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Assimilation of Sentinel 1 and SMAP – based satellite soil moisture retrievals into SWAT hydrological model: the impact of satellite revisit time and product spatial resolution on flood simulations in small basins

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Abstract

In runoff generation process, soil moisture plays an important role as it controls the magnitude of the flood events in response to the rainfall inputs. In this study, we investigated the ability of a new era of satellite soil moisture retrievals to improve the Soil & Water Assessment Tool (SWAT) daily discharge simulations via soil moisture data assimilation for two small (< 500 km²) and hydrologically different catchments located in Central Italy. We ingested 1) the Soil Moisture Active and Passive (SMAP) Enhanced L3 Radiometer Global Daily 9 km EASE-Grid soil moisture, 2) the Advanced SCATterometer (ASCAT) H113 soil moisture product released within the EUMETSAT Satellite Application Facility on Support to Operational Hydrology and Water Management (H-SAF) which has a nearly daily temporal resolution and sampling of 12.5 km, and 3) a fused ASCAT/Sentinel-1 (S1) satellite soil moisture product named SCATSAR-SWI with temporal and spatial sampling of 1 day and 1 km, respectively into SWAT hydrological model via the Ensemble Kalman Filter (EnKF).

Different configurations were tested with the aim of exploring the effect of the hydrological regime, the land use conditions, the spatial sampling and the revisit time of the products (which controls the amount of available data to be potentially ingested).

Results show a general improvement of SWAT discharge simulations for all products in terms of error and Nash Sutcliffe efficiency index. In particular, we found a relatively good behavior of

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.jhydrol.2019.124367>.

both the active and the passive products in terms of low flows improvement especially for the catchment characterized by a higher baseflow component. The benefit of the higher spatial resolution of SCATSAR-SWI obtained via S1 over ASCAT was small, likely due to very challenging areas for the S1 retrieval. Eventually, better performances were obtained for the passive product in the more forested catchment.

With the aim of exploring the benefit of having more frequent satellite soil moisture observations to be ingested, we tested the performance of the ASCAT product with a reduced temporal sampling obtained by temporally matching ASCAT observations to that of SMAP. The results show a significant reduction of the performance of ASCAT, suggesting that the correction frequency (due to the higher number of observations available) for small catchments is an important aspect for improving flood forecasting as it helps to adjust more frequently the pre-storm soil moisture conditions.

Keywords

Data assimilation; SWAT; EnKF, small basins; Satellite soil moisture

1. Introduction

Soil moisture controls the exchange of water, energy and carbon fluxes between the land surface and the atmosphere and has a key role in many applications (Seneviratne et al., 2010; Massari et al., 2015; Kumar et al., 2015; Leroux et al., 2014; Pan et al., 2003).

In runoff generation, soil moisture regulates the magnitude of flood events to the precipitation inputs via the partition of precipitation into runoff (Brocca et al., 2009; Beck et al., 2010; Trambly et al., 2010, 2011, 2012). Hydrological models are the most viable way for obtaining soil moisture spatial distribution, however the landscape diversity (i.e., soil type and topography) along with the intermittence character of rainfall and inherent model simplifications make its estimation highly challenging (Brocca et al., 2017).

In the last decade, there has been a considerable interest in using soil moisture observations derived from ground stations and remote sensing for monitoring and improving the representation of pre-storm soil moisture conditions of hydrological models (Massari et al., 2014a,b; Crow et al., 2017) as, under certain circumstances (i.e., when their accuracy is relatively high), these observations provide a better representation of the true catchment pre-storm soil moisture conditions with respect to hydrologic and land surface models (e.g. Crow et al., 2017). Therefore, the monitoring and the ingestion of soil moisture observations in models is particularly important for flood forecasting.

The collection of a large number of in situ measurements via gravimetric sampling or Time Domain Reflectometry (TDR) sensors (Vereecken et al., 2014) is the most direct way for the estimation of the soil moisture spatial distribution within a catchment. These techniques have the advantages of easy installation, and the ability to measure soil moisture at different soil depths. However, huge economic and time efforts are often required and optimal results are not always guaranteed given the limited spatial representativeness of the measurements

caused by the large spatial heterogeneity of soil moisture over a range of scales (Crow et al., 2012).

