A Method to Assess the Performance of SAR-Derived Surface Soil Moisture Products

John Beale, Toby Waine, Jonathan Evans, and Ronald Corstanje

***Abstract*—Synthetic aperture radar (SAR) is a remote sensing technique for mapping of soil moisture with high spatial resolution. *C*-band SAR can resolve features at field scale, or better, but responds to moisture only within the top 1 to 2 cm of the soil. When validating SAR-derived soil moisture products against standard *in situ* measurements at 5 to 10 cm depth, the greater moisture variability at the soil surface may be inaccurately categorized as measurement error. An alternative method was developed where the *C*-band SAR product is validated against soil moisture simulated at 2 cm depth by the HYDRUS-1D model. This reproduces soil moisture depth profiles from daily meteorological observations, leaf area index, and soil hydraulic parameters. The model was fitted at 13 COSMOS-UK sites so that the model output at 10 cm depth closely reproduced the cosmic ray neutron sensor data. At ten of the sites studied, there was an improvement of up to 8% in root-mean-squared difference by validating the Copernicus surface soil moisture (SSM) product at 2 cm compared to 10 cm. This suggests that Copernicus SSM and other *C*-band SAR surface soil moisture algorithms may be more accurate than have hitherto been acknowledged.**

***Index Terms*—Land surface, moisture measurement, remote sensing, soil moisture.**

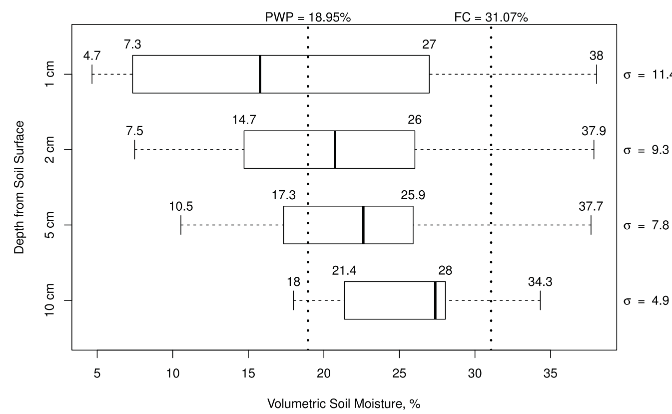

Fig. 1. Boxplot of soil moisture variability at shallow depths, in a Dark Brown Chernozemic soil (41% sand, 34% clay) at Lethbridge, Alberta, Canada over nine days of various wetting and drying regimes, analysis of data from Boisvert *et al.* [14]. The whiskers define the extremes of the data, the thick bars the median, and the box ends represent the first and third quartile values. The standard deviation σ at each depth is shown on the right, with estimates of field capacity (FC) [16] and permanent wilting point (PWP) [17] by the method of Saxton [18] as vertical, dotted lines.

I. Introduction

SOIL moisture remote sensing is of significant interest to agriculture, hydrological modeling, and weather forecasting. Satellite active microwave systems have the ability to operate over wide areas in almost all weather conditions, with *C*-band synthetic aperture radar (SAR) systems being able to achieve field-scale resolution or better. Soil moisture estimation by SAR exploits the dependence of radar backscatter on soil water content, but there are other dependencies on factors that are often unknown. These include soil texture, surface roughness, topography, and the effect of vegetation. A number of advanced algorithms have been and are being developed to address this problem.

The quantitative assessment, or validation, of SAR-based soil moisture retrieval algorithms [1] is commonly undertaken by statistical comparison to *in situ* soil moisture measurements. The instruments used include soil moisture probes [2]–[6] and Cosmic Ray Neutron Sensors (CRNS) [7]–[9]. A review of the International Soil Monitoring Network (ISMN) [10] reveals that probes are generally installed at a nominal depth of at least 5 cm and have a sample volume extending 5–6 cm in depth. This measurement depth is appropriate for validation of *L*-band SAR-derived soil moisture products, where it matches the microwave penetration depth [11] in bare soil. CRNS have an effective measurement depth of at least 10 cm (depending on soil moisture). Due to the practical problems of measuring soil moisture with probes at 1–2 cm [12], [13], there is no established measurement network that matches the penetration depth of *C*-band SAR.

Reliable soil moisture measurements very near the surface can be achieved by soil sampling and laboratory analysis, as in a previous study by Boisvert *et al.* [14]. Gravimetric soil moisture was measured at 1 cm depth increments from the surface to 10 cm depth in various sample plots subjected to a range of irrigation and drying profiles. The statistics of these measurements

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(converted to volumetric soil moisture) are summarized in the box plot of Fig. 1, annotated with the sample standard deviation (σ). This shows that the variability of soil moisture decreases significantly with depth. It is very high at the surface where the soil is subject to rapid wetting and drying due to rainfall, irrigation, and evaporation [15], while drainage to lower layers is a much slower process. At deeper levels soil moisture varies more slowly and over a smaller range. It cannot be assumed that soil moisture measured at 5 or 10 cm is similar to that at 1 to 2 cm depth. The consequence of doing as part of a validation process of any soil moisture estimates derived from *C*-band SAR has not previously been quantified.

The speed and range of movement in soil moisture at the surface also challenges the interpretation of soil moisture products that are published as a dimensionless and relative soil moisture index (SMI) [19]. An example is the Copernicus surface soil moisture (SSM) product [20], based on *C*-band Sentinel-1 data. For applications, such as irrigation scheduling, absolute soil moisture values will be derived by site specific scaling. The field capacity (FC) [16] and permanent wilting point (PWP) [17] of the soil are commonly used for this purpose, to define the range of possible soil moisture values. Fig. 1 shows that, while this may be acceptable at 10 cm depth, FC and PWP do not define the limits of soil moisture at very shallow depths. This issue is overlooked in the performance assessment of SMI-based products using scale-independent metrics, such as the coefficient of determination (R^2). This study uses, for the first time, alternative scale-sensitive metrics in an assessment of the Copernicus SSM product. The SMI values are scaled to VWC, having first identified the van Genuchten model [21] parameters, saturated water content (θ_S), and residual water content (θ_R), as suitable alternative limits of soil moisture content at the surface.

Modeling is an alternative to *in situ* measurement of soil moisture where the latter is impractical. HYDRUS-1D (v4.17) [22] is a model that has been successfully used in previous work [23], [24] to simulate soil moisture profiles near the surface. It is a finite-element model which simulates the 1-D movement of water in porous media by numerically solving the Richards equation [25] for water flow. Soil hydraulic parameters are key inputs to the model, but they are not static and vary with soil texture, land use, and management. Values obtained previously by laboratory measurements or indirectly from soil maps may not reflect contemporary conditions or local heterogeneity. They need to be optimized by an iterative process using *in situ* measurements of soil moisture as the benchmark.

The aim of this study was to establish, for the first time, a scalable method for generating soil moisture time-series at 2 cm depth or less, that may be used for objective assessment of *C*-band SAR-derived surface soil moisture data. The study evaluates the impact of this on the apparent performance assessments of an example product, compared to assessment at a greater depth of measurement. Having identified new limits on soil moisture variability at the surface, the additional errors due to scaling were estimated, contrasting the use of the new limits with the common choice of FC and PWP.

