, up from 0.62 in Version 3 (Table A2). Moreover, there is only a slight wet bias in Version 4 ($0.009 \text{ m}^3 \text{ m}^{-3}$) compared to the much stronger wet bias in Version 3 ($0.037 \text{ m}^3 \text{ m}^{-3}$). The root zone soil moisture dynamic range is noticeably smaller in Version 4 than in Version 3. Nevertheless, the root zone soil moisture ubRMSE, bias, and R metrics of both versions are very similar, with both including a considerable wet bias of $0.07 \text{ m}^3 \text{ m}^{-3}$.

For the present report we used a revised upscaling function for the in situ surface soil moisture at the 33 km Little River reference pixel. The Little River site is largely a mix of agricultural areas and ephemeral wetlands. Using additional measurements from recent intensive field campaigns and additional new sensors placed in the ephemeral wetland areas, the new upscaling function is able to correct for the uneven distribution of the long-term sensors, which were preferentially installed in the agricultural areas (Michael Cosh, personal communication, 2018). As a result, the above-mentioned bias of $0.037 \text{ m}^3 \text{ m}^{-3}$ in Version 3 surface soil moisture is much smaller than the $\sim 0.1 \text{ m}^3 \text{ m}^{-3}$ bias determined for Version 2 by Reichle et al. (2017a), even though the L4_SM data are essentially unchanged at this location between Version 2 and Version 3. Unfortunately, it is not yet possible to similarly correct the upscaling function for the 9 km surface soil moisture measurements or the 9 km and 33 km root zone soil moisture measurements.

At the 9 km South Fork reference pixel #16070911 (Figure 7), the bias in surface soil moisture is $0.031 \text{ m}^3 \text{ m}^{-3}$ in Version 4, down from $0.053 \text{ m}^3 \text{ m}^{-3}$ in Version 3 (Table A1), whereas ubRMSE and R values are essentially unchanged. Here, too, the reduction in the upward recharge of the surface excess reservoir in the Catchment model results in generally drier and less biased surface soil moisture conditions. For root zone soil moisture, the ubRMSE is $0.025 \text{ m}^3 \text{ m}^{-3}$ in Version 4, down from $0.031 \text{ m}^3 \text{ m}^{-3}$ in Version 3, while

the R values are very similar in both versions. There is, however, a dry bias of $0.017 \text{ m}^3 \text{ m}^{-3}$ in Version 4 root zone soil moisture, whereas Version 3 was essentially unbiased ($-0.003 \text{ m}^3 \text{ m}^{-3}$).

In the remainder of this section, we investigate the summary metrics for soil moisture and surface soil temperature, which are illustrated in Figures 8-11. Probably the most important result is that the average ubRMSE values for surface and root zone soil moisture for the Version 3 and Version 4 L4_SM products at both the 9 km and the 33 km scales all meet the accuracy requirement of $0.04 \text{ m}^3 \text{ m}^{-3}$.

For a more in-depth analysis, we first compare the skill of the L4_SM and Nature Run estimates. For the ubRMSE metrics at the 9 km and the 33 km scales (Figure 8a), the surface and root zone soil moisture skill of the Version 4 product exceeds that of NRv7.2, demonstrating the positive impact of the assimilation of SMAP brightness temperatures. For example, at the 9 km scale the surface soil moisture ubRMSE is $0.039 \text{ m}^3 \text{ m}^{-3}$ for Tv4000 surface soil moisture and $0.043 \text{ m}^3 \text{ m}^{-3}$ for NRv7.2. Likewise, the skill of the Version 3 product exceeds that of NRv4.1. For surface soil moisture at the 33 km scale, the ubRMSE improvements are statistically significant at the 5% level as indicated by the non-overlapping 95% confidence intervals. (Note that the confidence intervals are themselves uncertain and only provide rough guidance as to whether the skill differences are meaningful.)

The average bias (Figure 8b) and average absolute bias (Figure 8c) values for surface and root zone soil moisture tend to be slightly worse for the Version 4 product than for NRv7.2. These changes, however, are not statistically significant except for the average bias in root zone soil moisture at the 33 km scale, which is only around $0.01 \text{ m}^3 \text{ m}^{-3}$.

Across-the-board improvements are seen in the L4_SM product over the model-only Nature Run estimates in terms of R (Figure 9a) and anomaly R (Figure 9b) skill. The improvements are statistically significant for surface soil moisture in both L4_SM product versions at the 9 km and 33 km scales. Moreover, for root zone soil moisture the anomaly R values for both product versions at the 33 km scale are significantly improved over the corresponding Nature Run values.

Next, we compare the skill of the Version 4 product to that of the Version 3 product. The slight (and statistically insignificant) increase in the surface soil moisture ubRMSE values from Version 3 to Version 4 is balanced by a slight decrease in the root zone soil moisture ubRMSE values (Figure 8a). Similarly small differences between the two versions are seen for the correlation metrics (Figure 9). The average bias in surface soil moisture is considerably smaller in Version 4 than in Version 3, but the average bias in root zone soil moisture at the 9 km scale is somewhat worse in Version 4 (Figure 8b). The average absolute bias in Version 4 surface soil moisture is better than that of Version 3, whereas the average absolute bias in root zone soil moisture is essentially unchanged between the two versions (Figure 8c). On balance, there is no net improvement or degradation in Version 4 soil moisture compared to Version 3 in terms of core site metrics.

Next, we compare the skill values at 9 km to those at 33 km. The L4_SM and Nature Run skill values at 33 km are better for nearly all metrics than the corresponding values at 9 km (Figures 8 and 9), which is consistent with the fact that the model forcing data and the assimilated SMAP brightness temperature observations are all at resolutions of about 30 km or greater. The information used to downscale the assimilated information primarily stems from the land model parameters, which are at the finer, 9 km resolution; this information is expected to have a modest impact at best. It is therefore not a surprise that the estimates at 33 km are more skillful than those at 9 km.

Finally, we compare the skill of the surface estimates to that of the root zone estimates. Across both scales, for nearly all metrics and for both the L4_SM and Nature Run estimates, the skill of the root zone soil moisture estimates is better than that of the surface estimates. This result makes sense because there is much more variability in surface soil moisture.

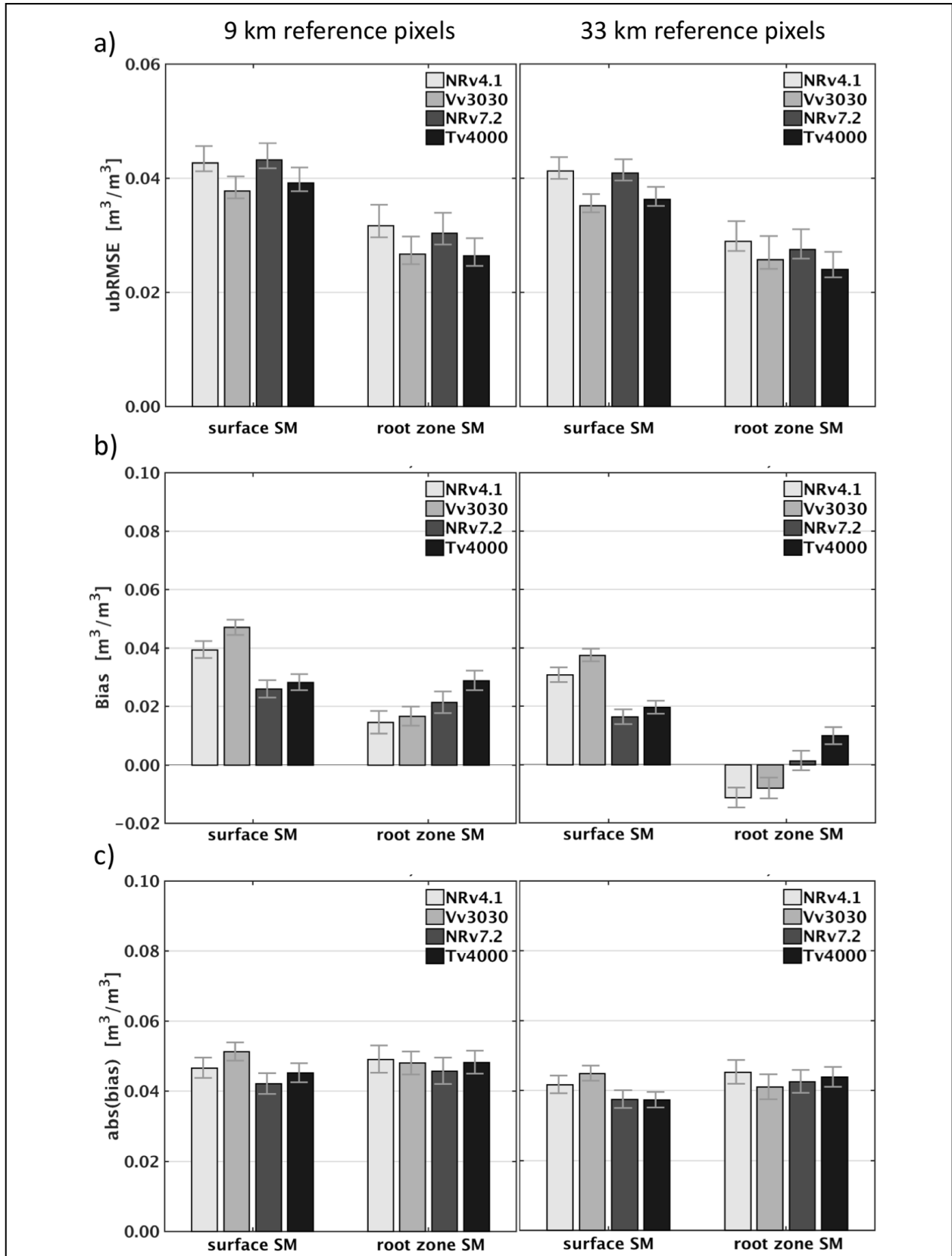


Figure 8. Surface and root zone soil moisture (a) ubRMSE, (b) bias and (c) absolute bias averaged across (left) 9 km and (right) 33 km core site reference pixels for Nature Run estimates and L4_SM products.

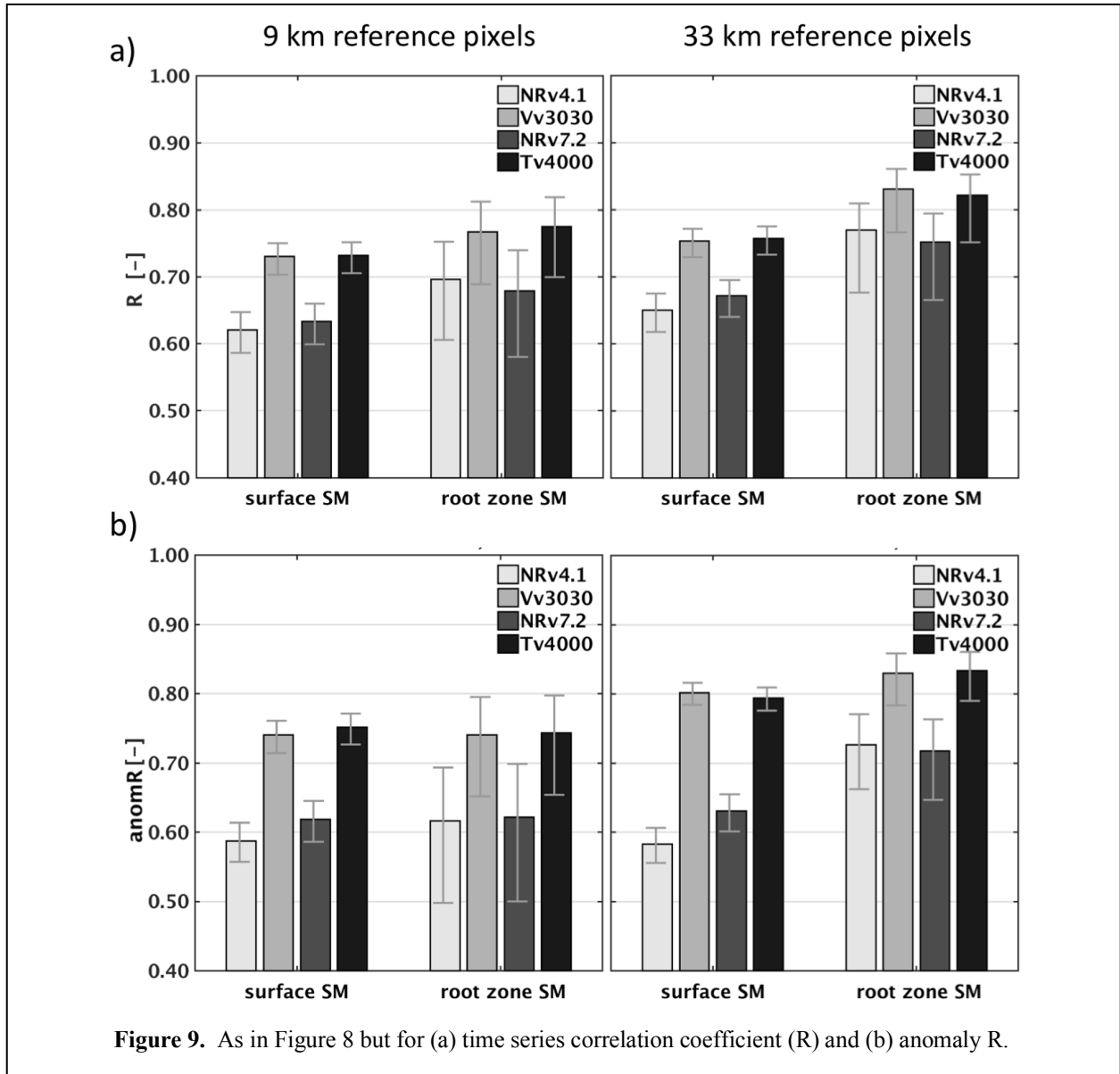


Figure 9. As in Figure 8 but for (a) time series correlation coefficient (R) and (b) anomaly R.

Most core sites that provide surface soil moisture measurements (Table 1) also provide surface soil temperature data. (Sufficient temperature data are not available for Tonzi Ranch, Valencia, Niger, Benin, and the 9 km Monte Buey reference pixel.) The surface soil temperature metrics are summarized in Figures 10 and 11. The ubRMSE values for the L4_SM products and Nature Run estimates at the 9 and 33 km scales range from 1.6 to 1.9 K, with slightly smaller values for 6am than for 6pm (Figure 10a). The skill differences between the various products, times of day and scales, however, are not statistically significant at the 5% level. Small improvements in the L4_SM products relative to the Nature Run estimates are seen in the mean bias and the mean absolute bias at 6am, whereas at 6pm the mean bias and mean absolute bias are slightly larger in the L4_SM products than in the Nature Run estimates (Figure 10b,c). At the 9 km scale, for example, the mean bias at 6am is around -2.4 K for the NRv7.2 estimates and around -2.0 K for the Version 4 L4_SM product, whereas the mean bias at 6pm is around 0.2 K for NRv7.2 and -0.8 K for the Version 4 L4_SM product (Figure 10b). Some but not all of the improvements or degradations are statistically significant.

As with the ubRMSE, there are no statistically significant differences in R values across all products, overpass times, and scales, with values ranging from 0.96 to 0.98 (Figure 11a). There is a consistent, small improvement in anomaly R values for the L4_SM products relative to the respective Nature Run results, but the improvements are not statistically significant (Figure 11b).

Across all metrics, there are no statistically significant differences in surface soil temperature skill between the Version 3 and Version 4 L4_SM products (Figures 10 and 11), although the R and anomaly R values for Version 4 are very slightly but consistently worse than those of Version 3. One reason for the slight degradation in correlation may be the change in the very definition of the top layer soil temperature (section 5.3.2). This change implies that the in situ measurements, which are typically at 5 cm depth, are less representative of the 5-15 cm layer-depth of the Version 4 surface soil temperature estimates (section 5.3.2).

Generally, the results presented here, which are based on 3 years of core site measurements, are consistent with those of Version 2, which were based on a validation period of 2 years (Reichle et al. 2017a). In summary, the results discussed here demonstrate that Version 4 of the L4_SM product is of sufficient maturity and quality for dissemination to the public.