Remote sensing is therefore a viable alternative to in situ measurements. In the last decade two important satellite missions have been specifically launched for the measurement of soil moisture from space, namely, the Soil Moisture Ocean Salinity-(SMOS) (Kerr et al., 2001) and the Soil Moisture Active and Passive mission SMAP (Entekhabi et al., 2010). Nevertheless, other active and passive sensors on board of operational and non-operational satellites have been (and are still) used to retrieve soil moisture. Notable examples are the Advanced Scatterometer ASCAT (Wagner et al., 2013) and the Advanced Microwave Scanning Radiometer for Earth observation science (AMSRE) (Njoku et al., 2003) and its successor AMSRE-2 (Lu et al., 2009). These sensors offer the possibility to measure soil moisture continuously in all-sky conditions and thus are extremely important for many applications.

Despite these great advantages, the small penetration depth (i.e., smaller than 5 cm) and the large spatial support (i.e., greater than 25 km) of these observations pose important challenges in flood and flash flood forecasting (Chen et al., 2011; Han et al., 2012a,b; Matgen et al., 2012). Indeed, unless the runoff generation is mainly driven by fast runoff and thus controlled by upper soil layers, root zone soil moisture (i.e., > 5 cm depth depending on the vegetation type) has often a larger influence on the runoff generation (Mao et al., 2018). Additionally, the evident contrast between small scale applications and the coarse spatial resolution suggests that the utility of satellite soil moisture observations for flood forecasting in medium-small basins (< 500–1000 km²) is limited (Matgen et al., 2011). Moreover, despite the value of satellite soil moisture observations has been partially demonstrated for continental and large-scale hydrology (Reichle et al., 2008; Chen et al., 2014), at smaller scales its utility appears much more controversial (Draper et al., 2011; Chen et al., 2011; Brocca et al., 2012; Wanders et al., 2014; Massari et al., 2015; Alvarez-Garreton et al., 2015; Lievens et al., 2015; Mao et al., 2018).

The new generation of satellite soil moisture observations characterized by higher temporal resolutions and relatively higher precision and accuracy can potentially provide more useful information for flood forecasting in small basins with respect to the past. For instance, ASCAT sensors are currently mounted on three satellites (i.e., Metop-A, Metop-B, and Metop-C) which can provide – with more than one observation per day – information on the daily soil moisture cycle. Also, SMAP soil moisture retrievals are characterized by a relatively high signal to noise ratio (i.e. Chen et al., 2018) thus being very informative across all the range of soil moisture values (i.e., from dry to wet). However, as highlighted before, the spatial support of these products is often much larger than the area of a small basin with the risk of not being representative of their true soil moisture conditions in the catchment.

To circumvent this problem, various downscaling/data fusion methods of satellite soil moisture products (Zhan et al., 2006; Piles et al., 2011; Merlin et al., 2012; Malbêteau et al. 2016, Bauer-Marschallinger et al., 2018b), incorporating geophysical variables such as land surface temperature and vegetation, have been studied for improving their spatial resolution. These methods differ in (1) the type of input data (radar data, optical/thermal data,

topography, and soil depth) and (2) the characteristics of the scaling model (physical and statistical). The reader is referred to Peng et al. (2017) for a detailed review on these methods.

In this respect, the recent launch of Sentinel-1 (S1) satellites has provided new information for potentially retrieving soil moisture from Synthetic Aperture Radar (SAR) at plot scale (< 100 m). However, the noise associated with the retrieval of soil moisture has limited the spatial resolution at values larger than 1 km while temporal resolution varies from 1.5 to 4 days in Europe (Balenzano et al. 2012; Bauer-Marschallinger et al. 2018a). Particularly the errors induced by vegetation and roughness have been demonstrated to be not negligible. For instance, a recent validation of surface soil moisture retrieved from S1 by Bauer-Marschallinger et al. (2018a) has highlighted a relatively good behavior of the product in flat agricultural areas and low vegetation density landscapes whereas poorer results were obtained on hilly and moderately vegetated areas. The latter can be an important limitation for the use of these products in flood and flash flood forecasting in complex terrain. In addition, their lower temporal resolution is often not appropriate for small scale flood forecasting applications as the response of small basins to precipitation inputs is very quick (i.e., it generally depends on the catchment size, topography and soil type).