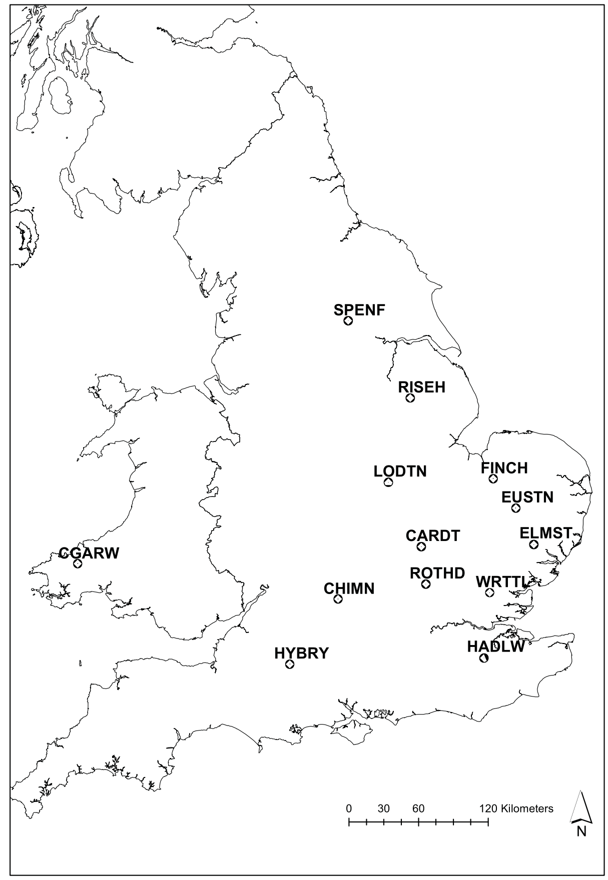


Fig. 2. Locations of the subset of COSMOS-UK sites selected for this study. The labels are the site identifiers.

II. Study Sites and Time Period

The COSMOS-UK network [9] comprises a total of 50 soil moisture monitoring stations across the U.K., operated by the U.K. Centre for Ecology and Hydrology (UKCEH). The primary soil moisture sensor at each site is a CRNS [7], which has a measurement footprint of approximately 200 metres in diameter [26]. By mitigating against the spatial heterogeneity of soil hydraulic properties, CRNS data are more suited to validation of remotely sensed soil moisture products without having to upscale the measurements from a densely spaced network of point sensors.

The COSMOS-UK sites are also instrumented to measure a range of meteorological and environmental parameters. COSMOS-UK sites were selected for this study for their ability to supply high quality daily time-series measurements of soil moisture from the CRNS sensor, with colocated measurements of potential evapotranspiration and rainfall.

Thirteen sites were selected for this study, as shown in Fig. 2. They represent agricultural sites as opposed to forested sites where the vegetation canopy would be too dense for *C*-band SAR to be able to sense soil moisture. The land uses are permanent grass, ley grass, and arable crops, where farmers and agronomists would hope that SAR remote sensing would be of

TABLE I
SUBSET OF COSMOS-UK SITES SELECTED FOR THIS STUDY

Site identifier	Site name	Soil type	Land cover	Dominant soil series
CARDT	Cardington	Loam to Silt Loam	Permanent Grass	Efford
CHIMN	Chimney Meadows	Clay Loam	Permanent Grass	Kelmscot
CGARW	Cwm Garw	Peaty Mineral Soil	Permanent Grass	Hafren
ELMST	Elmsett	Loam	Arable	Beccles
EUSTN	Euston	Sandy loam	Permanent Grass	Newport
FINCH	Fincham	Sandy loam, lime-rich	Arable	Swaffham Prior
HADLW	Hadlow	Clay Loam	Ley Grass	Wickham
HYBRY	Heytesbury	Shallow silt loam, lime-rich	Permanent Grass	Andover
LODTN	Loddington	Clay	Arable	Denchworth
RISEH	Riseholme	Humose Clay loam	Permanent Grass	Elmton
ROTHD	Rothamsted	Silty Loam	Arable	Batcombe
SPENF	Spen Farm	Clay loam	Arable	Aberford
WRTTL	Writtle	Loam with impeded drainage	Arable	Hornbeam

benefit to them in monitoring soil moisture. The chosen sites also vary in soil textures, as shown by Table I.

During 2018, the U.K. experienced a very cold and wet spring followed by a prolonged heatwave and drought. Using this year in the study made it probable that the soil moisture would vary between the wettest and driest conditions—well outside the range between FC and PWP—posing the greatest challenge to fit the model to *in situ* data.

III. DATA

The HYDRUS-1D model requires a number of input parameters and time series data in order to predict soil moisture profiles over time, and *in situ* soil moisture measurements for model fitting.

A. CRNS Soil Moisture

CRNS soil moisture measurements were obtained from the COSMOS-UK network for model fitting. The effective measurement depth of a CRNS sensor is defined by its 86% cumulative sensitivity depth, $D_{86}(\theta, r)$ [27] where θ is the soil moisture and r is the radius from the sensor. It may be calculated by the methods proposed by Kohli *et al.* [28] who also define a sensitivity weighting as a function of depth

$$W(d, \theta, r) \propto e^{-2\ d/D_{86}(\theta,r)} \tag{1}$$

where d is the soil depth in cm. A cumulative sensitivity depth function $S(d, \theta, r)$ can be derived by integrating this function and setting the constant value so that $S(d_\infty, \theta, r) = 1$

$$S(d, \theta, r) = 1 - e^{-2\ d/D_{86}(\theta,r)}. \tag{2}$$

To find the depth equivalent to 50% of the cumulative response, setting $S(d_{50}, \theta, r) = 0.5$

$$d_{50}(\theta, r) = -0.5.D_{86}(\theta, r).ln(0.5) = 0.3466.D_{86}(\theta, r). \tag{3}$$

Values of $d_{50}(\theta, r)$ were calculated for each daily COSMOS-UK CRNS measurement of soil moisture, θ, for 2018 at all 13 sites for r = (1, 5, 25, and 75 m). They were then weighted by the factors w = (1.89E+05, 2.45E+04, 8.22E+03, 4.90E+03),

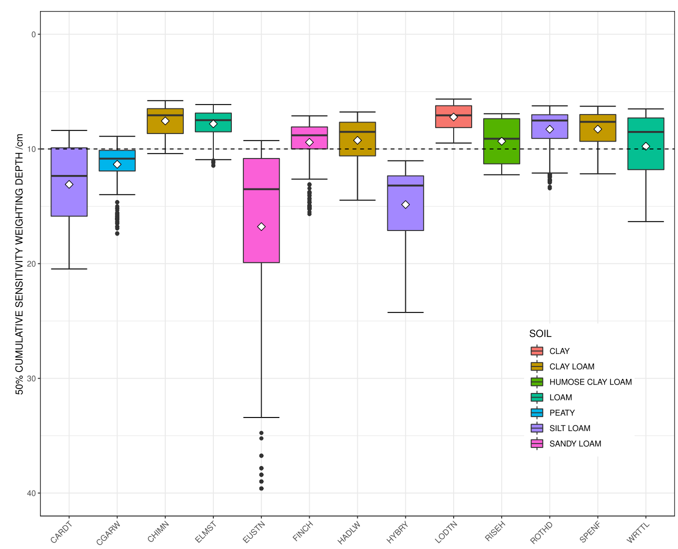


Fig. 3. Boxplot representing the variation in the 50% cumulative sensitivity depth d_{50} (weighted by radius) during 2018 at the COSMOS-UK sites used in this study. The whiskers define the extremes of the data, the thick bars the median, and the box ends represent the first and third quartile values. The mean for each site is plotted as the white diamond. The box colors represent the site soil classification for the surface layer.

respectively, these weightings used by the COSMOS-UK team based on [28]. Fig. 3 summarizes the statistics of d_{50} in the form of a boxplot. For most sites, the mean of d_{50} is close to 10 cm and the mean across all sites is 10.27 cm. This result agrees with a recent study in China [29], that found that CRNS measurements were more highly correlated with soil moisture at 10 cm from the surface than at any other depth.