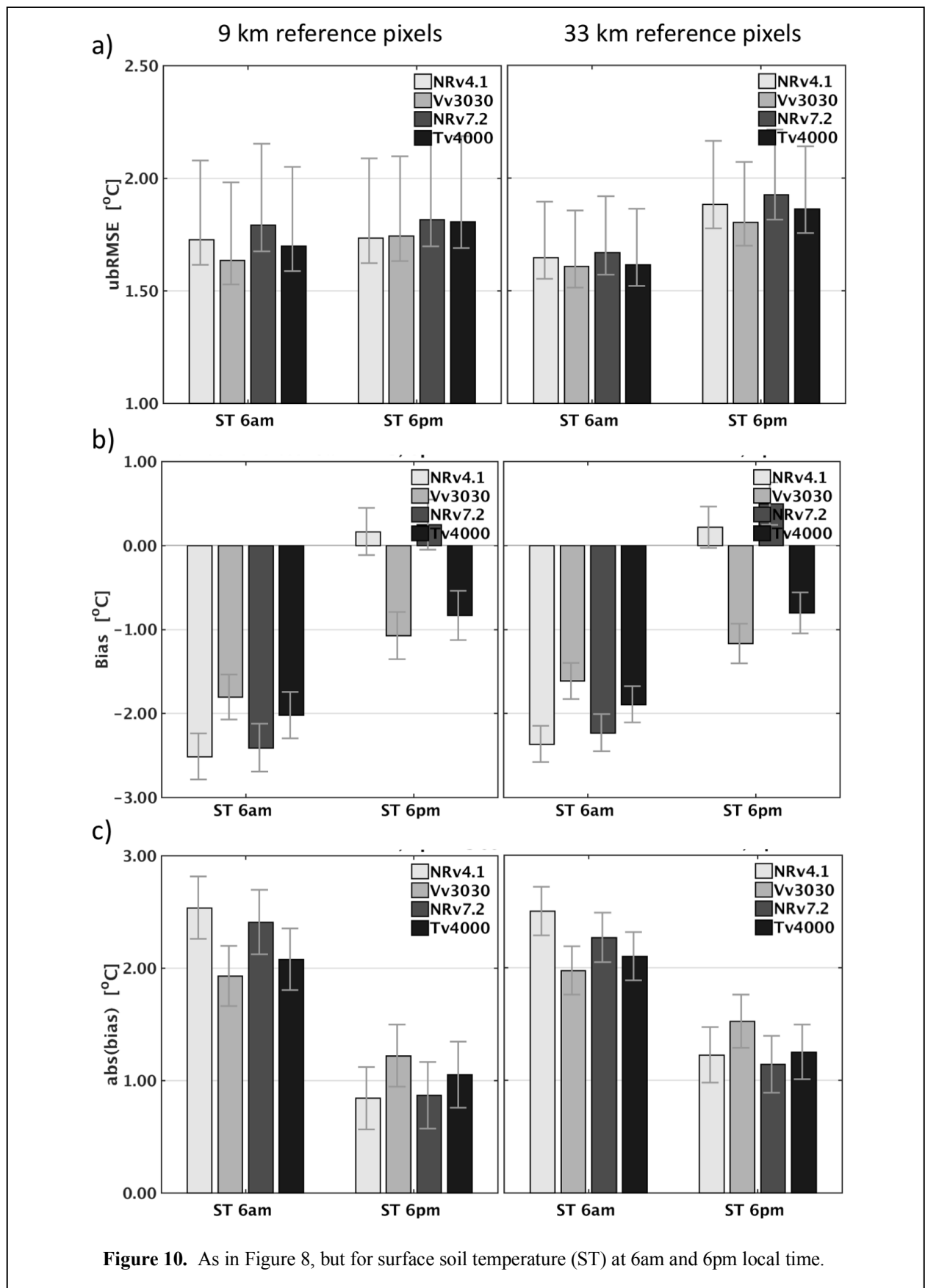
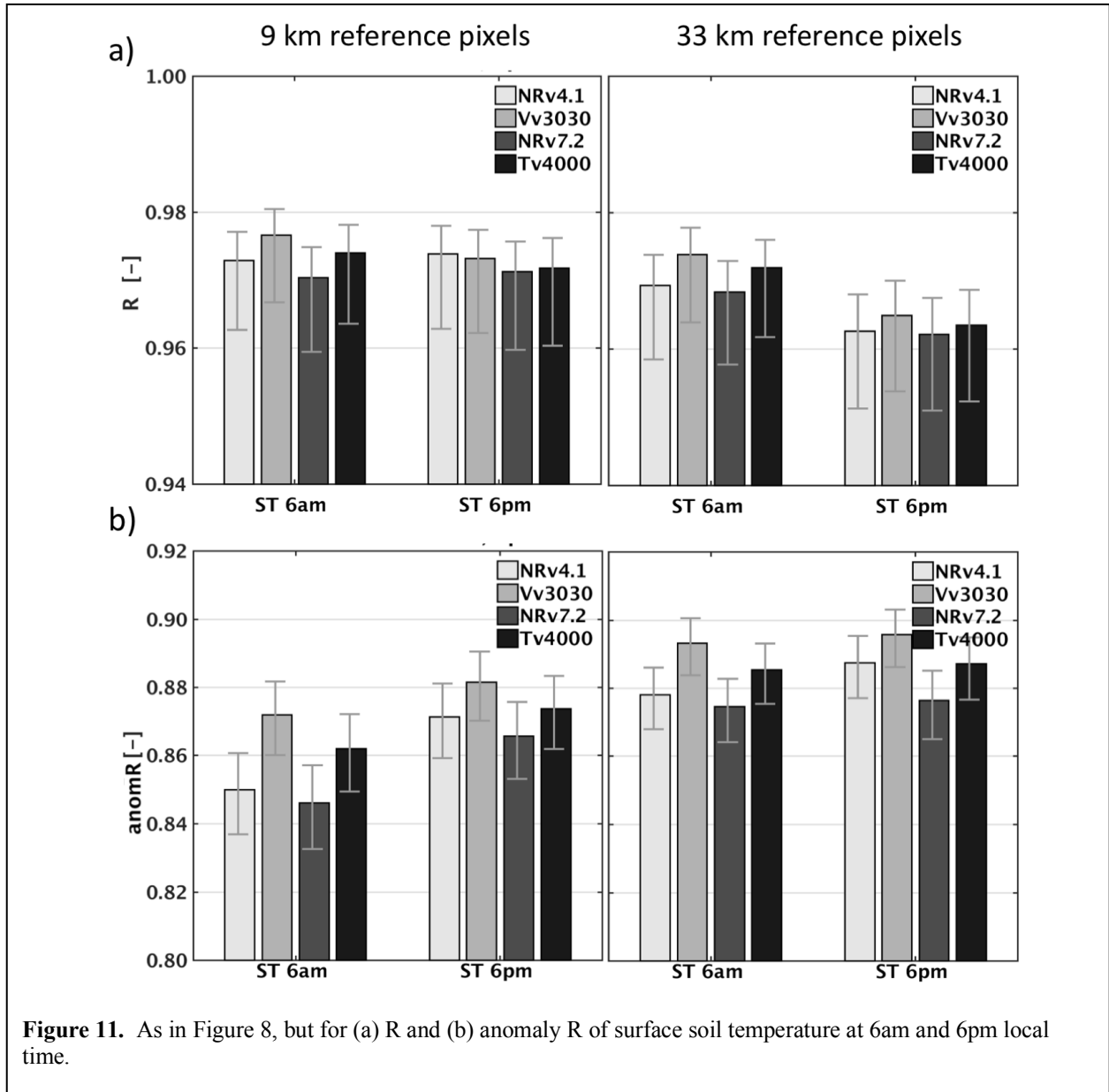


Figure 10. As in Figure 8, but for surface soil temperature (ST) at 6am and 6pm local time.



6.3 Sparse Networks

6.3.1 Method

The locally dense networks of the core validation sites are complemented by regional to continental-scale “sparse” networks. The defining feature of the sparse networks is that there is usually just one sensor (or profile of sensors) located within a given 9 km EASEv2 grid cell. Such point-scale measurements are, of course, generally not representative of the grid cell average conditions that the L4_SM algorithm is trying to estimate. Although sparse networks are not ideal for soil moisture validation for this and other reasons, they offer in situ measurements in a larger variety of environments and provide data operationally with very short latency. See Reichle et al. (2015) for further discussion of the advantages and limitations of using sparse networks in the L4_SM validation process.

This assessment report focuses on metrics obtained from a direct comparison of the L4_SM product to in situ measurements, that is, metrics derived without using triple collocation approaches that attempt to correct for errors in the in situ measurements (Chen et al. 2016; Gruber et al. 2016). The values of the time series correlation metrics provided here are thus lower than those that would be obtained with the aid of triple collocation, and they are therefore conservative estimates of the true skill. Note also that the *relative* performance of the products under investigation does not depend on the use of triple collocation approaches.

The skill of the L4_SM estimates was computed using all available in situ measurements (after quality control) at 3-hourly time steps, and this skill was then compared to that of the Nature Run estimates. For sparse networks, we used the same requirements for the minimum number of data values as for core validation sites (section 6.2). Note that quality control generally excludes in situ measurements when the ground is frozen (see Reichle et al. 2015, Appendix C). Instantaneous L4_SM data from the “aup” Collection and Nature Run data were taken directly from the standard 9 km EASEv2 grid cell that includes the sensor location (that is, the data product estimates are not interpolated bilinearly or otherwise to the precise location of the in situ sensor locations). Metrics were computed for surface and root zone soil moisture against in situ measurements from the SCAN, USCRN, OK Mesonet, OZNet-Murrumbidgee, and SMOSMania networks (Table 2). The average metrics were computed based on a clustering algorithm that assigns the weights given to each location based on the density of sites in the surrounding region (De Lannoy and Reichle 2016).

Table 2. Overview of sparse networks, with indication of the sensor depths and the number of sites (N) used here. Values in parentheses indicate the number of sites for which the anomaly R metric was computed. The anomaly R metric was only available for sites with sufficient data to compute a seasonally varying climatology.

Network	Area	Sensor Depths (cm)	Number of Sites		Period
			Surface	Root Zone	
SCAN	USA	5, 10, 20, 50	134 (112)	106 (74)	1 Apr 2015 - 31 Mar 2018
USCRN	USA	5, 10, 20, 50	111 (106)	77 (65)	
OK Mesonet	Oklahoma	5, 25, 60	118 (115)	77 (76)	
OZNet	Australia	4, 45	43 (36)	19 (16)	
SMOSMania	France	5, 20	21 (0)	21 (0)	1 Apr 2015 - 31 Dec 2016
All Networks			427 (369)	300 (231)	

Measurements used for L4_SM validation cover most of the contiguous United States (SCAN, USCRN, OK Mesonet), parts of the Murrumbidgee basin in Australia (OZNet), and an area in southwestern France (SMOSMania). The in situ measurements from the sparse network sites were subjected to extensive automated and manual quality control procedures by the L4_SM team following (Liu et al. 2011), which removed spikes, temporal inhomogeneities, oscillations, and other artifacts that are commonly seen in these automated measurements. Table 2 also lists the number of sites with sufficient data after quality control.

A total of 427 sites provided surface soil moisture measurements, and 300 provided root zone soil moisture measurements. Most of the sites are in the continental United States, including about 100 each in the USCRN and SCAN networks, and another ~100 sites in Oklahoma alone from the OK Mesonet. The OZNet network contributes 43 sites with surface soil moisture measurements, of which 19 sites also provide root zone measurements. Finally, 21 sites with surface and root zone soil moisture measurements were used from the SMOSMania network. For most networks, around 10-20% of the sites do not have sufficient numbers of measurements for the computation of the climatology that is needed to determine the anomaly R skill. Anomaly R values are not available for any of the SMOSMania sites because SMOSMania data were only available through 2016.

Table 2 also lists the sensor depths that were used to compute the in situ root zone soil moisture. As with the core validation sites, vertical averages for SCAN, USCRN, and OK Mesonet are weighted by the spacing of the sensor depths within the 0-100 cm layer corresponding to the L4_SM estimates, and the average is only computed if all sensors within a given profile provide measurements after quality control. For SCAN and USCRN sites, some measurements at 100 cm depth are available, but these deeper layer measurements are not of the quality and quantity required for L4_SM validation and are therefore not used here. For OZNet and SMOSMania, in situ root zone soil moisture is given by the measurements at the 45 cm and 20 cm depth, respectively; that is, no vertical average is computed.

6.3.2 Results

Figure 12 shows the average L4_SM and Nature Run metrics across all sparse network sites. When validated against the sparse network measurements, both versions of the L4_SM products show generally lower ubRMSE and higher R and anomaly R values than the corresponding Nature Run estimates, with improvements that are statistically significant at the 5% level for the surface soil moisture correlation metrics. This again demonstrates the additional information contributed by the assimilation of the SMAP brightness temperature observations in the L4_SM system.

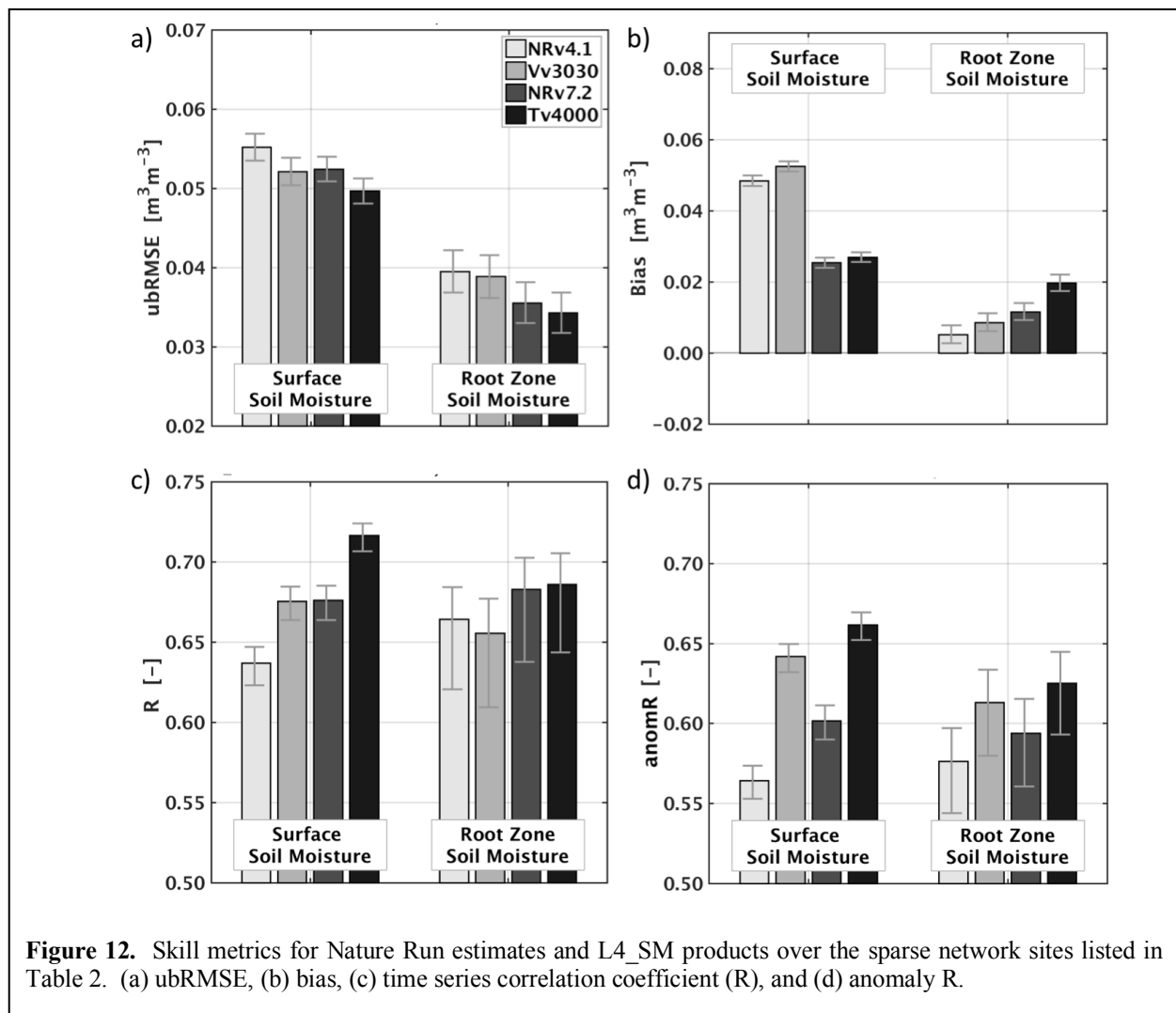
As with the core site validation results, the ubRMSE and bias values vs. the sparse network measurements are smaller (better) for root zone soil moisture than for surface soil moisture, which again reflects the fact that root zone soil moisture generally varies less in time than surface soil moisture.

The sparse network results suggest an improvement in the Version 4 L4_SM product compared to Version 3 across all metrics except the bias in root zone soil moisture. Specifically, the Version 4 product has lower ubRMSE values and higher R and anomaly R values for the surface and root zone, with statistically significant improvements in the Version 4 surface soil moisture correlation metrics compared to Version 3. Moreover, the average surface soil moisture bias at the sparse network sites has been reduced to about $0.025 \text{ m}^3 \text{ m}^{-3}$ in Version 4, compared to $0.05 \text{ m}^3 \text{ m}^{-3}$ in Version 3, although the root zone soil moisture bias increased to $0.02 \text{ m}^3 \text{ m}^{-3}$ in Version 4 from $0.01 \text{ m}^3 \text{ m}^{-3}$ in Version 3.

As with the core validation sites, the validation of the L4_SM and Nature Run estimates vs. sparse network measurements is within regions where the surface meteorological forcing takes advantage of high-quality, gauge-based precipitation measurements. Larger improvements from the assimilation of SMAP

observations can be expected in areas where the precipitation forcing inputs are not as well informed by gauge measurements.

Overall, the evaluation of skill for the sparse network sites yields results that are very similar to those obtained for the core validation sites. The beneficial impact of assimilating SMAP brightness temperature observations is greatest for surface soil moisture, with smaller improvements in root zone soil moisture estimates. Finally, it is important to keep in mind that all of the skill metrics presented here underestimate the true skill because these metrics are based on a direct comparison against in situ measurements (which are subject to error). Therefore, the sparse network ubRMSE values suggest that the L4_SM estimates would meet the formal accuracy requirement across a very wide variety of surface conditions, beyond those that are covered by the few core validation sites that have been available to date for formal verification of the accuracy requirement. One caveat, however, is that the sparse network results do not provide an entirely independent validation because SCAN and USCRN measurements were used to calibrate the NRv7.2 model (section 5.3.2). Nevertheless, the sparse network results provide additional confidence in the conclusions drawn from the core validation site comparisons.



6.4 Data Assimilation Diagnostics

This section provides an evaluation of the L4_SM data assimilation diagnostics, including the statistics of the observation-minus-forecast (O-F) residuals, the observation-minus-analysis (O-A) residuals, and the analysis increments. Because the L4_SM algorithm assimilates brightness temperature observations, the O-F and O-A diagnostics are in terms of brightness temperatures (that is, in “observation space”). The analysis increments are, strictly speaking, in the space of the Catchment model prognostic variables that make up the “state vector”, including the “root zone excess”, “surface excess”, and “top-layer ground heat content” (Reichle et al. 2014b). For the discussion below, the soil moisture increments have been converted into equivalent water flux terms in units of mm d^{-1} .

A key element of the analysis update is the downscaling and inversion of the observational information from the 36 km grid of the assimilated brightness temperatures into the modeled geophysical variables on the 9 km grid, based on the modeled error characteristics, which vary dynamically and spatially. An example and illustration of a single analysis update can be found in Reichle et al. (2017b, their section 3b).

6.4.1 Observation-Minus-Forecast Residuals

Figure 13 shows the global coverage of the SMAP L1C_TB observations that were used in the Tv4000 L4_SM analysis for 7 June 2015, 0z. The analysis window includes brightness temperature observations between 22:30z on 6 June 2015 and 01:30z on 7 June 2015. Within this window, a total of 17,702 observations were used, including 6,412 H-pol and 6,385 V-pol observations from two descending half-orbits over eastern Asia and 2,454 H-pol and 2,451 V-pol observations from two ascending half-orbits over the Americas.

Note that SMAP L1C_TB observations were used over China and central Asia where L-band radio-frequency interference (RFI) is common. This was not possible in Versions 1 and 2 of the L4_SM product (Reichle et al. 2015, 2016, 2017b) because the L4_SM algorithm requires knowledge of the long-term L-band brightness temperature climatology to address observation-minus-forecast bias in the system (Reichle et al. 2014b). In Versions 1 and 2, this knowledge was extracted from SMOS data, for which RFI in these regions prevents good quality observations. SMAP, in contrast, is equipped with a variety of hardware and software tools to correct for RFI and generally provides near-global coverage. Beginning with Version 3 of the L4_SM algorithm, the required climatological information has been computed from SMOS brightness temperatures and, additionally, from SMAP observations for times and locations where sufficient numbers of SMOS data are not available (section 5.3.1), thus enabling the assimilation of SMAP observations with near-global coverage. Note that in Version 2, only ~8,900 observations were used for the 7 June 2015, 0z analysis (compare Figure 13 to Figure 12 of Reichle et al. 2016).

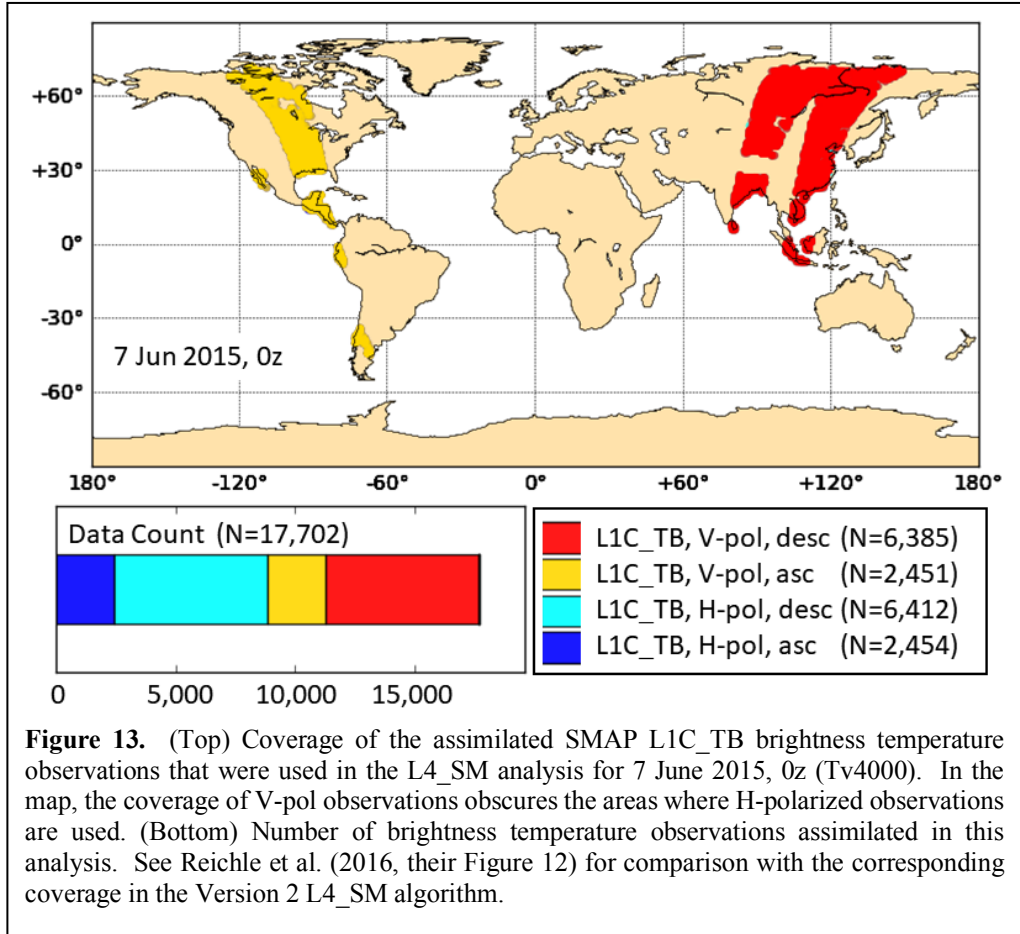


Figure 13. (Top) Coverage of the assimilated SMAP L1C_TB brightness temperature observations that were used in the L4_SM analysis for 7 June 2015, 0z (Tv4000). In the map, the coverage of V-pol observations obscures the areas where H-polarized observations are used. (Bottom) Number of brightness temperature observations assimilated in this analysis. See Reichle et al. (2016, their Figure 12) for comparison with the corresponding coverage in the Version 2 L4_SM algorithm.

The increase in spatial coverage is further illustrated in Figure 14, which shows the total number of L1C_TB observations that were assimilated at each grid cell in Version 4 during the assessment period (1 Apr 2015, 0z, to 1 Apr 2018, 0z). This count includes H- and V-pol observations from ascending and descending orbits. The average data count across the globe is approximately 1,423 for the 1,096-day period. (Results are very similar for Version 3.) Few or no SMAP brightness temperatures are assimilated in high-elevation and mountainous areas (including the Rocky Mountains, the Andes, the Himalayas and Tibet), in the vicinity of lakes (such as in northern Canada), and next to major rivers (including the Amazon and the Congo). In the high latitudes, the much shorter warm (unfrozen) season also results in lower counts of assimilated brightness temperature observations, although this is somewhat mitigated by SMAP's polar orbit, which results in more frequent revisit times there. The remaining gaps in coverage might reflect a lack of sufficient numbers of SMOS and SMAP observations to provide the required climatological information for the computation of the (seasonally varying) brightness temperature scaling parameters during the times of the year when conditions are suitable for a soil moisture analysis. Note, however, that the L4_SM product provides soil moisture estimates everywhere, even if in some regions the L4_SM estimates are not based on the assimilation of SMAP observations and rely only on the information in the model and forcing data.

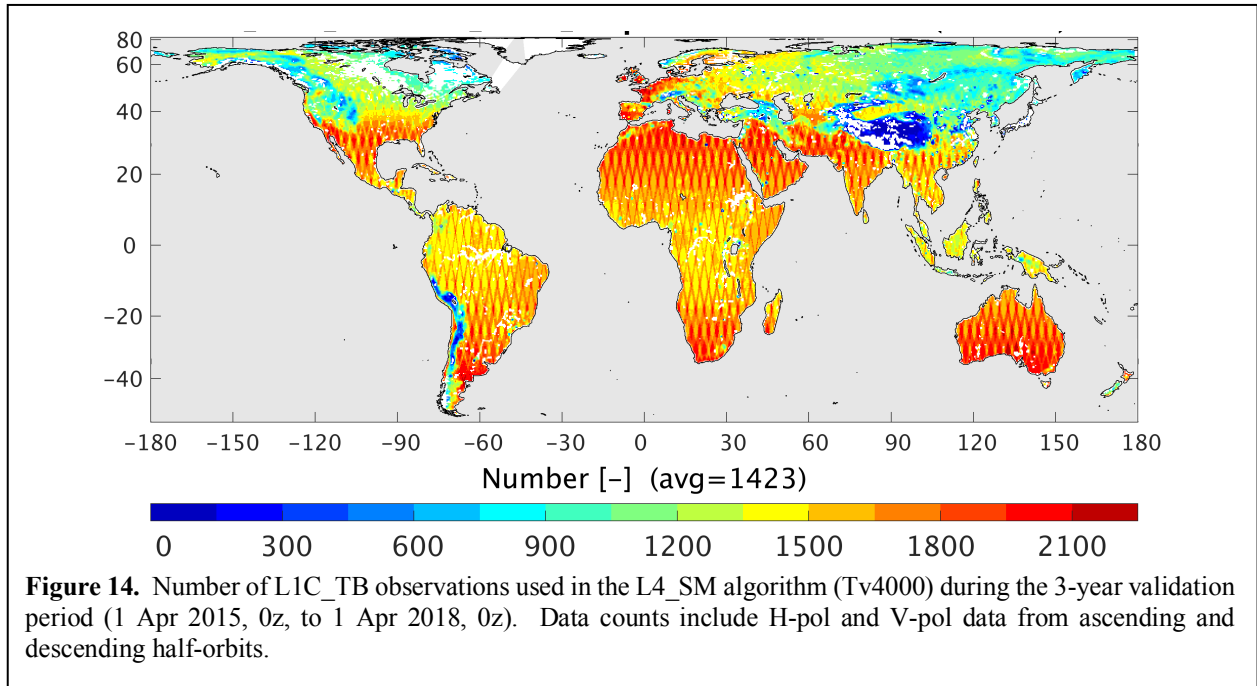
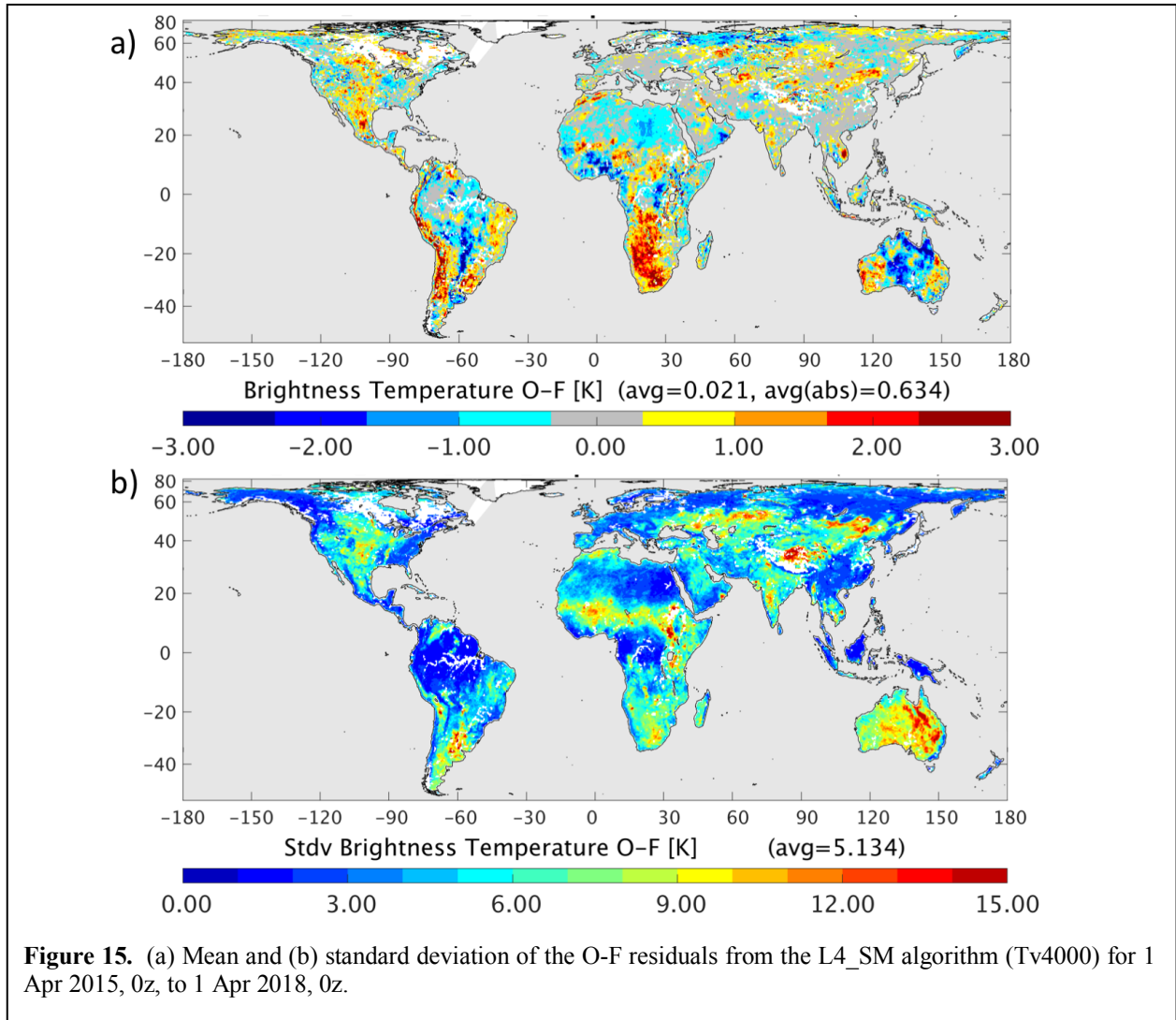
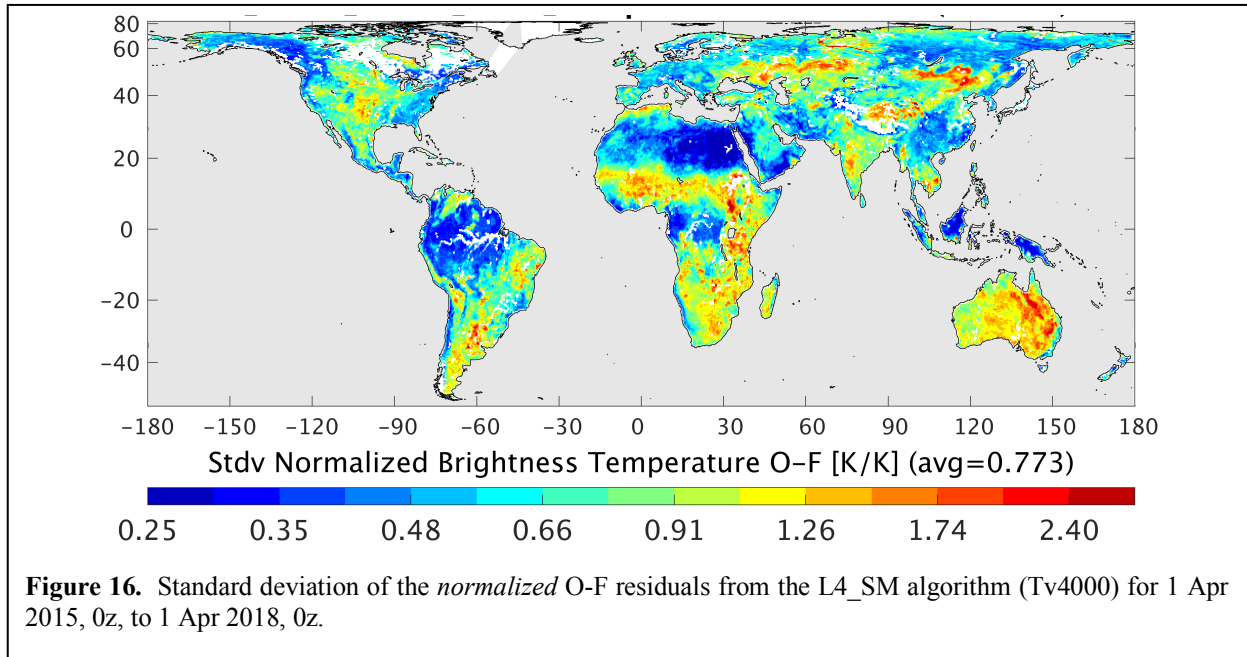