A depth of 10 cm is within the upper mineral soil layer (A horizon) for all of the sites chosen for this study. According to a recent review [30], the coefficient of variation of clay content in a typical A horizon is low (8%). This allows us to assume that the soil hydraulic properties are approximately the same at 10 and 2 cm, and to perform the model fitting at 10 cm against COSMOS-UK data using a single layer model. A multilayer

TABLE II
HYDRUS-1D INITIAL SOIL HYDRAULIC PROPERTIES OBTAINED FROM LANDIS HORIZON HYDRAULICS DATA [34] FOR THE 13 STUDY SITES. THESE ARE PARAMETERS OF THE VAN GENUCHTEN–MUALEM MODEL [21], [31]; WATER CONTENT AT QUASI-SATURATION (θ_S), RESIDUAL WATER CONTENT (θ_R), SATURATED HYDRAULIC CONDUCTIVITY (K_s), AND MODEL FITTING PARAMETERS (n, α)

Site identifier	Soil hydraulic parameters				
	$\theta_S(vol.\%)$	$\theta_R(vol.\%)$	α	n	K_s
CARDT	48.36	9.59	0.0492	1.2438	109.3
CGARW	90.0	9.0	0.1158	1.383	6540.5
CHIMN	54.56	11.36	0.054	1.2326	101.4
ELMST	32.5	7.32	0.0591	1.2488	76.4
EUSTN	45.21	7.31	0.0908	1.348	115.5
FINCH	36.98	7.71	0.0784	1.2984	92.05
HADLW	57.47	12.22	0.0441	1.2229	105.3
HYBRY	69.09	13.47	0.0406	1.2321	117.6
LODTN	44.09	11.35	0.0384	1.2131	71.5
RISEH	72.3	14.59	0.0468	1.2247	107.3
ROTHD	33.9	7.46	0.0406	1.2385	107.3
SPENF	40.33	9.34	0.051	1.2387	76.4
WRTTL	35.38	7.65	0.0489	1.2483	76.4

configuration of the model would have been impractical to optimize due to the number of variables this would introduce.

B. Soil Hydraulic Properties

The soil hydraulic properties required by HYDRUS-1D are the water retention parameters of the van Genuchten–Mualem model [21], [31]; water content at quasi-saturation (θ_S), residual water content (θ_R), saturated hydraulic conductivity (K_s), and model fitting parameters (n, α). Initial values were obtained from the National Soil Map of England and Wales (NATMAP) [32]. At each site, the dominant soil series was identified by overlaying the 200 m radius footprint of the CRNS sensor over the soil map. The main land use within the 200 m radius was categorized by inspection of phenocam images and site metadata as either permanent grass (PG), ley grass (LE), arable (AR), or other (OT). The depth of the upper soil horizon, its soil texture, and bulk density were obtained from the LANDIS Horizon Fundamentals [33], [34] table, by looking up the appropriate soil series and land use. In the same way, the soil hydraulic properties were obtained from the LANDIS Horizon Hydraulics table [34], [35]; these are summarized in Table II. For the Cwm Garw site, which has a very peaty soil, the initial soil hydraulics parameters were taken from a previous study of a site with peat soil by Fields *et al.* [36]. An alternative set of van Genuchten–Mualem model water retention parameters may be estimated using the Rosetta Lite v1.1 [37] pedotransfer function provided within the HYDRUS-1D model, by supplying it with the soil texture and bulk density.

C. Vegetation Properties

The drying mechanisms of the soil near the surface are drainage to a lower soil layer, direct evaporation, E_E, and transpiration through plant roots E_T. The drainage element is

TABLE III
CANDIDATE WET AND DRY REFERENCES FOR THE SURFACE SOIL LAYER AT COSMOS-UK SITES USED IN THIS STUDY, BASED ON LANDIS HORIZON HYDRAULICS DATA. OPTIMIZED VALUES θ_{SX} & θ_{RX} DERIVED FROM MODEL FITTING ARE SHOWN IN TABLE IV. VALUES ARE IN VOLUMETRIC WATER CONTENT (VOL.%)

Site Label	Wet References			Dry References		
	P	θ_S	θ_{FC}	θ_{PWP}	θ_{HC}	θ_R
CARDT	53.2	48.36	44.2	21.1	17.66	9.59
CGARW	>90	90	53	26.4	6.70	9
CHIMN	56.2	54.56	47	23.4	19.58	11.36
ELMST	44.2	32.5	36.7	19.9	15.21	7.32
EUSTN	52.9	45.21	41.4	17.1	11.33	7.31
FINCH	47.7	36.98	38.2	19.9	13.61	7.71
HADLW	56.9	57.47	48.2	24.2	21.02	12.22
HYBRY	60.8	69.09	51.4	23.7	21.15	13.47
LODTN	50.7	44.09	44.5	26.1	21.34	11.35
RISEH	62.2	72.33	52.5	25.1	22.18	14.59
ROTHD	44.7	33.86	38.5	19.7	16.17	7.46
SPENF	49.2	40.33	41.6	22.8	17.88	9.34
WRTTL	46	35.38	38.8	19.9	15.77	7.65

modeled by HYDRUS-1D, but the aggregate of the other two is dependent on weather conditions. This is the potential evapotranspiration ($E_0 = E_E + E_T$) and is a standard component of the COSMOS-UK site data. The HYDRUS-1D model requires E_0 to be partitioned into E_E and E_T; this is driven by the state of the vegetation. A common approximation is to assume that areas of bare soil are subject only to evaporation and areas covered by vegetation subject only to transpiration. Leaf area index (LAI) is a vegetation parameter that is inversely related to the proportion of bare soil, so a form of Beer's law [38], [39], may be used for the partitioning: $E_E = E_0 e^{-\alpha LAI}$ where the default extinction coefficient, $\alpha = 0.463$. HYDRUS-1D includes the option to perform this calculation automatically if daily time series of E_0 and LAI are supplied.

For this study, LAI data were obtained from the MODIS optical instrument on the Terra and Aqua satellites. The MODIS data (MCD15A3H V6 level 4) [40] suffer, especially over the U.K., from unreliable data due to cloud cover. To minimise the impact of this, the 4-day time series was smoothed by weighting according to the confidence values ("SCF_QC" bits) provided with the product, by the following:

$$LAI_{i+1} = LAI_i + \Delta_{i+1}/(1 + C_{i+1}) \quad (4)$$

where LAI_i, LAI_{i+1} represent the time series of LAI, C is the confidence level (0 = High to 4 = No Data), and Δ is the change in the LAI value between the previous time-step and the MODIS measurement. The data were then aligned to the COSMOS-UK data time-series by linear interpolation.