Figure 15 shows the global distributions of the time series mean and standard deviation of the O-F brightness temperature residuals. The time mean values of the O-F residuals are typically small and mostly range from -3 to 3 K, with an overall bias of just 0.02 K. Larger values are found in southern South America, western and southern Africa, and Australia. These biases are slightly larger in Version 4 compared to Version 3. Over Africa, the L4_SM precipitation forcing is not corrected to the gauge-based product (Reichle and Liu 2014). Therefore, in Africa the L4_SM algorithm relies heavily on the consistency between the present forcing data from the $\frac{1}{4}$ degree GEOS operational forward processing (FP) system (GEOS-5.13.0 through GEOS-5.17) and the historic forcing data from the $\frac{1}{2}$ degree MERRA-2 system (GEOS-5.12.4) that contributed to the derivation of the brightness temperature scaling parameters in the calibration of the L4_SM algorithm. On the other hand, Version 4 no longer shows the larger bias in the center of the United States that was seen in Version 3 (not shown). While the results suggest that the L4_SM algorithm is reasonably unbiased, the system could obviously benefit from further calibration.

The time series standard deviation of the O-F residuals ranges from a few Kelvin to around 15 K. The highest values are found in central North America, southern South America, southern Africa, the Sahel, central Asia, India, and (particularly) Australia. These regions have sparse or modest vegetation cover and typically exhibit strong variability in soil moisture conditions. The O-F residuals are generally smallest in more densely vegetated regions, including the eastern United States, the Amazon basin, and tropical Africa. Small values are also found in the high latitudes, including Alaska and Siberia, and in the Sahara Desert. The global (spatial) average of the O-F standard deviation is about 5.1 K in Version 4 (Figure 15b), which is reduced from about 5.9 K in Version 3 and suggests that the modeling system of Version 4 is better able to predict the observed brightness temperatures just prior to each analysis. The spatially averaged time series standard deviation of the O-A residuals is 3.7 K (not shown), which again reflects the impact of the SMAP observations in the L4_SM system. The corresponding value in Version 3 is 4.0 K (not shown).



Finally, Figure 16 shows the standard deviation of the *normalized* O-F residuals, which measures the consistency between the expected (modeled) errors and the actual errors. Specifically, the O-F residuals are normalized with the standard deviation of their expected total error, which is the sum (in a covariance sense) of the error in the observations (including instrument errors and errors of representativeness) and the error in the brightness temperature model forecasts (Reichle et al. 2015, their Appendix B). The parameters that determine the expected error standard deviations are key inputs to the ensemble-based L4_SM assimilation algorithm. If they are chosen such that the expected errors are fully consistent with the actual errors, the metric shown in Figure 16 should be unity everywhere. If the metric is less than one, the actual errors are overestimated by the assimilation system, and if the metric is greater than one, the actual errors are underestimated.



The global average of the metric in Version 4 is 0.77, which suggests that, on average, the modeled errors are overestimating the actual errors (Figure 16). The metric, however, varies greatly across the globe. Typical values are either too low or too high. In the Amazon basin, the eastern US, tropical Africa, and portions of the high northern latitudes, values range from 0.25 to 0.5, and thus errors there are considerably overestimated. Conversely, in central North America, the Sahel, southern Africa, India, portions of central Asia and most of Australia, values range from 1.5 to 3, meaning that errors in these regions are considerably underestimated. In Version 3, the global pattern of low and high values of the normalized O-F standard deviation was very similar, but with nearly uniformly greater values and a global average of almost exactly unity (not shown). This global average would suggest that Version 3 was better calibrated than Version 4 in terms of this metric. But in the regions where the soil moisture analysis is most relevant, including central North America, the Sahel, and Australia, Version 4 has less underestimation of the actual errors than Version 3. The enhanced overestimation of actual errors in Version 4 (relative to Version 3) is primarily in densely vegetated regions where the SMAP brightness temperatures are mostly insensitive to soil moisture. In any case, more work is needed to further improve the calibration of the input parameters that determine the model and observation errors in the L4_SM system.

6.4.2 Increments

Figure 17 shows the average number of increments that the L4_SM algorithm generated per day during the validation period. The global mean is 0.81, which means that for a given location, there are approximately four increments applied every five days on average, either from an ascending or a descending overpass. The overall pattern of the increments count follows that of the count of the assimilated observations shown in Figure 14. The coverage of the increments, however, is somewhat greater than that of the observations due to the spatial interpolation and extrapolation of the observational information in the distributed analysis update of the L4_SM algorithm. The figure also reveals the diamond patterns resulting from SMAP's regular 8-day repeat orbit. The corresponding map for Version 3 (not shown) is very similar, except that Version 3 (and all prior versions) exhibited a few patches of slightly elevated data counts where fore- and aft-looking brightness temperatures for the same location and from the same half-orbit were inadvertently assimilated at different analysis times. This has been fixed in Version 4 (section 5.3.2).

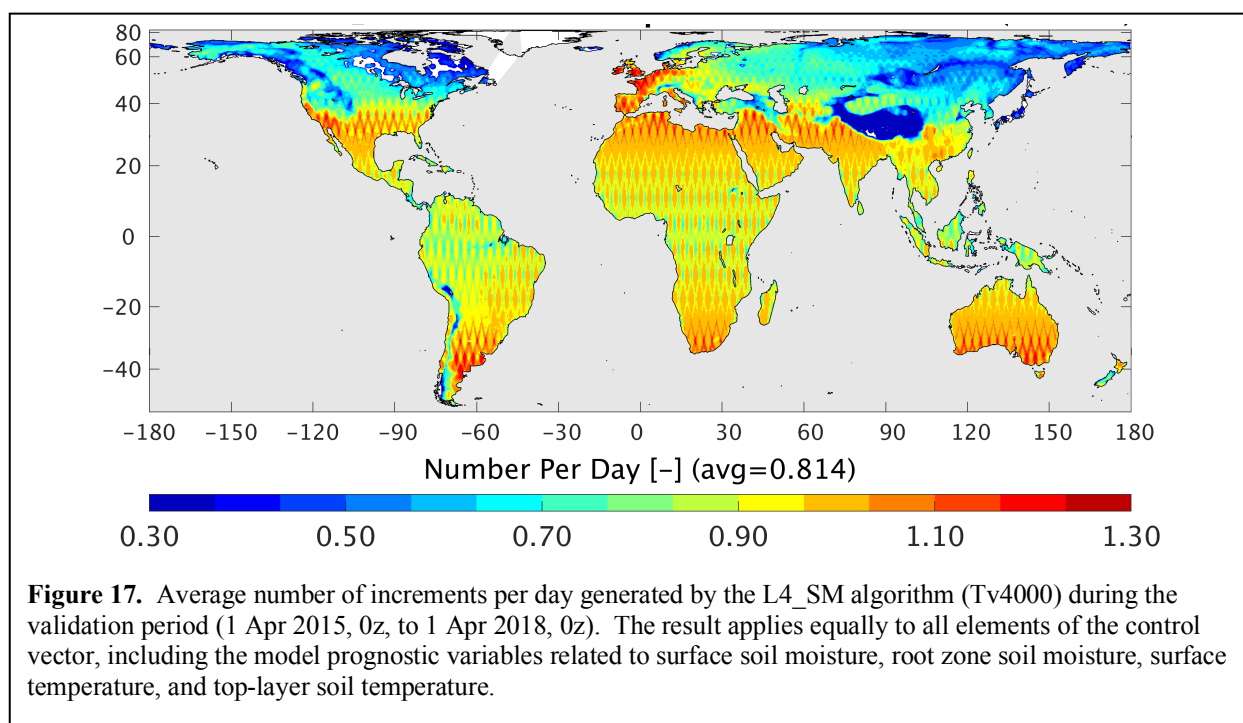
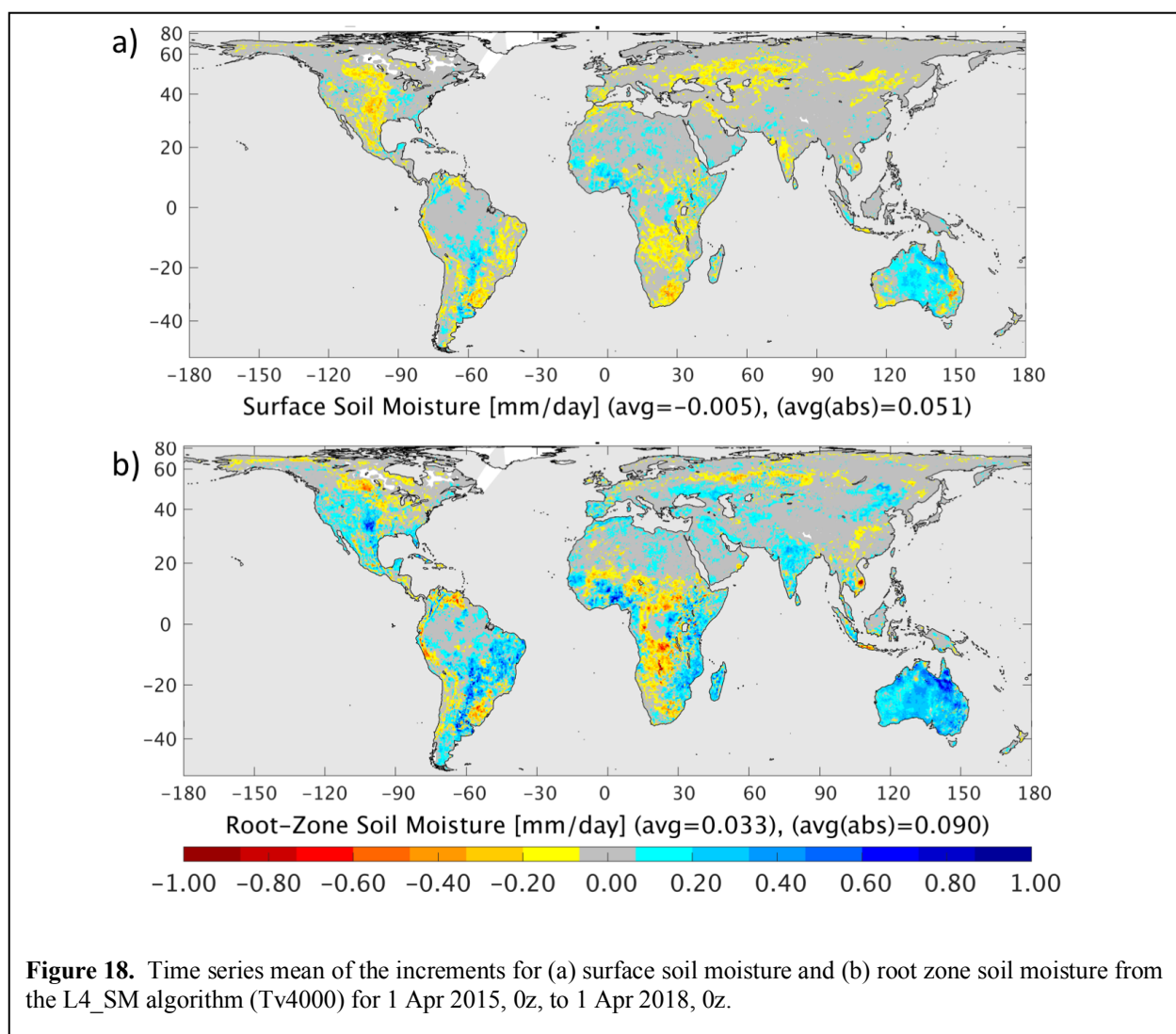


Figure 17. Average number of increments per day generated by the L4_SM algorithm (Tv4000) during the validation period (1 Apr 2015, 0z, to 1 Apr 2018, 0z). The result applies equally to all elements of the control vector, including the model prognostic variables related to surface soil moisture, root zone soil moisture, surface temperature, and top-layer soil temperature.

Figure 18 shows the time mean values of the analysis increments for surface and root zone soil moisture. In the global average, the net increments are only -0.005 mm d^{-1} for surface soil moisture and 0.03 mm d^{-1} (or $\sim 10 \text{ mm per year}$) for root zone soil moisture. Regionally, however, the mean increments are larger and constitute a non-negligible fraction of the water balance. The average absolute increment is about 0.05 mm d^{-1} for surface soil moisture and 0.09 mm d^{-1} for root zone soil moisture. Central North America, eastern South America, southern Africa, and portions of central Asia experience net drying increments in surface soil moisture, whereas Australia experiences net wetting increments. Root zone soil moisture increments similarly have a net wetting effect in Australia. Interestingly, there is a net wetting in the root zone in central North America, where the surface layer experiences a net drying. Generally, the pattern of the net increments reflects the long-term mean bias in the O-F residuals (Figure 15a). Compared to Version 4, the long-term mean increments in Version 3 are typically smaller by a factor of two for surface soil moisture and larger by the same factor for root zone soil moisture (not shown).

Figure 19 shows the time series standard deviation of the increments in surface and root zone soil moisture. This metric measures the typical magnitude of instantaneous increments. Typical increments in surface soil moisture are on the order of 0.2 mm d^{-1} in the central US, the Sahel, southern South America, southern Africa, India, portions of central Asia, and most of Australia. In the same regions, root zone soil moisture increments are typically on the order of 0.1 mm d^{-1} . Over densely vegetated regions, in particular the tropical forests, surface and root zone soil moisture increments are generally negligible, reflecting the fact that in those areas the measured SMAP brightness temperatures are mostly sensitive to the dense vegetation and are only marginally sensitive to soil moisture.