HYDRUS-1D uses rooting depth and the root density profile to calculate the transpiration profile with depth. For the purposes of this study, these parameters were set the same for each site, with the root density decreasing linearly with depth over the

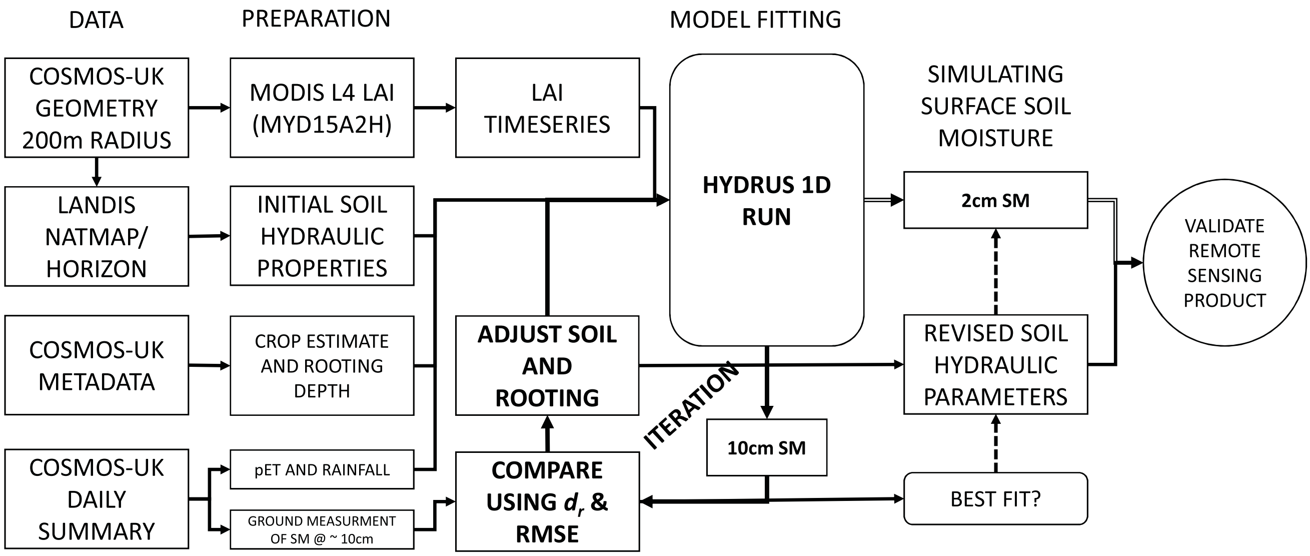


Fig. 4. Block diagram of the method for model fitting of HYDRUS-1D and using the fitted model to generate a time series of soil moisture at 2 cm soil depth.

upper 15 cm only. This is an estimate typical of many grass species, and will be suitable for many of the sites used in this study. For others, this assumption could introduce a small error in the model fitting.

D. SAR-Derived Soil Moisture

To illustrate the effectiveness of the method through a case study, a remote sensing soil moisture product based on *C*-band Sentinel-1 SAR data, Copernicus SSM [20], was selected. This product estimates soil moisture by the change detection method [41], and presents it as an SMI value between 0% and 100% relative to the range of historically observed values at each geospatial location. The spatial resolution of the Copernicus SSM product is nominally 1 km, and the temporal resolution is governed by the orbital coverage of Sentinel-1, being approximately once every 2–6 days within the U.K. A time series was obtained by averaging the SMI values of the pixels overlapping the CRNS 200 m radius footprint (weighted by their intersection) at each of the 13 monitoring stations selected. For the purposes of comparison to the HYDRUS model output, the predicted values (P_i) are the remote sensing predictions and the HYDRUS-1D modeled soil moisture at 2 cm are the independent observations (O_i). Prior to analysis, the remotely sensed soil moisture values (S_i) were converted from an SMI to volumetric water content (VWC) by scaling, as shown in (5), where θ_{wet} and θ_{dry} are the selected wet and dry soil moisture references as determined in Section IV.B

$$P_i = \theta_{\text{dry}} + S_i(\theta_{\text{wet}} - \theta_{\text{dry}}). \tag{5}$$

IV. Methods

A. Simulating Soil Moisture at Shallow Depth

The method for generating a soil moisture time series at 2 cm is depicted in Fig. 4. The HYDRUS-1D model was configured for a single soil layer the same thickness as the upper horizon using the initial soil hydraulic properties derived from LANDIS data [34]. Excess water at the surface was set to run off and free drainage to a lower soil layer was defined at the lower interface. The daily time series of potential evapotranspiration, rainfall, and LAI were imported into the HYDRUS-1D model as time-varying boundary conditions.

The soil hydraulic parameters were optimized by iteration until the model predictions at 10 cm depth (P_i) matched *in situ* soil moisture observations, (O_i) from the COSMOS-UK CRNS, as closely as possible. The approach of Harmel *et al.* [42] was used; selecting an index of agreement based on the Willmott index [43], d, which quantifies the relative covariability of the predictions about the mean of the observations. The refined version d_r [44] is reported to be less sensitive to extreme values and better suited for model evaluation than R^2 [45]. It is a dimensionless number, calculated according to (6) and (7) that varies between -1 (no fit) and +1 (ideal fit) and is particularly suitable where a 1:1 relationship between prediction and observation is expected. The root-mean-squared difference (RMSD), as defined by (8), was also calculated. According to the recommendation of Harmel *et al.* [42], the optimization sought to maximize d_r but without allowing RMSD to increase significantly

$$d_r = 1 - \frac{\sum_{i=1}^{n} |P_i - O_i|}{2\sum_{i=1}^{n} |O_i - \overline{O}|}, \text{when} \sum_{i=1}^{n} |P_i - O_i| \leq 2\sum_{i=1}^{n} |O_i - \overline{O}| \tag{6}$$

$$d_r = \frac{2\sum_{i=1}^{n}|O_i - \overline{O}|}{\sum_{i=1}^{n}|P_i - O_i|} - 1, \text{when} \sum_{i=1}^{n}|P_i - O_i| > 2\sum_{i=1}^{n}|O_i - \overline{O}| \quad (7)$$

$$RMSD = \sqrt{\frac{\sum_{i=1}^{n}(P_i - O_i)^2}{n}}. \quad (8)$$

To optimize the fit of the HYDRUS-1D model to CRNS data, d_r and RMSD were calculated as a function of each soil hydraulic parameter ($\theta_R, \theta_S, \alpha, n, K_s$) to locate a value close to a maximum in d_r and a minimum in RMSD. Some interdependence between the parameters was evident, so the whole process was repeated several times for each study site until no further improvement could be achieved. Having established an optimum set of values of the soil hydraulic parameters that appear to describe the local soil properties well, the HYDRUS-1D model output at the desired simulation depth of 2 cm was then obtained using these values.

B. Identifying Soil Moisture Limits at the Surface

A review was conducted to identify soil moisture parameters that are candidates for natural limits on the movement of soil moisture due to drying or wetting processes. These are all related to soil physics or attributes of the drying mechanisms. Starting at the highest value of soil moisture are the following.

1) Porosity (P) defines the total pore space available to be filled with water and sets an effective upper limit for soil water content, probably achieved only if the soil surface is under water for some time.
2) Water content at quasi-saturation (θ_S) is one of the van Genuchten model [21] parameters, and is typically 5%–15% below P, due to entrapment of air during wetting. Soil is unlikely to wet above this value, excess water will run off. After wetting to this point, the soil will dry rapidly due to drainage (mostly) and evapotranspiration.
3) FC or θ_{FC} [16] is the point below which soil will no longer drain to a lower layer under gravity. Further drying is by evapotranspiration only.
4) PWP or θ_{PWP} [17] is a point at which transpiration by plants falls to zero and evaporation becomes the only drying mechanism.
5) Hygroscopic coefficient (θ_{HC}), or natural air-dried moisture value, defines the water content of soil that has dried by evaporation then allowed to reach equilibrium in a saturated atmosphere. Most of the pore water has been removed. Further drying is possible in very hot conditions by evaporating some capillary water, but this requires significantly more energy. When the temperature falls, the soil moisture will tend to return to this value naturally, without rainfall, provided there is sufficient humidity in the air.
6) Residual water content (θ_R) is another of the van Genuchten model [21] parameters, and is an approximate lower limit of the soil drying process in natural conditions rather than at the much higher temperature of an oven.

To identify which, if any, of these candidates are suitable as wet or dry reference points, values of P, θ_S, θ_{FC}, θ_{PWP}, and θ_R were obtained from the LANDIS Horizon data for each of the 13 COSMOS-UK sites, as shown in Table III . θ_{HC} was calculated using the van Genuchten model [21], (9), where $h =$ 3100 kPa and n and m were obtained initially from the LANDIS Horizon Hydraulics data [34]. The HYDRUS-1D model fitting process also generated optimized values for θ_S and θ_R which will be referred to as θ_{SX} and θ_{RX}, respectively

$$\theta_{HC} = \theta_R + \frac{(\theta_S - \theta_R)}{(1 + (\alpha h)^n)^m}. \quad (9)$$

Pairs of candidate references were evaluated by using them to scale the remotely sensed SMI time series of the Copernicus SSM product to VWC. The results were compared to the 2 cm depth soil moisture simulation of the model. As previously discussed, scale-independent statistical measures of accuracy, such as the coefficient of determination (R^2), are inappropriate as they are not sensitive to scaling errors introduced in the conversion of SMI to VWC. Scale-dependent measures, such as RMSD (8) are also unsuitable because the scaling process serves to amplify or attenuate any systematic noise in the time-series, affecting the RMSD value independently of the trend. Alternative metrics were identified based on range and offset. Linear regression was used to find the best-fit straight line to describe the relationship between the calibrated volumetric soil moisture from remote sensing (y) and the model output at 2 cm (x). This line was expected to be of the form $y = a + bx$ where a is the offset and b is the slope. Since the ideal scaling has no offset ($a = 0$) and unity slope ($b = 1$), metrics in the form of $|a|$ and $|1 - b|$ were used, in addition to d_r and RMSD, to find the most effective combinations of candidate references for each site.

V. Case Study

To assess the relative benefits of validating a *C*-band SAR derived surface soil moisture product against the simulated soil moisture at 2 cm, a limited performance assessment of the Copernicus SSM product [20] was undertaken. This product is based on data from ESA's Sentinel-1 satellites [46] and processed with a change detection algorithm [41]. Using the methods described earlier, daily soil moisture predictions for 2018 were generated at 2, 5, 10, and 15 cm soil depth for each of the study sites. SSM-derived VWC was obtained by calibrating the SMI values against wet and dry soil moisture references, θ_{wet} and θ_{dry}, respectively. As the SSM data do not provide a daily time series at any particular location, values for the days within the SSM time series were paired with the equivalent days in the model output for comparison.

Inspection of the SSM data showed that it was characterized by significant, apparently random, errors, that were much larger in magnitude than the soil moisture variation. To mitigate this, a simple exponential filter, defined by (10) was implemented.

TABLE IV
OPTIMIZED VAN GENUCHTEN–MUALEM SOIL HYDRAULIC PARAMETERS AND MODEL FIT STATISTICS (HYDRUS-1D AT 10 CM VERSUS CRNS) FOR 2018 AT 13 COSMOS-UK SITES. θ_{SX} IS THE WATER CONTENT AT SATURATION AND θ_{RX} IS THE RESIDUAL WATER CONTENT. α AND n ARE PARAMETERS OF THE WATER RETENTION FUNCTION AND K_s IS THE SATURATED (VERTICAL) HYDRAULIC CONDUCTIVITY. THE MODEL FIT STATISTICS ARE THE WILLMOTT INDEX, d_r, AND RMSD

SITE ID	Optimised Soil Hydraulic Properties					Model Fit Metrics	
	$\theta_{SX}(vol.\%)$	$\theta_{RX}(vol.\%)$	$\alpha(cm^{-1})$	n	$K_s(cm.day^{-1})$	d_r	$RMSD(vol.\%)$
CARDT	47.0	5.20	0.0008	1.66	6.0	0.779	4.62
CGARW	90.0	9.00	0.0990	1.23	8580	0.659	7.75
CHIMN	61.4	3.50	0.0070	1.27	95.0	0.827	3.68
ELMST	48.5	0.05	0.0015	1.19	7.0	0.829	3.17
EUSTN	49.7	0.01	0.0140	1.61	95.0	0.867	2.52
FINCH	40.4	1.00	0.0120	1.29	38.0	0.775	2.93
HADLW	64.3	4.50	0.0032	1.49	15.0	0.832	4.23
HYBRY	61.2	4.30	0.0070	1.42	50.0	0.762	5.35
LODTN	69.8	10.00	0.0030	1.30	15.0	0.834	4.62
RISEH	73.0	12.00	0.0235	1.46	265	0.837	3.20
ROTHD	37.9	2.20	0.0080	1.27	3.0	0.774	4.30
SPENF	41.1	4.00	0.0010	1.29	10.0	0.855	2.76
WRTTL	57.5	1.90	0.0020	1.62	1.5	0.807	5.78

The decay constant α_i is a function of the time interval between measurements in days $\Delta T = T_i - T_{i-1}$, according to (11). The values of $\alpha_0 = 0.8$ and $\lambda = 0.1$ were chosen to reduce the noise level without significantly reducing the data sensitivity to short term changes in soil moisture. The time constant of this filter is $\lambda^{-1} = 10$ days, which is similar to the 12-day repeat cycle of each Sentinel-1 satellites. A significant component of the noise that the filter is attenuating may be artefacts of multiple platforms and overlapping orbit image footprints that are otherwise beneficial in enabling more frequent measurements. A full optimization of such a filter, or an alternative mitigation strategy is outside the scope of this study, and is not necessary to achieving the objectives

$$P_i' = (1 - \alpha_i)P_i + \alpha_i P_{i-1} \tag{10}$$

$$\alpha_i = \alpha_0 e^{\lambda(1-\Delta T)} \text{ where } \alpha_0 = 0.8, \lambda = 0.1. \tag{11}$$

The performance of the SSM derived VWC was assessed against the HYDRUS-1D simulations using the refined Wilmott index of agreement, d_r [44], RMSD, linear regression slope error ($|1 - b|$), and offset ($|a|$). For the purpose of calculating d_r, the HYDRUS-1D simulation provides the observations against which to test the predictions from the SSM product. A good level of performance is characterized by a high value of d_r, and low values of RMSD, $|1 - b|$, and $|a|$.

VI. RESULTS

A. Model Fitting

Results of the model fitting at 10 cm depth to the CRNS data for all 13 selected COSMOS-UK sites and the whole of 2018 are presented in Table IV. This shows the final values of the soil hydraulic parameters after optimization and the values of d_r and RMSD achieved. The Cwm Garw site (CGARW) is a slight outlier, but here the soil depth is relatively shallow so the free drainage assumption for the bottom of the A horizon may not be valid. The models used may also not work as well for peat soils with a high organic matter content. Across the other sites the d_r value ranges from 0.774 to 0.862 and the RMSD from 2.52 to 5.78 vol.%. An example of the time series fit at the Fincham (FINCH) site is shown in Appendix A; the optimization process is very effective in matching the prediction to the observations. Remaining variance may be due, to some degree, to the effective measurement depth of the CNRS sensor, which is a function of soil moisture.

Having established an optimized set of soil hydraulic properties for each site, the candidates for use as reference soil moisture values (θ_{wet} and θ_{dry}) for converting SMI's to VWC may be revised also.

B. Predicting Soil Moisture at 2 Cm

The HYDRUS-1D model with its optimized soil hydraulic parameters were used to simulate soil moisture at each of the 13 selected COSMOS-UK sites, for the whole of 2018. Observation nodes were set at soil depths of 2, 5, 10, and 15 cm from the surface. An example of the prediction at the Chimney Meadows (CHIMN) site is shown in Fig. 5, which plots about four months of data in the summer, which was a drought and heatwave period. In such conditions, the profile of soil moisture is expected to vary significantly with depth. The time series demonstrates this, with the prediction at 2 cm showing the greatest range of soil moisture values and the prediction at 15 cm showing the least. The 2 cm data are reacting well to the short rainfall events and longer dry spells.