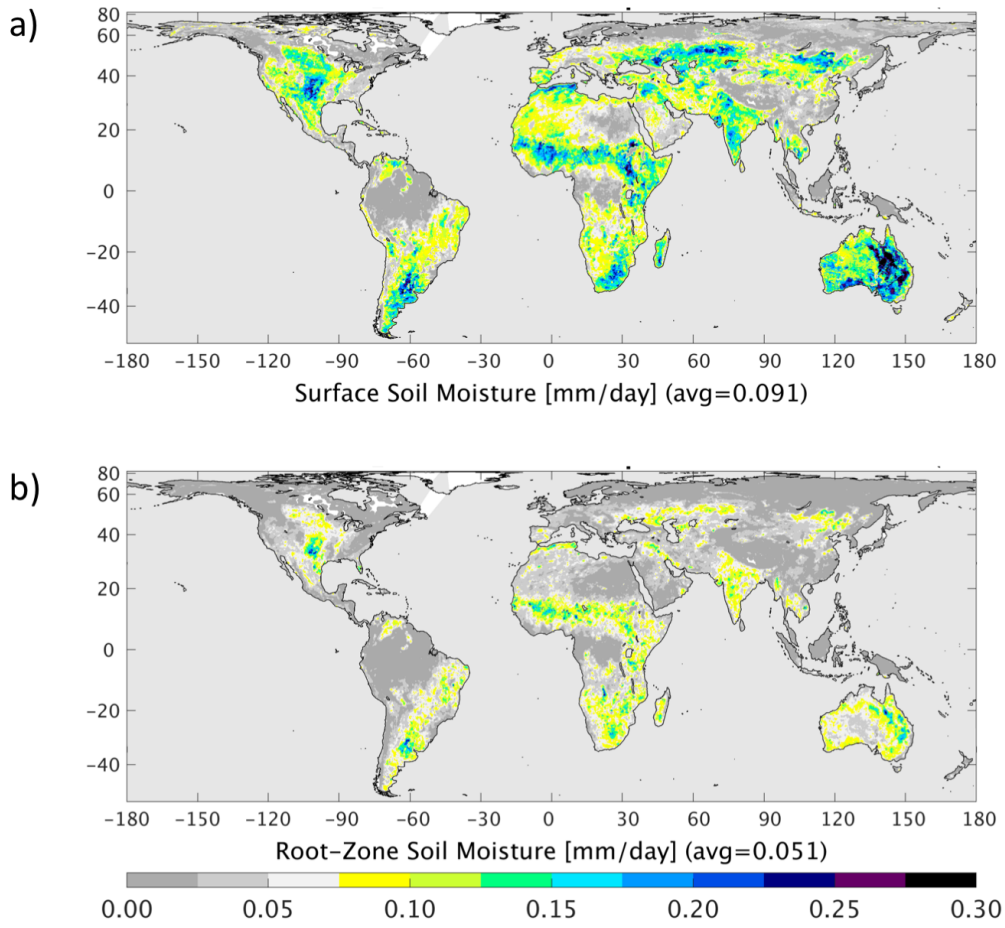


Figure 19. Same as Figure 18 but for time series standard deviation of the increments.

6.4.3 Uncertainty Estimates

The L4_SM data product also includes error estimates for key output variables, including surface and root zone soil moisture as well as surface soil temperature. These uncertainty estimates vary dynamically and geographically because they are computed as the standard deviation of a given output variable across the ensemble of land surface states at a given time and location. (The ensemble is an integral part of the ensemble Kalman filter employed in the L4_SM algorithm, and the ensemble mean provides the estimate of the variable under consideration (Reichle 2008).) By construction, the uncertainty estimates represent only the random component of the uncertainty. Bias and other structural errors such as errors in the dynamic range are not included.

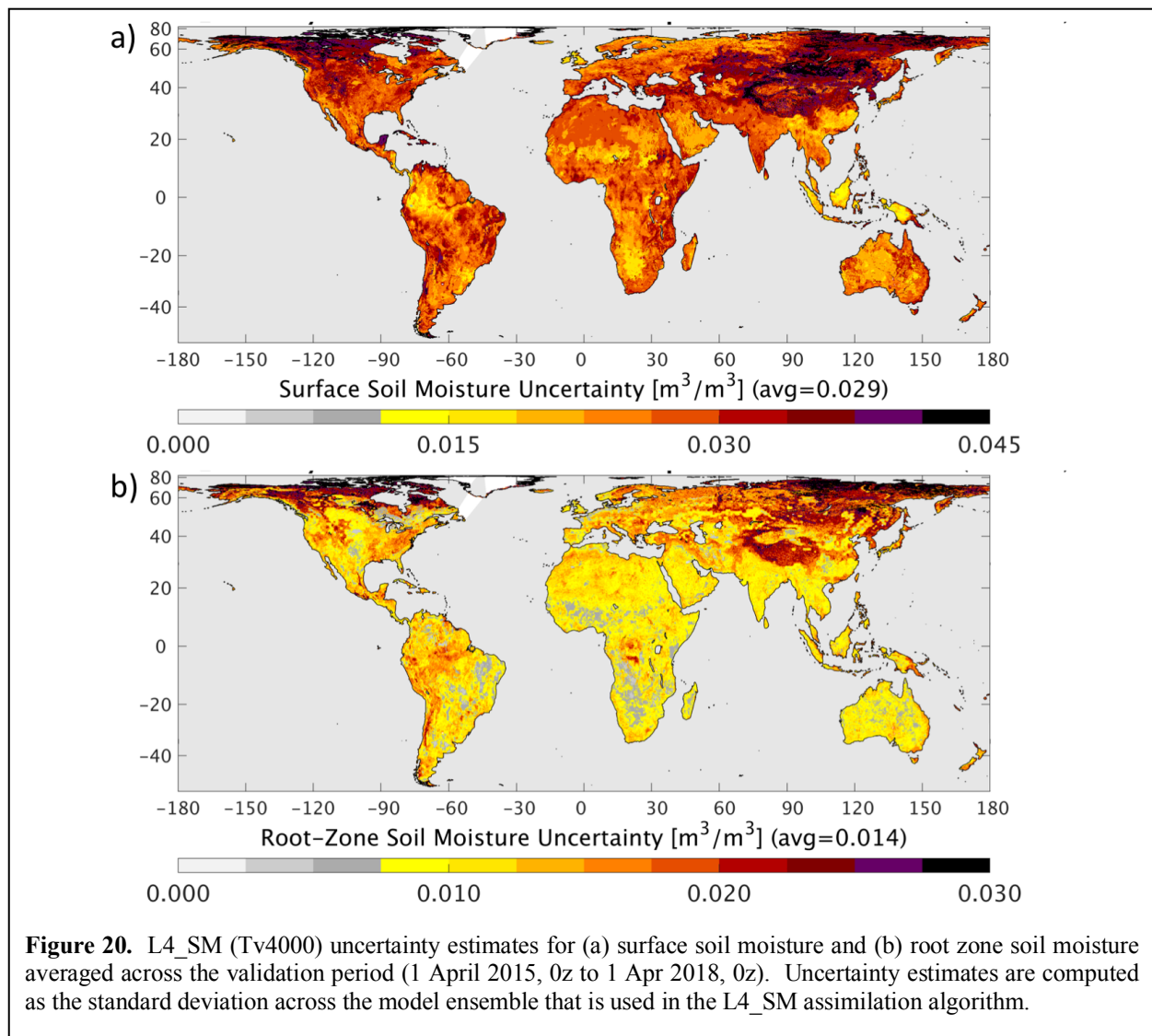


Figure 20 shows the time mean of the uncertainty estimates for the validation period. Across the globe, surface soil moisture uncertainty typically ranges from 0.02 to 0.04 m³ m⁻³ in Version 4, with the larger uncertainties in regions where the lowest number of SMAP brightness temperatures are assimilated (Figure 14), including northwestern North America and northeastern Asia, which are subject to frozen or snow-covered conditions for a large part of the year. The less frequent brightness temperature analysis in these

regions implies less reduction in ensemble spread. The uncertainty in root zone soil moisture exhibits a similar pattern, albeit with uncertainty estimates typically ranging from 0.01 to 0.02 m³ m⁻³. The lower uncertainty estimates in root zone soil moisture primarily reflect the fact that root zone soil moisture is less variable in time than surface soil moisture.

In Version 4, the uncertainty estimates are larger than in Version 3 by ~50% for surface soil moisture and ~20% for root zone soil moisture (not shown), bringing the uncertainty estimates more in line with ubRMSE results from the core site validation. Moreover, the spatial patterns of the uncertainty estimates in Version 4 are more plausible. In Version 3, the highest surface soil moisture uncertainty estimates were counter-intuitively concentrated in the driest regions such as the Sahara Desert. Moreover, in Version 3 the global patterns of the uncertainty estimates were very different for surface and root zone soil moisture, which is also counter-intuitive. The greater similarity in Version 4 of the patterns in surface and root zone soil moisture uncertainty is likely an improvement.

7 LIMITATIONS AND PLAN FOR FUTURE IMPROVEMENTS

The assessment of Version 4 of the L4_SM product presented in the previous section reveals a number of current limitations as well as avenues for future development.

7.1 Bias and L4_SM Algorithm Calibration

Compared to earlier versions, the calibration of the Version 4 L4_SM algorithm utilized (i) longer records of SMAP and SMOS brightness temperature observations and (ii) surface meteorological forcing data from longer and more consistent GEOS products. The improved algorithm calibration reduced the residual bias between the predicted brightness temperatures from the L4_SM modeling system and the (rescaled) SMAP observations, resulting in a less biased analysis. Figure 15a, however, showed that there are still regions with a modest bias in the brightness temperature O-F residuals, which in turn leads to non-zero long-term mean analysis increments in surface and root zone soil moisture (Figure 18).

Eventually, further improvements in the L4_SM algorithm calibration will be facilitated by an even longer record of SMAP observations, in combination with further improvements in and perhaps even convergence of the calibration of the SMAP and SMOS brightness temperature records. It is unlikely, however, that there will be a suitable long-term, consistent record of GEOS products to alleviate the issues associated with breaks (or inhomogeneities) in the surface meteorological forcing data.

A long-term reanalysis dataset such as MERRA-2 is needed for L4_SM algorithm calibration. The GEOS system used to generate this reanalysis, however, is always going to be different (in both model version and resolution) from the near-real time forward-processing (FP) system required to force the SMAP L4_SM algorithm during the SMAP period. Put differently, the climatological parameters derived from Nature Run data do not necessarily reflect the true climatology of the L4_SM system's model component, and this results in errors in L4_SM algorithm calibration and, consequently, some bias in long-term mean O-F residuals and analysis increments. Moreover, this climatological inconsistency negatively impacts the quality of the soil moisture output in *percentile* units from the “gph” Collection. More research is needed to ascertain the quality of these percentile outputs.

Another aspect of algorithm calibration involves the tuning of the L4_SM observation and model error parameters. Attempts to tune the model and observation error parameters manually or by using a poor man's adaptive filter have been inconclusive. Such tuning has so far failed to consistently improve the skill metrics versus independent in situ observations.

7.2 Impact of SMAP Observations and Ensemble Perturbations

The assessment of the L4_SM product presented herein uses NRv7.2 estimates as the model-based reference. Both estimates use the same gauge-corrected precipitation forcing. Not surprisingly, the assessment of the L4_SM and NRv7.2 estimates versus in situ soil moisture measurements is focused on regions for which the model forcing data can take advantage of typically dense and reliable precipitation gauge observations. The generally good skill of the NRv7.2 estimates in these regions therefore presumably leads to an underestimation of the impact of the SMAP brightness temperature observations in the L4_SM assimilation system. In regions with poor precipitation data, the impact of the SMAP observations should be larger, but because of the lack of observations of any kind in those regions, the precise impact remains unknown.

Secondly, the NRv7.2 and L4_SM estimates differ partly because the NRv7.2 estimates are from a single-member model run without perturbations, whereas the L4_SM estimates are based on an ensemble

of model realizations that experiences perturbations to its surface meteorological forcing and prognostic variables. An undesirable, yet at this time unavoidable, side effect of such perturbations is that they lead to biases between the ensemble mean estimates and the estimates from the unperturbed NRv7.2 model integration. These biases are particularly acute in very arid regions such as the Sahara Desert, southern Africa, and Australia, where the perturbations in soil moisture are, by construction, biased wet because the unperturbed, single-member model run typically remains at the lowest possible soil moisture value, thereby making negative (that is, drying) perturbations unphysical and thus disallowed. Some of the differences between the NRv7.2 and L4_SM estimates will therefore partly reflect the impact of the perturbations regime rather than the use of SMAP observations.

To investigate these two issues, ensemble model runs with and without gauge-based precipitation corrections were conducted for Version 3. Preliminary results (not shown) suggest that the impact of SMAP is indeed greater when gauge-based precipitation corrections are unavailable. Moreover, the ensemble model runs also revealed that the long-term mean impact of the perturbations on the water balance rivals that of the long-term mean analysis increments. Similar ensemble model runs for the Version 4 system will be conducted along with the reprocessing of the Version 4 L4_SM data.

Another shortcoming of the L4_SM product is the relative lack of predictive power in the L4_SM uncertainty estimates (section 6.4.3). While the bias of the Version 4 uncertainty estimates has been considerably reduced relative to earlier versions, there is no correlation between the uncertainty estimates and actual L4_SM errors (vs. in situ soil moisture measurements). Unfortunately, it is not clear at this time how the uncertainty estimates could be improved.

7.3 Expanded Site Locations, Record Length, and Data Sets

The assessment of the Version 4 product is still limited by the relatively short period of record. Only 3 years of data were available for this assessment report, which is too short to adequately assess inter-annual variations. The anomaly R values provided in this assessment only provide a first glance at the ability of the L4_SM product to describe year-to-year variations in soil moisture. As the SMAP observatory continues to provide measurements, the length of the data record that can be assessed, and therefore the reliability of the assessment, will continue to increase. With time, we also hope to see a further increase in the volume of validation data, with additional soil moisture and soil temperature measurements becoming available from core sites and sparse networks that are currently still under development. Moreover, tower measurements of latent and sensible heat fluxes, which are typically published with a couple years latency, should soon be of sufficient number during the SMAP period to evaluate the L4_SM latent and sensible heat flux estimates.

7.4 L4_SM Algorithm Refinements

Despite its overall complexity, the L4_SM algorithm includes many simplifications. For example, SMAP brightness temperatures are not assimilated when the water fraction of the observed field-of-view exceeds a threshold of 5%. The Version 4 L1C_TB product newly includes water-corrected brightness temperatures (Peng et al. 2018), which may be suitable for assimilation into the L4_SM algorithm beyond the current 5% threshold for water within the field-of-view. Alternatively, the L4_SM algorithm could be refined to include the brightness temperature of open water in its forward operator. This would require a dynamic model of the surface temperature of lakes and large rivers in the L4_SM modeling system, as well as a corresponding radiative transfer model, based, for example, on the model by Klein and Swift (1977).

Another avenue worth exploring is the assimilation of the enhanced-resolution brightness temperatures from the SMAP L1C_TB_E product (Peng et al. 2018). The L1C_TB_E algorithm exploits the

oversampling in the SMAP radiometer observations and employs a Backus-Gilbert algorithm to increase the resolution of the brightness temperature estimates to ~27 km, compared to the ~40 km resolution of the standard L1C_TB product. The L1C_TB_E product is posted on the 9 km EASEv2 grid and thus is oversampled relative to its true resolution, which may have adverse effects on the L4_SM analysis. Additional research is needed to determine if and how the L4_SM product could be improved through the assimilation of enhanced-resolution brightness temperatures.

The CPCU gauge-based precipitation observations contribute considerably to the skill of the L4_SM soil moisture estimates, but they are by no means perfect. Precipitation corrections, for example, are not applied in Africa and the high-latitudes owing to the sparsity of the precipitation gauge network there. The monitoring of the L4_SM O-F residuals and a verification of the L4_SM precipitation against observations from the Australian Bureau of Meteorology have revealed further that the quality of the CPCU product is relatively poor in central Australia (Reichle et al. 2017b). This result rests on a comparison of CPCU estimates with a continent-wide, gauge-based precipitation dataset from the Australian Bureau of Meteorology. The latter product is publicly available within a latency that would likely permit its integration into the L4_SM algorithm as a replacement for the CPCU precipitation observations over Australia. More work is needed, however, to implement and test the Australian precipitation data within the L4_SM algorithm.

8 SUMMARY AND CONCLUSIONS

This report provides an assessment of Version 4 of the SMAP L4_SM product based on Tv4000 test data. The L4_SM test data cover the period from 1 April 2015, 0z to 1 April 2018, 0z and are based on the assimilation of a matching pre-release test dataset of LIC_TB observations. The test data are very similar to the official Version 4 data product (ECS Version ID 4) that is being generated and published beginning on 14 June 2018.