TABLE V
RECOMMENDED CHOICES OF WET AND DRY REFERENCE PARAMETERS FOR CONVERSION OF COPERNICUS SSM SMI TO VWC AT 13 COSMOS-UK SITES, BASED ON 2018 DATA, AND COMPARISON WITH HYDRUS-1D PREDICTIONS AT 2 CM DEPTH OF SOIL. THE ADDITIONAL ERROR ESTIMATE FOR USING 2ND CHOICE OVER 1ST CHOICE OR FC/PWP IS THE MEAN OF THE DIFFERENCES BETWEEN THE PAIRS OF WET/DRY REFERENCES REFERENCES AT EACH SITE

Site	Wet Reference		Dry Reference		Error Est. vol.%	
identifier	1st Choice	2nd Choice	1st Choice	2nd Choice	1st vs. 2nd	1st vs. FC/PWP
CARDT	θ_{SX}	θ_S	θ_{RX}	θ_R	2.9	6.6
CGARW	θ_{SX}	θ_S	θ_{RX}	θ_R	0	9.8
CHIMN	θ_{SX}	P	θ_{RX}	θ_R	1.3	2.8
ELMST	θ_{SX}	P	θ_{RX}	θ_R	1.5	4
EUSTN	P	θ_{SX}	θ_{RX}	θ_R	2.1	2.8
FINCH	θ_{SX}	θ_S	θ_{RX}	θ_R	1.6	8.4
HADLW	θ_{SX}	θ_S	θ_{RX}	θ_R	0.4	1.8
HYBRY	θ_{SX}	θ_S	θ_{RX}	θ_R	8.5	4.8
LODTN	θ_{SX}	P	θ_R	θ_{RX}	10.2	5.3
RISEH	P	FC	θ_{RX}	θ_R	3.6	1.7
ROTHD	P	FC	θ_{RX}	θ_R	0.5	5.7
SPENF	θ_{SX}	P	θ_{RX}	θ_R	6.7	9.7
WRTTL	θ_{SX}	P	θ_{RX}	θ_R	2.9	0.4

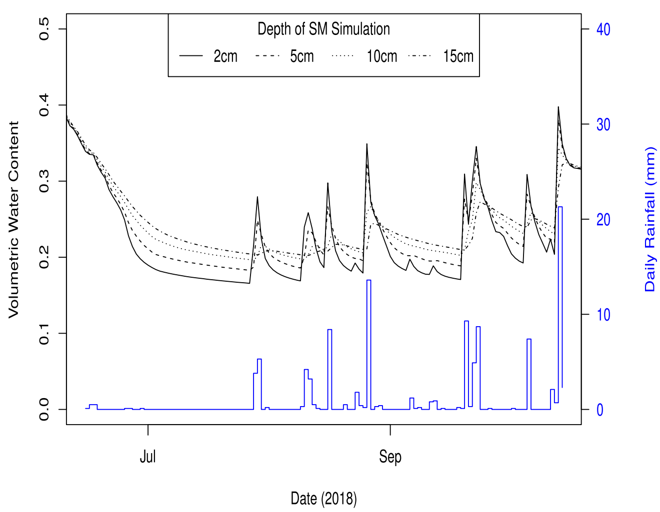


Fig. 5. HYDRUS-1D [47] simulation of soil moisture at the Chimney Meadows COSMOS-UK site at various depths from the surface.

C. Identifying Wet and Dry Reference Values for Converting SMI to Absolute VWC

For each of the 13 selected COSMOS-UK sites, a best fit straight line between the SSM-derived VWC and the HYDRUS-1D prediction at 2 cm soil depth was found by linear regression in R. The slope error ($|1 - b|$) and offset ($|a|$) relative to the expected $y = x$ relationship are tabulated in Appendix B. Analysis of this data yield recommendations of first and second choices for wet and dry references, as shown in Table V. The additional error estimate for using second choice over first choice reference recommendations was calculated as the mean of the differences between the first and second choice references at each site. In most cases, this is less than 5 vol.% except for LOTDN, HYBRY, and SPENF sites where the error is up to 10 vol.%. A similar estimate was calculated for using the common choice of FC and PWP as references compared to the first choice recommendations. The error in this case is generally larger. It should be noted that these are estimates of the average error, the actual error will be soil moisture dependents and will be greatest toward the extremes of the range, where the error could be up to 20 vol.%.

D. Case Study—Assessment of the Copernicus SSM-Derived VWC

Fig. 6 illustrates, for one site, the beneficial impact of the exponential smoothing filter that was applied to the Copernicus SSM derived soil moisture data. The remotely sensed time series in Fig. 6(b) is much better matched to the HYDRUS-1D simulations, but retains a similar dynamic range and responsiveness to soil moisture changes. The maximum deviation is between May and July, which may be due to vegetation effects in the remotely sensed data, and is currently subject to further study by the authors.

Appendix B summarizes the performance metrics for the SSM-derived volumetric soil moisture assessed against simulated soil moisture at 2 and 10 cm, at all 13 of the selected COSMOS-UK sites. The assessment was repeated for SSM data with and without the smoothing by exponential filter.

VII. DISCUSSION

A. Model Fitting

The optimized soil hydraulic properties model fit in Table IV is characterized by an RMSD value of less that 5 vol.% in almost all cases, which is a significant achievement in light of the fact that the CRNS sensor has a variable depth sensitivity. The results provided enough confidence in the model to use it at a shallower soil depth.

Comparing the optimized (see Table IV) to initial (Table II soil hydraulic properties, the deviation is quite large at some sites. Generally, the fitted values of θ_R are lower than the initial

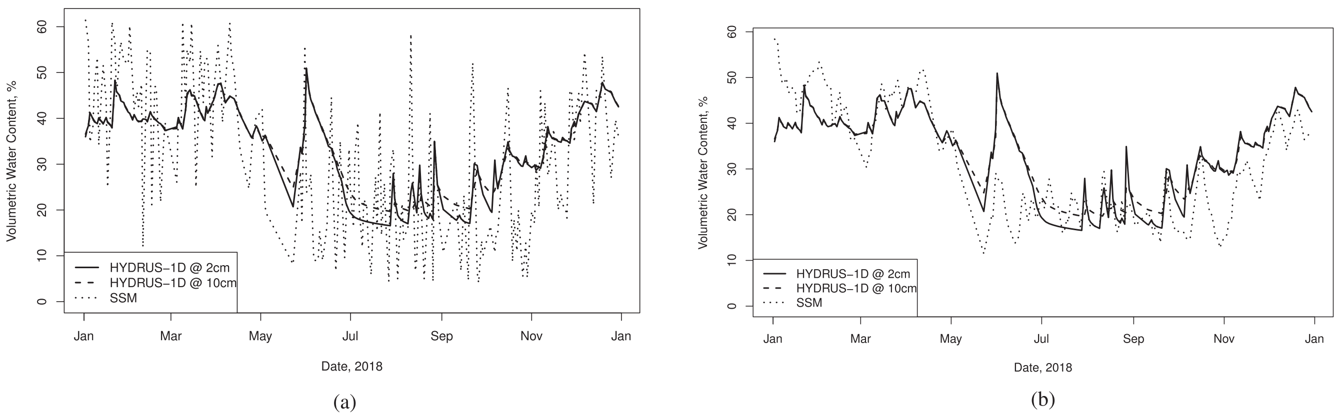


Fig. 6. HYDRUS-1D [47] Copernicus SSM-derived VWC time series for 2018 compared to the HYDRUS-1D simulation at 2 and 10 cm depths. The site is Chimney Meadows (CHIMN).

values form the soil maps, in some cases very close to 0% SM. For some sites the value of θ_S is much higher than the starting value (CHIMN, ELMST, LODTN, WRTTL) which might suggest that the soil texture is not as expected from the soil map. Some of the optimized values of K_s were very different to that expected from the LANDIS Horizon Hydraulics data (CARDT, ELMST, FINCH, HADLW, HYBRY, LODTN, RISEH ROTHD, SPENF, and WRTTL). Possible reasons for this include; local heterogeneity not represented in the soil map, localized soil compaction, tillage operations, and fissures and other drainage channels that have developed.