Version 4 of the L4_SM algorithm is based on a revised land surface modeling system. The model changes include revised parameters and parameterizations of (i) the surface energy balance, (ii) recharge from below of the model's surface excess reservoir, and (iii) the snow depletion curve. Updated ancillary inputs include improved datasets for land cover, topography, and vegetation height. Moreover, the new modeling system includes a revised approach to precipitation corrections that improves the precipitation climatology in Africa and the high-latitudes. For system calibration, the model is forced retrospectively with MERRA-2 reanalysis data, which are closer to the near-real time GEOS FP forcing used during the SMAP period than are the retrospective GEOS data that were available for previous L4_SM versions. In short, Version 4 benefits from an improved L4_SM modeling component along with retrospective data that are as consistent as possible with the present-day data in terms of their climatology.

The microwave radiative transfer model parameters and the brightness temperature scaling parameters used in the Version 4 algorithm are based on longer and improved SMOS records. Moreover, beginning with Version 3 of the L4_SM algorithm, the brightness temperature scaling parameters are derived from SMAP observations wherever SMOS data are impacted by radio-frequency interference. This facilitates the assimilation of SMAP brightness temperatures with near-global coverage and overcomes the considerable spatial gaps in the brightness temperature analysis of earlier L4_SM versions.

In this report, the Tv4000 L4_SM test product was validated using in situ soil moisture measurements from core validation sites and sparse networks. The product was further evaluated through an assessment of the data assimilation diagnostics generated by the L4_SM algorithm, such as the observation-minus-forecast residuals and the increments.

An analysis of the time-averaged surface and root zone soil moisture shows that the global pattern of arid and humid regions is captured by the Version 4 L4_SM estimates. Owing to the changes in the land surface modeling system, surface soil moisture is typically drier by several volumetric percent in Version 4 compared to Version 3, whereas root zone soil moisture is wetter in Version 4 in some regions and drier in others. Because of these climatological differences, the Version 3 and Version 4 products should *not* be combined into a single dataset for use in applications.

Based on the comparisons with the core validation site measurements, the L4_SM Tv4000 estimates of surface and root zone soil moisture meet the accuracy requirement ($\text{ubRMSE} < 0.04 \text{ m}^3 \text{ m}^{-3}$). For surface soil moisture the ubRMSE is $0.039 \text{ m}^3 \text{ m}^{-3}$ at the 9 km scale and $0.036 \text{ m}^3 \text{ m}^{-3}$ at the 33 km scale. For root zone soil moisture, the ubRMSE is $0.029 \text{ m}^3 \text{ m}^{-3}$ at the 9 km scale and $0.020 \text{ m}^3 \text{ m}^{-3}$ at the 33 km scale. The assimilation of SMAP brightness temperatures in the L4_SM algorithm is beneficial for surface and root zone soil moisture estimates, with improvements over the model-only Nature Run (NRv7.2) that are consistent across the 9 km and 33 km scales and across the ubRMSE and R metrics. For surface soil moisture, the improvements are statistically significant at the 5% level in most cases. The comparison with in situ measurements from a global set of sparse networks corroborate the results obtained for the core validation sites.

The data assimilation diagnostics further broaden the validation to the global domain and indicate that the L4_SM system is reasonably unbiased in the global average sense. The time mean, globally averaged analysis increments in surface and root zone soil moisture are very small. Regionally, however, time mean increments can be as large as 1 mm d^{-1} . These biases are caused by modest biases in the observation-minus-

forecast residuals of brightness temperature in the L4_SM product that can be up to ± 3 K in some regions. The assimilation diagnostics further reveal that, on a regional basis, the errors in brightness temperature are typically over- or underestimated considerably by the L4_SM system.

Uncertainty estimates for the analyzed surface soil moisture, root zone soil moisture, surface temperature, and top layer soil temperature are also provided with the product. These uncertainty estimates are designed to reflect the random error in key geophysical product fields. While the uncertainty estimates appear more reasonable in Version 4 compared to earlier versions, it is not yet clear how well they reflect actual uncertainties.

It is important to keep in mind that the comparisons against the in situ measurements are impacted by the fact that the in situ measurements themselves are prone to errors. Therefore, the metrics presented here underestimate the true skill of the product. In fact, the ubRMSE results presented in the report should be interpreted as the unbiased RMS *difference* between the model estimates and the in situ measurements, rather than errors with respect to actual (or true) soil moisture conditions. Moreover, whereas the surface soil moisture in situ measurements are typically at 5 cm depth, and thus mostly represent the moisture in the 3-7 cm soil layer, the L4_SM estimates are for the 0-5 cm soil layer. As with the error in the in situ measurements themselves, this mismatch in layer depths adversely impacts the validation.

Based on the results presented in this report, the public release of Version 4 of the L4_SM data product is recommended. The results, however, also uncovered limitations in the Version 4 product and possible avenues for future development. Further calibration of the system is needed to reduce the residual regional bias in the observation-minus-forecast brightness temperature residuals and the resulting impact of non-zero long-term mean analysis increments on the water balance. Improved system calibration will be facilitated by the increasing length of the SMAP record. Similarly, new and longer records of in situ measurements will permit more extensive validation, including the evaluation of L4_SM latent and sensible heat fluxes and runoff estimates. Finally, the assimilation of newly available water-body corrected and enhanced-resolution brightness temperatures instead of the standard L1C_TB data may result in further improvements in the L4_SM estimates. These developments will be addressed in future work.

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APPENDIX

Performance Metrics at Core Validation Site Reference Pixels

Tables A1-A8 in this Appendix provide a complete listing of the performance metrics, including ubRMSE, bias, R, and anomaly R, for all 9 km and 33 km core site reference pixels. Metrics are provided for surface soil moisture, root zone soil moisture, and surface soil temperature at 6am and 6pm local time for the L4_SM Tv4000 and Vv3030 product versions as well as for the NRv7.2 and NRv4.1 estimates.

Table A1. Surface soil moisture ubRMSE and bias at individual reference pixels and averaged over 33 km and 9 km reference pixels, including average and average absolute bias (bottom rows labeled “All sites”). Information for 33 km reference pixels is shown in bold font. Italics indicate Version 4 L4_SM metrics.

Site name	Reference pixel		Surface soil moisture									
	ID	Horiz. scale (km)	ubRMSE (m3 m-3)					Bias (m3 m-3)				
			NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.	NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.
REMEDIHUS	03013302	33	0.024	0.026	0.028	0.035	0.005	0.072	0.084	0.057	0.053	0.007
	03010903	9	0.025	0.029	0.030	0.040	0.005	0.139	0.162	0.132	0.135	0.007
	03010908	9	0.034	0.036	0.036	0.044	0.006	0.016	0.030	-0.004	-0.006	0.009
Reynolds Creek	04013302	33	0.041	0.035	0.045	0.046	0.017	0.031	0.042	0.008	0.008	0.022
	04010907	9	0.032	0.031	0.045	0.050	0.013	-0.005	0.004	-0.020	-0.024	0.017
	04010910	9	0.037	0.031	0.041	0.047	0.022	0.034	0.040	0.008	-0.006	0.026
Yanco	07013301	33	0.061	0.041	0.054	0.039	0.010	-0.002	0.021	-0.016	-0.013	0.014
	07010902	9	0.083	0.060	0.075	0.059	0.015	-0.031	-0.011	-0.046	-0.043	0.021
	07010916	9	0.061	0.041	0.054	0.045	0.013	0.026	0.061	0.015	0.025	0.017
Carman	09013301	33	0.035	0.038	0.038	0.040	0.005	-0.020	-0.001	-0.034	-0.029	0.007
	09010906	9	0.038	0.040	0.043	0.041	0.006	0.059	0.082	0.039	0.043	0.008
Ngari	12033301	33	0.044	0.035	0.040	0.033	0.010	-0.013	-0.003	-0.028	0.003	0.013
Walnut Gulch	16013302	33	0.026	0.027	0.027	0.027	0.003	0.041	0.056	0.031	0.054	0.004
	16010906	9	0.027	0.029	0.026	0.027	0.003	0.015	0.034	0.011	0.046	0.004
	16010907	9	0.026	0.030	0.027	0.027	0.003	0.033	0.051	0.027	0.060	0.004
	16010913	9	0.033	0.032	0.031	0.035	0.004	0.071	0.081	0.096	0.097	0.006
Little Washita	16023302	33	0.038	0.033	0.040	0.034	0.003	-0.010	-0.019	-0.021	-0.032	0.005
	16020905	9	0.051	0.045	0.050	0.043	0.006	0.013	0.009	0.001	-0.003	0.008
	16020906	9	0.041	0.037	0.043	0.038	0.005	0.020	0.012	0.006	-0.007	0.007
Fort Cobb	16020907	9	0.037	0.034	0.040	0.035	0.006	-0.016	-0.025	-0.030	-0.042	0.008
	16033302	33	0.039	0.032	0.041	0.033	0.003	0.014	0.025	-0.006	-0.007	0.004
	16030911	9	0.047	0.038	0.051	0.036	0.006	0.023	0.039	-0.032	-0.030	0.008
Little River	16030916	9	0.039	0.033	0.042	0.036	0.004	-0.005	-0.005	-0.018	-0.024	0.006
	16043302	33	0.047	0.041	0.040	0.038	0.004	0.040	0.037	0.008	0.009	0.005
	16040901	9	0.043	0.039	0.034	0.030	0.003	0.110	0.113	0.085	0.089	0.005
St Josephs	16040906	9	0.031	0.033	0.033	0.030	0.005	0.070	0.081	0.046	0.053	0.008
	16063302	33	0.052	0.046	0.044	0.042	0.007	0.157	0.154	0.118	0.112	0.009
	16060907	9	0.055	0.048	0.046	0.042	0.015	0.103	0.100	0.067	0.057	0.020
South Fork	16073302	33	0.059	0.042	0.054	0.040	0.008	0.074	0.049	0.036	0.025	0.011
	16070909	9	0.064	0.048	0.060	0.043	0.007	0.036	0.009	-0.001	-0.014	0.010
	16070910	9	0.067	0.048	0.063	0.047	0.008	0.076	0.049	0.037	0.025	0.011
	16070911	9	0.070	0.051	0.066	0.050	0.009	0.082	0.053	0.043	0.031	0.012
Monte Buey	19023301	33	0.044	0.037	0.045	0.037	0.009	-0.053	-0.044	-0.087	-0.075	0.013
	19020902	9	0.037	0.036	0.038	0.033	0.009	-0.041	-0.026	-0.058	-0.043	0.012
Tonzi Ranch	25013301	33	0.040	0.034	0.038	0.032	0.010	0.031	0.049	0.006	0.015	0.013
	25010911	9	0.043	0.037	0.043	0.036	0.010	0.031	0.044	-0.001	0.012	0.013
Kenaston	27013301	33	0.040	0.033	0.045	0.035	0.008	0.045	0.062	0.023	0.014	0.011
	27010910	9	0.032	0.031	0.033	0.035	0.007	0.014	0.038	-0.010	-0.016	0.010
	27010911	9	0.042	0.040	0.045	0.035	0.009	-0.001	0.018	-0.027	-0.033	0.012
Valencia	41010906	9	0.023	0.019	0.031	0.027	0.006	0.089	0.085	0.072	0.065	0.008
Niger	45013301	33	0.033	0.027	0.043	0.035	0.006	0.002	0.027	0.038	0.061	0.008
	45010902	9	0.034	0.028	0.045	0.037	0.004	0.010	0.033	0.046	0.071	0.006
Benin	45023301	33	0.048	0.047	0.046	0.047	0.011	0.056	0.042	0.105	0.103	0.015
	45020902	9	0.050	0.048	0.047	0.048	0.012	0.053	0.040	0.104	0.102	0.016
TxSON	48013301	33	0.044	0.034	0.039	0.033	0.006	0.078	0.083	0.054	0.056	0.008
	48010902	9	0.042	0.036	0.040	0.039	0.005	0.110	0.108	0.092	0.099	0.006
	48010911	9	0.051	0.042	0.044	0.039	0.006	0.115	0.131	0.098	0.100	0.008
HOBE	67013301	33	0.028	0.029	0.030	0.030	0.007	0.013	0.009	0.001	-0.004	0.010
	67010901	9	0.046	0.044	0.048	0.046	0.022	-0.002	0.008	-0.004	-0.004	0.028
All sites	Average	33	0.041	0.035	0.041	0.036	0.002	0.031	0.037	0.016	0.020	0.002
	Average	9	0.042	0.038	0.043	0.039	0.002	0.040	0.048	0.027	0.029	0.003
	Average Abs	33	n/a	n/a	n/a	n/a	n/a	0.042	0.045	0.037	0.037	0.002
	Average Abs	9	n/a	n/a	n/a	n/a	n/a	0.048	0.052	0.044	0.047	0.003

Table A2. As in Table A1 but for R and anomaly R.

Site name	Reference pixel		Surface soil moisture									
	ID	Horiz. scale (km)	R (dimensionless)					anomaly R (dimensionless)				
			NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.	NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.
REMEDHUS	03013302	33	0.81	0.82	0.83	0.83	0.06	0.73	0.78	0.70	0.75	0.07
	03010903	9	0.50	0.50	0.51	0.54	0.13	n/a	n/a	n/a	n/a	n/a
	03010908	9	0.71	0.70	0.74	0.70	0.09	0.55	0.64	0.55	0.61	0.11
Reynolds Creek	04013302	33	0.44	0.62	0.40	0.48	0.29	n/a	n/a	n/a	n/a	n/a
	04010907	9	0.34	0.45	0.11	0.11	0.32	n/a	n/a	n/a	n/a	n/a
	04010910	9	0.60	0.73	0.54	0.55	0.26	n/a	n/a	n/a	n/a	n/a
Yanco	07013301	33	0.79	0.90	0.85	0.91	0.06	0.74	0.87	0.78	0.88	0.06
	07010902	9	0.79	0.90	0.85	0.89	0.07	0.68	0.86	0.76	0.83	0.08
	07010916	9	0.77	0.90	0.82	0.89	0.07	0.72	0.86	0.75	0.86	0.08
Carman	09013301	33	0.60	0.59	0.48	0.63	0.10	0.38	0.77	0.37	0.68	0.11
	09010906	9	0.55	0.58	0.42	0.63	0.11	0.25	0.69	0.25	0.62	0.13
Ngari	12033301	33	0.68	0.70	0.71	0.67	0.19	n/a	n/a	n/a	n/a	n/a
Walnut Gulch	16013302	33	0.75	0.80	0.77	0.76	0.06	0.71	0.80	0.72	0.75	0.05
	16010906	9	0.74	0.74	0.74	0.70	0.06	0.69	0.72	0.68	0.66	0.06
	16010907	9	0.74	0.74	0.75	0.70	0.06	0.71	0.75	0.71	0.71	0.05
	16010913	9	0.62	0.72	0.72	0.74	0.10	n/a	n/a	n/a	n/a	n/a
Little Washita	16023302	33	0.67	0.78	0.66	0.80	0.05	0.65	0.79	0.65	0.82	0.05
	16020905	9	0.64	0.73	0.64	0.76	0.06	0.61	0.73	0.62	0.76	0.06
	16020906	9	0.70	0.77	0.67	0.77	0.05	0.67	0.79	0.66	0.81	0.05
Fort Cobb	16020907	9	0.71	0.77	0.68	0.81	0.07	n/a	n/a	n/a	n/a	n/a
	16033302	33	0.70	0.81	0.67	0.84	0.04	0.67	0.81	0.64	0.84	0.04
	16030911	9	0.70	0.81	0.61	0.83	0.06	0.66	0.81	0.58	0.84	0.06
Little River	16030916	9	0.64	0.76	0.59	0.80	0.05	0.65	0.78	0.64	0.81	0.05
	16043302	33	0.57	0.62	0.72	0.74	0.08	0.58	0.69	0.69	0.74	0.07
	16040901	9	0.63	0.64	0.77	0.81	0.07	0.58	0.52	0.80	0.79	0.12
St Josephs	16040906	9	0.67	0.60	0.70	0.74	0.12	n/a	n/a	n/a	n/a	n/a
	16063302	33	0.45	0.61	0.64	0.71	0.14	0.02	0.82	0.47	0.81	0.16
South Fork	16060907	9	0.47	0.60	0.65	0.72	0.21	n/a	n/a	n/a	n/a	n/a
	16073302	33	0.38	0.73	0.56	0.77	0.10	0.31	0.77	0.51	0.77	0.09
	16070909	9	0.39	0.73	0.53	0.78	0.10	0.40	0.80	0.55	0.81	0.08
Monte Buey	16070910	9	0.32	0.72	0.49	0.74	0.10	0.28	0.78	0.46	0.75	0.09
	16070911	9	0.29	0.69	0.45	0.71	0.11	0.22	0.75	0.41	0.72	0.10
	19023301	33	0.59	0.74	0.57	0.76	0.07	0.55	0.83	0.54	0.80	0.10
Tonzi Ranch	19020902	9	0.60	0.80	0.59	0.81	0.09	n/a	n/a	n/a	n/a	n/a
	25013301	33	0.93	0.94	0.95	0.95	0.05	0.81	0.86	0.79	0.85	0.06
Kenaston	25010911	9	0.90	0.93	0.94	0.94	0.05	0.76	0.84	0.77	0.82	0.07
	27013301	33	0.69	0.78	0.52	0.76	0.09	0.71	0.77	0.56	0.79	0.08
	27010910	9	0.59	0.68	0.59	0.69	0.11	0.71	0.82	0.60	0.73	0.12
Valencia	27010911	9	0.70	0.69	0.58	0.78	0.09	0.72	0.72	0.56	0.78	0.09
	41010906	9	0.56	0.76	0.51	0.69	0.15	n/a	n/a	n/a	n/a	n/a
Niger	45013301	33	0.36	0.73	0.35	0.59	0.20	n/a	n/a	n/a	n/a	n/a
	45010902	9	0.28	0.65	0.26	0.51	0.17	n/a	n/a	n/a	n/a	n/a
Benin	45023301	33	0.70	0.72	0.76	0.74	0.14	n/a	n/a	n/a	n/a	n/a
	45020902	9	0.71	0.73	0.75	0.75	0.13	n/a	n/a	n/a	n/a	n/a
TxSON	48013301	33	0.78	0.88	0.83	0.88	0.06	0.73	0.86	0.77	0.85	0.06
	48010902	9	0.66	0.78	0.71	0.76	0.07	0.61	0.77	0.66	0.72	0.07
	48010911	9	0.71	0.82	0.78	0.83	0.08	0.63	0.77	0.71	0.79	0.08
HOBE	67013301	33	0.82	0.80	0.81	0.79	0.09	n/a	n/a	n/a	n/a	n/a
	67010901	9	0.81	0.85	0.82	0.84	0.12	n/a	n/a	n/a	n/a	n/a
All sites	Average	33	0.65	0.75	0.67	0.76	0.02	0.58	0.80	0.63	0.79	0.02
	Average	9	0.62	0.73	0.63	0.73	0.03	0.59	0.74	0.62	0.75	0.02

Table A3. As in Table A1 but for root zone soil moisture.