Where there is an appreciable organic layer overlying the mineral soil, the single layer model may not be ideal. HYDRUS-1D may be configured for two or more layers, but the optimization of additional soil hydraulic parameters may not be practical.

The methods could be used with alternative soil moisture sensors where no CRNS is available, provide that measurements of rainfall and PE can be made. The soil hydraulic parameters could also be determined direct by soil sampling and laboratory analysis, but this an expensive and resource intensive process. It is more scalable to start with values derived from existing soil maps and adjust them empirically to match field observations.

B. Wet and Dry References for Converting SMIs to VWC

The results of this study, summarized in Table V, confirm that FC and PWP are not the appropriate references to use when converting Copernicus SSM SMI values to VWC. For none of the 13 sites does PWP appear appropriate as a dry reference, and in only two cases does FC seem an acceptable choice as a wet reference. In most cases the Van Genuchten model parameters θ_S and θ_R are an appropriate choice for the wet and dry reference. Where optimized values are available from model fitting, these give even better results in most cases, as expected. In regions where values of θ_S and θ_R may not be readily available, the saturation value P, which may be approximately estimated by the porosity of the soil, would be a better estimate of wet reference than FC. For the dry reference a value of 0%–5% could be used, as the values of θ_{RX} are generally very low.

This finding may also be relevant to the calibration of other products presented as SMIs, where the sensing technology is only sensitive to a shallow surface layer of less than 5 cm. This may include all products based solely on *C*- and *X*-band SAR or optical remote sensing.

C. Application of the Method

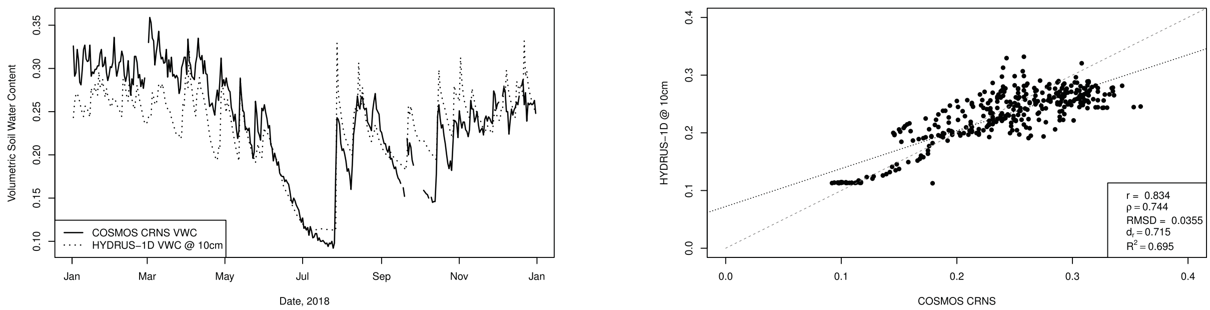
The HYDRUS-1D model has been fitted to the COSMOS-UK CRNS sensor with a foot print of around 400 m diameter, using MODIS LAI data at 500 m resolution to partition evapotranspiration into evaporation and transpiration. There will be some uncertainty due to the difference in scale. The HYDRUS-1D predictions of soil moisture at 2 and 10 cm depth are derived from, and therefore at the same scale as COSMOS-UK When using these predictions to validate the Copernicus SSM 1 km product, a representativeness error [1] may be introduced. For the purpose of this study, the magnitude of this error is assumed to be the same when validating at 2 and 10 cm soil depth.

The depth of penetration of *C*-band SAR depends on the dielectric constant of the soil, which is a function of soil moisture, and is in the range of 1–5 cm [11]. This appears as a source of noise when comparing the SAR-derived soil moisture to any fixed depth measurement. A depth of 2 cm is close to the average penetration depth and will minimise the noise compared to 5 or 10 cm where validation is typically undertaken.

The method of validation presented here should also be applicable to validation of SAR-based soil moisture products at, for example, *X*-band, which has an even shallower depth [11] of penetration than *C*-band.

D. Case Study Assessment of Copernicus SSM-Derived Soil Moisture

Fig. 6(a) compares the time series of volumetric soil moisture derived from remote sensing and the HYDRUS-1D model simulation at 2 and 10 cm depth. As anticipated, the overall trends of the remote sensing output and the model simulation match reasonably well, especially at 2 cm depth, but the SSM-derived-data appear to have a significant noise element. This varies so



(a) (b)

Fig. 7. HYDRUS-1D model fit at the Fincham COSMOS-UK site, before optimization, for 2018.

rapidly that it cannot be explained by variations in soil moisture, surface roughness, or vegetation. The source is likely to be a combination of random noise (speckle), heavy rain, frozen soil, or the occasional presence of scattering sources such as vehicles. Alternatively it may be systematic in nature, due to time of day or orbit geometry. This was the motivation for implementing the exponential filter in the course of this study. In implementing such a filter, some caution must be advised, as a similar approach may be used to estimate soil moisture at greater depths from surface soil measurements [48]. Soil moisture below the surface is dependent on the history of rainfall events and evaporation at the surface, with a time constant dependent on infiltration rates. When implementing an exponential filter for noise reduction, care must be taken to avoid damping the signal too much, and by doing so unwittingly predict soil moisture at a greater depth than the observations. Other types of filters will be the subject of further research.

Appendix B shows that, for 10 out of the 13 selected COSMOS-UK sites, the assessment of the SSM-derived soil moisture was more favorable overall when compared to HYDRUS-1D simulations at 2 cm depth than they were compared to HYDRUS-1D simulations at 10 cm depth. This is based mainly on d_r values. At seven sites CHIMN, ELMST, FINCH, LODTN, RISEH, ROTHD, and SPENF, the benefit of assessing at 2 cm is unambiguous, with improvements in almost all metrics. At CARDT, HADLW, and WRTTL, the results are a little mixed. The anomalous sites include CGARW and HYBRY. These are reported to have a relatively shallow overall soil depth over rock and chalk, so the CRNS data may be more strongly correlated to surface soil moisture at these sites. The results at RISEH are generally poor, which appears to be due to errors in setting the wet and/or dry references at this site (indicated by a large value of $|1 - b|$). At EUSTN, the performance metrics are similar at 2 and 10 cm. It is likely that rapid drainage due to the exceptionally high sand content $> 73\%$ has caused the whole 10 cm soil layer to have similar soil moisture to the top 2 cm layer.