Site name	Reference pixel		Root zone soil moisture										
	ID	Horiz. scale (km)	ubRMSE (m3 m-3)					Bias (m3 m-3)					
			NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.	NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.	
REMEDIHUS	03013302	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	03010903	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	03010908	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Reynolds Creek	04013302	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	04010907	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	04010910	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Yanco	07013301	33	0.010	0.025	0.011	0.009	0.012	-0.126	-0.107	-0.110	-0.092	0.013	
	07010902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	07010916	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Carman	09013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	09010906	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Ngari	12033301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Walnut Gulch	16013302	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	16010906	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	16010907	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	16010913	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Little Washita	16023302	33	0.030	0.025	0.031	0.029	0.004	-0.038	-0.041	-0.009	-0.006	0.005	
	16020905	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	16020906	9	0.026	0.022	0.027	0.024	0.005	-0.018	-0.020	0.004	0.007	0.006	
	16020907	9	0.031	0.029	0.031	0.030	0.008	-0.042	-0.043	-0.020	-0.018	0.011	
Fort Cobb	16033302	33	0.026	0.023	0.029	0.023	0.003	0.006	0.021	0.032	0.053	0.004	
	16030911	9	0.031	0.028	0.034	0.029	0.006	0.013	0.033	-0.006	0.016	0.008	
	16030916	9	0.026	0.025	0.027	0.021	0.004	-0.031	-0.024	-0.010	0.006	0.006	
Little River	16043302	33	0.037	0.030	0.029	0.028	0.004	0.074	0.071	0.066	0.071	0.006	
	16040901	9	0.039	0.034	0.028	0.026	0.004	0.108	0.108	0.097	0.103	0.006	
	16040906	9	0.025	0.025	0.025	0.022	0.007	0.048	0.057	0.047	0.056	0.010	
St Josephs	16063302	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	16060907	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
South Fork	16073302	33	0.041	0.029	0.030	0.024	0.006	0.021	-0.007	0.013	0.013	0.008	
	16070909	9	0.045	0.030	0.035	0.027	0.007	-0.030	-0.064	-0.038	-0.039	0.010	
	16070910	9	0.045	0.029	0.034	0.027	0.006	0.044	0.014	0.034	0.034	0.009	
	16070911	9	0.044	0.031	0.032	0.025	0.007	0.030	-0.003	0.018	0.017	0.009	
Monte Buey	19023301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	19020902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Tonzi Ranch	25013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	25010911	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Kenaston	27013301	33	0.024	0.016	0.028	0.022	0.007	-0.035	-0.017	-0.025	-0.021	0.010	
	27010910	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	27010911	9	0.028	0.022	0.033	0.025	0.008	-0.048	-0.029	-0.043	-0.036	0.010	
Valencia	41010906	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Niger	45013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	45010902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Benin	45023301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	45020902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
TxSON	48013301	33	0.035	0.032	0.035	0.033	0.011	0.018	0.024	0.043	0.052	0.015	
	48010902	9	0.032	0.028	0.033	0.032	0.006	0.083	0.087	0.108	0.120	0.008	
	48010911	9	0.027	0.025	0.028	0.027	0.008	0.082	0.094	0.113	0.121	0.011	
HOBE	67013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	67010901	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
All sites	Average	33	0.029	0.026	0.028	0.024	0.003	-0.011	-0.008	0.001	0.010	0.003	
	Average	9	0.032	0.027	0.030	0.026	0.002	0.015	0.017	0.021	0.029	0.003	
	Average Abs	33	n/a	n/a	n/a	n/a	n/a	0.045	0.041	0.043	0.044	0.003	
	Average Abs	9	n/a	n/a	n/a	n/a	n/a	0.049	0.048	0.046	0.048	0.003	

Table A4. As in Table A1 but for root zone soil moisture R and anomaly R.

Site name	Reference pixel		Root zone soil moisture										
	ID	Horiz. scale (km)	R (dimensionless)					anomaly R (dimensionless)					
			NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.	NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.	
REMEDHUS	03013302	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	03010903	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	03010908	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Reynolds Creek	04013302	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	04010907	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	04010910	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Yanco	07013301	33	0.93	0.92	0.94	0.95	0.24	n/a	n/a	n/a	n/a	n/a	n/a
	07010902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	07010916	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Carman	09013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	09010906	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Ngari	12033301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Walnut Gulch	16013302	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	16010906	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	16010907	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	16010913	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Little Washita	16023302	33	0.81	0.85	0.77	0.82	0.08	0.81	0.85	0.78	0.84	0.07	
	16020905	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	16020906	9	0.70	0.79	0.68	0.76	0.13	0.62	0.86	0.60	0.78	0.22	
Fort Cobb	16020907	9	0.83	0.80	0.81	0.83	0.14	n/a	n/a	n/a	n/a	n/a	
	16033302	33	0.74	0.82	0.66	0.82	0.09	0.70	0.83	0.61	0.84	0.09	
	16030911	9	0.70	0.78	0.64	0.78	0.14	0.66	0.82	0.62	0.83	0.15	
Little River	16030916	9	0.61	0.70	0.56	0.78	0.15	0.58	0.69	0.56	0.76	0.19	
	16043302	33	0.64	0.70	0.65	0.65	0.15	0.58	0.72	0.61	0.65	0.14	
	16040901	9	0.57	0.62	0.61	0.63	0.15	0.43	0.35	0.49	0.39	0.40	
St Josephs	16040906	9	0.66	0.62	0.66	0.74	0.28	n/a	n/a	n/a	n/a	n/a	
	16063302	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
South Fork	16060907	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	16073302	33	0.49	0.73	0.61	0.74	0.20	0.45	0.79	0.65	0.87	0.18	
	16070909	9	0.49	0.76	0.62	0.78	0.21	n/a	n/a	n/a	n/a	n/a	
Monte Buey	16070910	9	0.39	0.73	0.52	0.69	0.22	0.35	0.79	0.55	0.82	0.19	
	16070911	9	0.43	0.74	0.57	0.72	0.22	0.36	0.76	0.57	0.83	0.20	
	19023301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Tonzi Ranch	19020902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	25013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Kenaston	25010911	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	27013301	33	0.85	0.91	0.71	0.86	0.17	0.88	0.92	0.75	0.89	0.13	
	27010910	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Valencia	27010911	9	0.87	0.85	0.71	0.86	0.16	0.87	0.85	0.70	0.87	0.15	
	41010906	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Niger	45013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	45010902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Benin	45023301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	45020902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
TxSON	48013301	33	0.93	0.89	0.92	0.91	0.11	0.92	0.87	0.91	0.91	0.08	
	48010902	9	0.76	0.81	0.73	0.72	0.14	0.73	0.82	0.71	0.72	0.15	
	48010911	9	0.90	0.89	0.88	0.88	0.12	0.89	0.86	0.87	0.89	0.09	
HOBE	67013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
	67010901	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
All sites	Average	33	0.77	0.83	0.75	0.82	0.06	0.73	0.83	0.72	0.83	0.05	
	Average	9	0.70	0.77	0.68	0.78	0.06	0.62	0.74	0.62	0.74	0.09	

Table A5. As in Table A1 but for surface soil temperature at 6am local time.

Site name	Reference pixel		Surface Soil Temperature (6am)									
	ID	Horiz. scale (km)	ubRMSE (K)					Bias (K)				
			NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.	NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.
REMEDHUS	03013302	33	2.2	1.7	2.2	1.9	0.9	-4.5	-3.8	-4.3	-3.9	1.2
	03010903	9	2.1	1.7	2.2	1.9	0.9	-4.9	-4.3	-4.8	-4.5	1.1
	03010908	9	1.7	1.3	1.8	1.5	0.7	-3.8	-3.1	-3.7	-3.4	0.9
Reynolds Creek	04013302	33	1.5	1.9	1.6	1.8	1.4	1.0	2.7	0.3	1.6	1.6
	04010907	9	1.4	1.8	1.5	1.7	1.6	0.5	2.3	-0.4	1.1	1.7
	04010910	9	2.5	2.5	2.6	2.5	3.2	-2.4	-1.0	-2.5	-1.3	3.1
Yanco	07013301	33	1.8	1.5	1.9	1.6	0.5	-3.2	-1.9	-3.4	-2.6	0.7
	07010902	9	2.0	1.6	2.1	1.7	0.5	-3.2	-1.9	-3.5	-2.6	0.7
	07010916	9	2.6	1.9	2.8	2.3	0.7	-4.0	-2.8	-4.4	-3.6	0.9
Carman	09013301	33	2.7	2.5	2.8	2.6	0.8	-3.7	-3.1	-3.5	-3.2	1.0
	09010906	9	3.0	2.8	3.1	2.9	0.8	-4.0	-3.4	-3.8	-3.5	1.1
Ngari	12033301	33	2.1	1.8	1.9	1.7	0.7	-5.2	-3.5	-4.7	-4.4	0.9
Walnut Gulch	16013302	33	1.6	1.4	1.7	1.6	0.5	-2.3	-2.1	-1.9	-2.4	0.7
	16010906	9	1.8	1.5	2.0	1.9	0.5	-1.9	-1.7	-1.5	-2.1	0.7
	16010907	9	1.6	1.4	1.7	1.6	0.5	-3.3	-3.1	-2.8	-3.4	0.7
	16010913	9	2.0	1.6	2.1	1.9	0.8	-2.9	-2.6	-2.4	-2.6	1.0
Little Washita	16023302	33	1.7	1.8	1.7	1.7	0.8	-2.3	-1.7	-2.1	-1.9	1.0
	16020905	9	1.9	2.1	1.9	2.0	0.9	-2.3	-1.7	-2.0	-1.8	1.1
	16020906	9	1.7	1.9	1.7	1.8	0.7	-2.3	-1.7	-2.0	-1.8	0.9
Fort Cobb	16020907	9	1.5	1.6	1.5	1.6	0.9	-2.1	-1.5	-1.9	-1.7	1.0
	16033302	33	1.6	1.6	1.5	1.6	0.7	-2.3	-2.0	-2.0	-1.9	0.9
	16030911	9	1.3	1.3	1.3	1.3	0.7	-1.8	-1.5	-1.4	-1.4	0.8
Little River	16030916	9	1.4	1.4	1.4	1.4	1.4	-1.7	-1.0	-1.5	-1.3	1.5
	16043302	33	1.7	1.7	1.6	1.7	0.5	-2.8	-1.8	-2.9	-2.2	0.7
	16040901	9	1.6	1.6	1.5	1.5	0.4	-2.9	-1.9	-2.8	-2.2	0.6
St Josephs	16040906	9	1.3	1.4	1.3	1.4	1.7	-2.9	-2.1	-3.1	-2.6	1.7
	16063302	33	1.6	1.5	1.7	1.6	0.6	-1.9	-1.2	-1.8	-1.3	0.8
South Fork	16060907	9	1.6	1.6	1.7	1.6	0.8	-2.1	-1.4	-2.1	-1.5	1.0
	16073302	33	1.6	1.6	1.6	1.6	0.7	-2.3	-1.5	-2.2	-1.7	0.9
	16070909	9	1.5	1.4	1.5	1.4	0.6	-1.9	-1.1	-1.8	-1.3	0.7
Monte Buey	16070910	9	1.6	1.6	1.6	1.6	0.7	-2.4	-1.5	-2.2	-1.7	0.8
	16070911	9	1.5	1.5	1.6	1.5	0.6	-2.5	-1.7	-2.3	-1.9	0.8
Tonzi Ranch	19023301	33	1.4	1.3	1.3	1.3	0.4	-2.3	-2.3	-1.7	-2.0	0.5
	19020902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Kenaston	25013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	25010911	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Valencia	27013301	33	1.3	1.4	1.4	1.4	0.6	-1.4	-0.9	-1.1	-0.9	0.8
	27010910	9	1.3	1.1	1.4	1.2	0.5	-1.7	-1.2	-1.4	-1.2	0.6
	27010911	9	1.4	1.4	1.5	1.4	0.6	-1.7	-1.3	-1.4	-1.2	0.8
Niger	41010906	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	45013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Benin	45010902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	45023301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
TxSON	45020902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	48013301	33	1.2	1.2	1.2	1.2	0.3	-1.2	-0.8	-1.2	-1.0	0.4
	48010902	9	1.4	1.2	1.4	1.3	0.3	-2.7	-2.2	-2.5	-2.4	0.4
HOBE	48010911	9	1.3	1.2	1.5	1.4	0.3	-2.3	-1.9	-2.2	-2.1	0.4
	67013301	33	0.9	1.1	0.9	1.0	0.5	-1.0	-0.3	-1.1	-0.5	0.6
All sites	67010901	9	0.9	1.1	1.0	1.0	0.6	-1.1	-0.6	-1.1	-0.6	0.7
	Average	33	1.6	1.6	1.7	1.6	0.2	-2.4	-1.6	-2.2	-1.9	0.2
	Average	9	1.7	1.6	1.8	1.7	0.2	-2.5	-1.8	-2.4	-2.0	0.3
	Average Abs	33	n/a	n/a	n/a	n/a	n/a	2.5	2.0	2.3	2.1	0.2
Average Abs	9	n/a	n/a	n/a	n/a	n/a	2.5	1.9	2.4	2.1	0.3	

Table A6. As in Table A1 but for 6am surface soil temperature R and anomaly R.

Site name	Reference pixel		Surface Soil Temperature (6am)									
	ID	Horiz. scale (km)	R (dimensionless)					anomaly R (dimensionless)				
			NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.	NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.
REMEDHUS	03013302	33	0.98	0.98	0.97	0.98	0.02	0.87	0.89	0.87	0.90	0.03
	03010903	9	0.97	0.98	0.97	0.98	0.02	0.86	0.89	0.87	0.88	0.03
	03010908	9	0.98	0.99	0.98	0.99	0.02	0.90	0.92	0.90	0.91	0.03
Reynolds Creek	04013302	33	0.98	0.97	0.98	0.97	0.05	n/a	n/a	n/a	n/a	n/a
	04010907	9	0.98	0.98	0.98	0.97	0.04	n/a	n/a	n/a	n/a	n/a
	04010910	9	0.96	0.95	0.96	0.96	0.07	n/a	n/a	n/a	n/a	n/a
Yanco	07013301	33	0.97	0.98	0.97	0.98	0.02	0.84	0.89	0.84	0.87	0.03
	07010902	9	0.97	0.98	0.96	0.98	0.02	0.80	0.87	0.81	0.85	0.04
	07010916	9	0.96	0.98	0.96	0.97	0.02	0.79	0.87	0.78	0.85	0.04
Carman	09013301	33	0.93	0.94	0.92	0.93	0.05	0.57	0.64	0.56	0.61	0.10
	09010906	9	0.92	0.93	0.91	0.92	0.06	0.53	0.59	0.52	0.57	0.11
Ngari	12033301	33	0.90	0.92	0.92	0.93	0.12	n/a	n/a	n/a	n/a	n/a
Walnut Gulch	16013302	33	0.98	0.99	0.97	0.98	0.02	0.87	0.90	0.87	0.88	0.03
	16010906	9	0.97	0.98	0.96	0.97	0.03	0.86	0.88	0.85	0.85	0.03
	16010907	9	0.98	0.98	0.97	0.98	0.02	0.87	0.88	0.87	0.86	0.03
	16010913	9	0.98	0.99	0.98	0.98	0.03	n/a	n/a	n/a	n/a	n/a
Little Washita	16023302	33	0.98	0.98	0.98	0.98	0.01	0.91	0.91	0.91	0.91	0.02
	16020905	9	0.98	0.98	0.98	0.98	0.02	0.90	0.90	0.90	0.90	0.02
	16020906	9	0.98	0.98	0.98	0.98	0.01	0.91	0.91	0.90	0.90	0.02
Fort Cobb	16020907	9	0.98	0.98	0.98	0.98	0.02	n/a	n/a	n/a	n/a	n/a
	16033302	33	0.98	0.99	0.98	0.99	0.01	0.89	0.90	0.90	0.90	0.02
	16030911	9	0.99	0.99	0.99	0.99	0.01	n/a	n/a	n/a	n/a	n/a
Little River	16030916	9	0.97	0.98	0.97	0.98	0.04	n/a	n/a	n/a	n/a	n/a
	16043302	33	0.98	0.98	0.98	0.98	0.01	0.94	0.93	0.94	0.93	0.02
	16040901	9	0.98	0.98	0.98	0.98	0.01	0.95	0.94	0.94	0.94	0.02
St Josephs	16040906	9	0.99	0.99	0.99	0.99	0.04	n/a	n/a	n/a	n/a	n/a
	16063302	33	0.98	0.98	0.97	0.98	0.02	0.94	0.95	0.94	0.94	0.03
South Fork	16060907	9	0.97	0.98	0.97	0.98	0.02	n/a	n/a	n/a	n/a	n/a
	16073302	33	0.98	0.98	0.98	0.98	0.02	0.92	0.92	0.92	0.92	0.02
	16070909	9	0.98	0.98	0.98	0.98	0.02	0.93	0.93	0.93	0.93	0.02
	16070910	9	0.98	0.98	0.98	0.98	0.02	0.92	0.92	0.92	0.92	0.02
Monte Buey	16070911	9	0.98	0.98	0.98	0.98	0.02	0.92	0.92	0.92	0.92	0.02
	19023301	33	0.96	0.97	0.96	0.97	0.02	0.95	0.95	0.95	0.95	0.03
Tonzi Ranch	19020902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	25013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Kenaston	25010911	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	27013301	33	0.97	0.97	0.97	0.97	0.02	0.89	0.89	0.88	0.88	0.03
	27010910	9	0.98	0.99	0.98	0.98	0.02	0.89	0.91	0.89	0.91	0.03
Valencia	27010911	9	0.97	0.97	0.97	0.97	0.02	0.90	0.90	0.88	0.89	0.03
	41010906	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Niger	45013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	45010902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Benin	45023301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	45020902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
TxSON	48013301	33	0.99	0.99	0.98	0.99	0.01	0.94	0.95	0.93	0.93	0.01
	48010902	9	0.98	0.99	0.98	0.98	0.01	0.91	0.93	0.91	0.92	0.02
	48010911	9	0.98	0.99	0.98	0.98	0.01	0.92	0.93	0.91	0.91	0.02
HOBE	67013301	33	0.99	0.98	0.98	0.98	0.02	n/a	n/a	n/a	n/a	n/a
	67010901	9	0.99	0.99	0.98	0.98	0.03	n/a	n/a	n/a	n/a	n/a
All sites	Average	33	0.97	0.97	0.97	0.97	0.01	0.88	0.89	0.87	0.89	0.01
	Average	9	0.97	0.98	0.97	0.97	0.01	0.85	0.87	0.85	0.86	0.01

Table A7. As in Table A1 but for surface soil temperature at 6pm local time.

Site name	Reference pixel		Surface Soil Temperature (6pm)									
	ID	Horiz. scale (km)	ubRMSE (K)					Bias (K)				
			NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.	NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.
REMEDHUS	03013302	33	1.4	1.6	1.6	1.7	0.7	-0.5	-2.1	-0.2	-1.5	0.9
	03010903	9	1.6	1.9	1.8	2.0	0.8	-1.6	-3.3	-1.5	-2.8	1.0
	03010908	9	1.4	1.4	1.6	1.6	0.8	0.1	-1.6	0.2	-1.2	0.9
Reynolds Creek	04013302	33	1.8	1.6	1.9	1.7	1.5	3.2	1.6	3.0	1.7	1.6
	04010907	9	1.7	1.5	1.8	1.7	1.7	2.6	0.8	2.4	1.0	1.8
	04010910	9	2.4	2.4	2.5	2.5	2.8	0.3	-0.8	0.7	-0.3	2.8
Yanco	07013301	33	1.7	1.6	1.7	1.6	0.5	1.2	-0.2	1.4	0.0	0.6
	07010902	9	1.7	1.5	1.5	1.4	0.4	1.5	0.1	1.7	0.3	0.5
	07010916	9	1.7	1.6	1.6	1.7	0.4	0.8	-0.7	0.8	-0.7	0.5
Carman	09013301	33	2.2	2.1	2.1	2.0	0.7	1.8	0.7	1.7	0.8	1.0
	09010906	9	2.3	2.2	2.2	2.1	0.7	1.7	0.5	1.6	0.8	1.0
Ngari	12033301	33	4.3	3.9	4.0	3.8	1.1	-4.9	-8.6	-3.0	-7.2	1.5
Walnut Gulch	16013302	33	1.6	1.7	1.9	2.0	0.6	1.2	-1.4	1.3	-1.1	0.7
	16010906	9	2.0	2.1	2.3	2.5	0.6	1.0	-1.7	1.2	-1.5	0.8
	16010907	9	1.8	1.8	2.0	2.1	0.6	0.1	-2.5	0.7	-2.0	0.7
	16010913	9	2.1	2.3	2.4	2.4	0.8	-0.5	-2.9	0.0	-1.9	1.0
Little Washita	16023302	33	1.9	1.9	2.0	1.9	0.9	0.4	-0.5	0.5	-0.4	1.1
	16020905	9	2.1	2.1	2.1	2.1	1.1	0.5	-0.3	0.7	-0.1	1.3
	16020906	9	1.9	1.9	2.0	1.9	0.9	0.5	-0.4	0.6	-0.3	1.1
Fort Cobb	16020907	9	1.6	1.7	1.8	1.7	0.9	0.3	-0.6	0.3	-0.5	1.1
	16033302	33	1.8	1.7	1.8	1.7	0.8	0.4	-0.7	0.9	-0.2	1.0
	16030911	9	1.5	1.5	1.6	1.5	0.9	0.4	-0.7	1.0	0.0	1.1
Little River	16030916	9	1.4	1.4	1.5	1.4	1.4	0.6	-0.1	1.0	-0.1	1.5
	16043302	33	1.8	1.7	1.7	1.6	0.6	-0.6	-1.6	-0.5	-1.5	0.8
	16040901	9	1.7	1.7	1.6	1.6	0.5	-0.8	-1.8	-0.6	-1.6	0.7
St Josephs	16040906	9	1.6	1.5	1.6	1.5	2.0	-0.6	-1.8	-0.7	-1.7	2.0
	16063302	33	1.6	1.5	1.7	1.7	0.7	0.1	-0.7	0.2	-0.4	0.9
South Fork	16060907	9	1.6	1.5	1.7	1.6	1.0	-0.2	-1.0	0.0	-0.6	1.2
	16073302	33	1.7	1.7	1.8	1.7	0.8	0.2	-0.5	0.3	-0.4	1.0
	16070909	9	1.6	1.6	1.7	1.7	0.7	0.2	-0.5	0.2	-0.4	0.9
Monte Buey	16070910	9	1.8	1.8	1.8	1.8	0.8	-0.3	-0.9	-0.2	-0.9	1.1
	16070911	9	1.7	1.7	1.8	1.8	0.8	-0.4	-1.0	-0.2	-0.9	1.0
	19023301	33	1.8	1.8	1.8	1.9	0.5	-0.5	-1.5	1.1	-0.5	0.7
Tonzi Ranch	19020902	9	1.5	2.0	1.6	1.7	0.7	0.4	-1.1	0.3	-1.2	0.8
	25013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Kenaston	25010911	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	27013301	33	2.1	1.8	2.1	1.9	0.9	1.6	0.4	1.5	0.8	1.1
	27010910	9	1.8	1.6	1.9	1.7	0.6	0.8	-0.4	0.7	0.0	0.8
Valencia	27010911	9	2.1	1.8	2.1	2.0	0.8	1.0	-0.2	0.9	0.2	1.0
	41010906	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Niger	45013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	45010902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Benin	45023301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	45020902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
TxSON	48013301	33	1.5	1.4	1.7	1.6	0.4	0.7	-0.5	0.4	-0.6	0.6
	48010902	9	1.8	1.7	2.0	2.0	0.6	-1.2	-2.3	-1.3	-2.4	0.7
	48010911	9	2.1	2.0	2.4	2.3	0.7	-1.3	-2.6	-1.6	-2.6	0.9
HOBE	67013301	33	1.0	1.1	1.0	1.1	0.5	-1.1	-1.8	-1.0	-1.7	0.7
	67010901	9	1.1	1.3	1.2	1.5	0.7	-1.5	-2.1	-1.4	-1.9	0.8
All sites	Average	33	1.9	1.8	1.9	1.9	0.2	0.2	-1.2	0.5	-0.8	0.2
	Average	9	1.7	1.7	1.8	1.8	0.2	0.2	-1.1	0.2	-0.8	0.3
	Average Abs	33	n/a	n/a	n/a	n/a	n/a	n/a	1.2	1.5	1.1	1.2
	Average Abs	9	n/a	n/a	n/a	n/a	n/a	0.8	1.2	0.9	1.1	0.3

Table A8. As in Table A1 but for 6pm surface soil temperature R and anomaly R.

Site name	Reference pixel		Surface Soil Temperature (6pm)									
	ID	Horiz. scale (km)	R (dimensionless)					anomaly R (dimensionless)				
			NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.	NRv4.1	Vv3030	NRv7.2	Tv4000	95% conf. int.
REMEDHUS	03013302	33	0.99	0.99	0.98	0.98	0.02	0.91	0.93	0.90	0.91	0.03
	03010903	9	0.99	0.99	0.99	0.99	0.01	0.91	0.92	0.91	0.92	0.03
	03010908	9	0.99	0.99	0.98	0.98	0.02	0.89	0.90	0.88	0.89	0.03
Reynolds Creek	04013302	33	0.98	0.98	0.97	0.98	0.04	n/a	n/a	n/a	n/a	n/a
	04010907	9	0.98	0.98	0.97	0.98	0.04	n/a	n/a	n/a	n/a	n/a
	04010910	9	0.96	0.96	0.95	0.95	0.07	n/a	n/a	n/a	n/a	n/a
Yanco	07013301	33	0.98	0.98	0.98	0.98	0.02	0.86	0.88	0.84	0.86	0.03
	07010902	9	0.98	0.99	0.98	0.98	0.01	0.89	0.91	0.89	0.90	0.02
	07010916	9	0.98	0.98	0.98	0.98	0.01	0.87	0.90	0.88	0.89	0.03
Carman	09013301	33	0.95	0.95	0.95	0.95	0.04	0.75	0.75	0.77	0.76	0.07
	09010906	9	0.94	0.95	0.95	0.95	0.04	0.74	0.74	0.75	0.75	0.07
Ngari	12033301	33	0.79	0.81	0.82	0.83	0.16	n/a	n/a	n/a	n/a	n/a
Walnut Gulch	16013302	33	0.98	0.98	0.97	0.97	0.02	0.89	0.91	0.87	0.89	0.02
	16010906	9	0.97	0.97	0.97	0.96	0.02	0.86	0.88	0.84	0.85	0.03
	16010907	9	0.98	0.98	0.97	0.97	0.02	0.88	0.89	0.86	0.87	0.03
	16010913	9	0.98	0.98	0.98	0.98	0.02	n/a	n/a	n/a	n/a	n/a
Little Washita	16023302	33	0.98	0.98	0.98	0.98	0.02	0.91	0.90	0.89	0.90	0.02
	16020905	9	0.98	0.98	0.98	0.98	0.02	0.89	0.89	0.88	0.88	0.02
	16020906	9	0.98	0.98	0.98	0.98	0.02	0.90	0.90	0.88	0.89	0.02
	16020907	9	0.98	0.98	0.97	0.97	0.02	n/a	n/a	n/a	n/a	n/a
Fort Cobb	16033302	33	0.98	0.98	0.98	0.98	0.02	0.89	0.89	0.88	0.89	0.02
	16030911	9	0.99	0.99	0.98	0.98	0.02	n/a	n/a	n/a	n/a	n/a
	16030916	9	0.98	0.98	0.97	0.98	0.05	n/a	n/a	n/a	n/a	n/a
Little River	16043302	33	0.98	0.98	0.98	0.97	0.02	0.92	0.92	0.91	0.91	0.02
	16040901	9	0.98	0.98	0.97	0.97	0.02	0.90	0.91	0.90	0.91	0.03
	16040906	9	0.98	0.98	0.98	0.98	0.06	n/a	n/a	n/a	n/a	n/a
St Josephs	16063302	33	0.98	0.98	0.98	0.98	0.02	0.95	0.95	0.94	0.93	0.03
	16060907	9	0.98	0.98	0.98	0.98	0.03	n/a	n/a	n/a	n/a	n/a
South Fork	16073302	33	0.98	0.98	0.98	0.98	0.02	0.93	0.92	0.92	0.91	0.02
	16070909	9	0.98	0.98	0.98	0.98	0.02	0.93	0.92	0.92	0.92	0.02
	16070910	9	0.97	0.97	0.97	0.97	0.02	0.92	0.91	0.91	0.91	0.02
	16070911	9	0.98	0.98	0.98	0.98	0.02	0.92	0.91	0.91	0.91	0.02
Monte Buey	19023301	33	0.96	0.95	0.96	0.96	0.03	0.88	0.89	0.85	0.89	0.07
	19020902	9	0.96	0.94	0.96	0.96	0.04	n/a	n/a	n/a	n/a	n/a
Tonzi Ranch	25013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	25010911	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Kenaston	27013301	33	0.95	0.96	0.95	0.96	0.04	0.88	0.89	0.87	0.88	0.03
	27010910	9	0.97	0.98	0.96	0.97	0.02	0.89	0.90	0.88	0.89	0.03
	27010911	9	0.95	0.96	0.95	0.96	0.03	0.89	0.90	0.88	0.89	0.03
Valencia	41010906	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Niger	45013301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	45010902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Benin	45023301	33	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	45020902	9	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
TxSON	48013301	33	0.98	0.98	0.98	0.98	0.01	0.90	0.92	0.88	0.90	0.02
	48010902	9	0.98	0.98	0.97	0.98	0.02	0.87	0.90	0.86	0.88	0.03
	48010911	9	0.97	0.97	0.96	0.97	0.02	0.83	0.86	0.81	0.84	0.03
HOBE	67013301	33	0.99	0.98	0.98	0.98	0.02	n/a	n/a	n/a	n/a	n/a
	67010901	9	0.99	0.98	0.98	0.98	0.03	n/a	n/a	n/a	n/a	n/a
All sites	Average	33	0.96	0.96	0.96	0.96	0.01	0.89	0.90	0.88	0.89	0.01
	Average	9	0.97	0.97	0.97	0.97	0.01	0.87	0.88	0.87	0.87	0.01

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