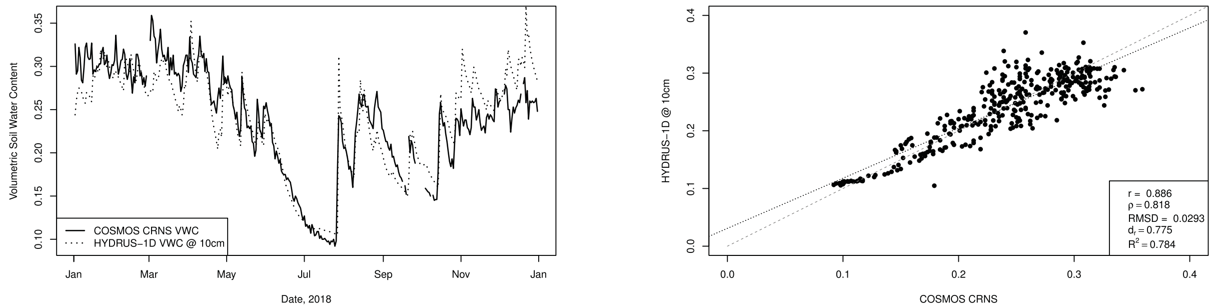
The practical implication of the results just presented is that previous assessments of products such as Copernicus SSM may have overestimated the error in these products due to validation at an inconsistent depth and that future analyzes should take account of this by adopting a similar method to that reported here.

The RMSD values associated with the Copernicus SSM-derived soil moisture compared to HYDRUS-1D 2 cm simulations, is in the range of 8.9 to 19.8 vol.% (unsmoothed data) or 7.6 to 18.3 vol.% (exponentially smoothed). The noise reduced by filtering will be partly random, but also seems to have a periodic component, which may be due to satellite orbit geometry, that should be further investigated.

VIII. Conclusion

Surface soil moisture products should ideally be assessed for performance against *in situ* observations that are consistent with the penetration depth of the frequency of SAR being used. In the case of *C*-band SAR, this is at no greater depth than 2 cm, where instrumented soil moisture measurements appear to be rare. As an alternative, the method developed offers a means to simulate *in situ* soil measurements at 2 cm or any other depth, by fitting the HYDRUS-1D model to *in situ* observations at a much greater depth. The data required to achieve this is a time series of soil moisture measurements at (for example) 10 cm, LAI, and potential evapotranspiration. There is a demonstrable improvement in the apparent performance of soil moisture derived from Copernicus-SSM between assessment at 2 and 10 cm in 10 out of 13 COSMOS-UK sites studied.

For many applications, the soil moisture indices (SMI) often used in remote sensing products, would be much more useful converted into absolute values of VWC, or plant available water. We have shown that for the Copernicus-SSM product, to convert SMI to VWC, the wet and dry references should ideally be the Van Genuchten model parameters θ_S and θ_R and not θ_{FC} and θ_{PWP} as commonly used. The potential error in using the latter is in the range 2 to 10 vol.% on average, but increases up to as much as 20 vol.% at high or low soil moisture values for some sites. The use of Van Genuchten model parameters θ_S and θ_R derived from model optimization can further improve accuracy over those obtained from soil maps, but this is site dependent and is generally less than a 10 vol.% improvement in average accuracy.



(a) (b)

Fig. 8. HYDRUS-1D model fit at the Fincham COSMOS-UK site, after optimization, for 2018.

TABLE VI
SSM PERFORMANCE METRICS ASSESSED AGAINST HYDRUS-1D SIMULATIONS OF SOIL MOISTURE AT 2 AND 10 CM SOIL DEPTHS AT 13 COSMOS-UK SITES IN 2018. BEST VALUES ARE SHOWN IN BOLD

Site identifier	Depth (cm)	SSM not smoothed				SSM Exponentially Smoothed			
		d_r	$RMSD$	$\|a\|$	$\|1-b\|$	d_r	$RMSD$	$\|a\|$	$\|1-b\|$
CARDT	**2**	**0.525**	9.807	3.809	**0.002**	**0.593**	7.670	4.819	**0.020**
	10	0.501	**9.737**	**2.478**	0.043	0.587	**7.509**	**3.432**	0.027
CGARW	2	0.024	**18.843**	18.746	0.414	0.355	12.876	**4.204**	**0.103**
	10	**0.026**	19.149	**15.409**	**0.348**	**0.371**	**12.775**	4.209	0.105
CHIMN	**2**	**0.381**	**13.069**	**1.899**	**0.006**	**0.629**	**8.343**	**0.535**	**0.043**
	10	0.304	13.359	4.863	0.067	0.594	8.354	4.769	0.069
ELMST	**2**	**0.245**	**13.677**	**12.217**	**0.054**	**0.306**	**12.170**	**9.311**	**0.024**
	10	0.112	14.377	16.642	0.159	0.181	12.659	15.143	0.121
EUSTN	2	**0.246**	14.574	10.915	**0.119**	**0.359**	11.530	11.981	0.147
	10	0.211	**14.572**	**10.652**	**0.119**	0.346	**11.218**	**11.077**	**0.102**
FINCH	**2**	**0.406**	**9.369**	**5.325**	**0.118**	**0.478**	**7.827**	**3.523**	**0.052**
	10	0.216	10.030	9.756	0.268	0.329	8.294	8.739	0.237
HADLW	**2**	**0.510**	**13.586**	3.639	0.123	**0.618**	**11.041**	2.721	0.093
	10	0.437	14.008	**1.859**	**0.089**	0.573	11.249	**0.313**	**0.023**
HYBRY	2	**0.477**	**13.219**	1.048	0.169	**0.667**	8.506	1.777	0.170
	10	0.455	13.323	**0.037**	**0.141**	0.665	**8.447**	**0.220**	**0.127**
LODTN	**2**	**0.539**	**12.431**	**14.766**	**0.233**	**0.658**	**9.416**	**14.056**	**0.202**
	10	0.458	13.272	19.505	0.321	0.591	10.160	19.953	0.318
RISEH	**2**	**0.046**	**19.926**	**1.443**	**0.513**	**0.079**	18.340	**0.390**	**0.494**
	10	-0.026	20.110	4.282	0.590	0.035	**18.194**	5.577	0.646
ROTHD	**2**	**0.510**	**9.356**	**1.277**	0.166	**0.567**	**8.119**	**0.365**	0.226
	10	0.346	10.127	6.520	**0.011**	0.407	8.720	5.287	**0.053**
SPENF	**2**	**0.525**	**8.932**	**4.714**	**0.013**	**0.558**	**8.043**	**3.132**	0.075
	10	0.492	9.117	6.395	0.037	0.534	8.109	5.158	**0.012**
WRTTL	**2**	**0.580**	**13.820**	10.794	0.240	**0.653**	11.170	11.120	0.247
	10	0.522	14.277	**10.147**	**0.238**	0.628	**11.018**	**9.059**	**0.195**

APPENDIX A MODEL FITTING RESULTS

An example of the time series fit at the Fincham (FINCH) site is given in Fig. 7 (before optimization) and Fig. 8 (after optimization). This demonstrates that the optimization process has been very effective in matching the prediction to the observations. The remaining errors may be due, to some degree, to the effective measurement depth of the CNRS sensor, which varies with soil moisture.

Appendix B Depth Influence on Assessment of Copernicus SSM-Derived Soil Moisture

Table VI summarizes the performance metrics for the SSM-derived volumetric soil moisture assessed against simulated soil moisture at 2 and 10 cm, at all 13 of the selected COSMOS-UK sites. The assessment was repeated for SSM data with and without the smoothing by exponential filter.

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This study brought together existing research data obtained from a number of different sources, some of which were upon request and subject to licence restrictions. Full details of how these data may be obtained may be found at doi: 10.17862/cranfield.rd.13028123.

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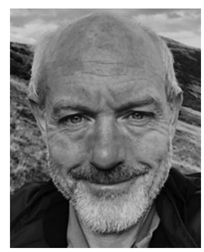

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