Despite this, Cenci et al. (2017) demonstrated that SAR derived soil moisture observations obtained from S1 are able to improve discharge simulations in a small Mediterranean catchment located in northern Italy provided that some preprocessing steps are carried out prior to the assimilation. In addition, S1 observations can be very important for obtaining products at higher spatial resolutions via disaggregation of either the coarse scale soil moisture products (Das et al. 2011) or the brightness temperature (Das et al. 2014), or alternatively via direct fusion of the two (Montzka et al., 2016). In this respect, Bauer-Marschallinger et al. (2018b) developed an approach to fuse two data streams of satellite soil moisture retrieved from ASCAT and S1 observations, respectively, providing a product with a resolution more commensurable with small scale flood forecasting applications (i.e., 1 km and daily time stamp, with an effective spatial resolution of 5–10 km, i.e. 5×5 km, 10×10 km).

Flood forecasting applications using downscaled soil moisture products are quite rare. One notable case is the one of López López et al. (2016). In the study, a downscaled soil moisture product derived by applying a smoothing filter modulation technique to AMSRE brightness temperatures was jointly assimilated with discharge measurements into a large-scale hydrological model. The authors showed that the assimilation of soil moisture observations resulted in the largest improvement of the model estimates of streamflow (the joint assimilation of both streamflow and downscaled soil moisture observations led to further but smaller improvements). The product of Gevaert et al. (2016) is substantially different from the fused one of Bauer-Marschallinger et al. (2018b) as it does not use SAR information but relies upon brightness temperatures from the C band (~ 50 km $\times$ 50 km) which are adjusted based on data from the Ka band (~ 10 km $\times$ 10 km) (see Gevaert et al., 2016 for additional details). A conceptually similar approach (i.e., relying only on brightness temperature) was also used to obtain SMAP L3 9 km daily Global Radiometer Enhanced Soil Moisture (given the radar failure after only 3 months after the launch of the SMAP mission). In this case, the

Backus–Gilbert (BG) optimal interpolation technique to antenna temperature measurements in the original SMAP Level 1B brightness temperature product was applied (Chan et al., 2018).

The effect of the revisit times and thus the number of remotely sensed soil moisture data available for correcting the model is also another important and under discussed aspect in hydrological data assimilation. While many data assimilation experiments have criticized and discussed the limitation associated to the spatial resolution (Matgen et al., 2011), little can be found about the limitation associated to the revisit time. In a nutshell, shorter revisit times would guarantee a more accurate estimation of the daily soil moisture value or in case of sub-daily hydrological model simulations a more frequent correction and thus potentially more value for flood forecasting in small basins (where flood events can be observed at sub-daily scale). For instance, after the launch of Metop-B satellite in 2012, ASCAT can provide more than one observation per day in Central Italy (although very close each other) and potentially up to three with last launch of Metop-C in 2018 (as third Metop satellite), whereas SMOS and SMAP, having long revisit times, have in general less observations to build the daily composite L3 products.

In this context, it is interesting to analyze if medium to coarse scale products and their derived downscaled versions have a value for flood forecasting in small basins and to investigate the potential benefit of having a larger number of observations within a period. Understanding these issues is a relevant research question and may have potential benefits for water resources management and for the design of future satellite missions.

In this study, we investigated the ability of three satellite soil moisture data products to improve the Soil & Water Assessment Tool (SWAT) (Arnold et al., 1998) discharge simulations for two small and hydrologically different catchments in Central Italy (one dominated by highly permeable soils, a larger baseflow component and a smaller presence of forests and the other dominated by more clayey soils, a much smaller baseflow component and a larger presence of forests). The products assimilated are one passive (downscaled) soil moisture product (i.e., the SMAP L3 9 km), and two active products, namely, the EUMETSAT Satellite Application Facility on Support to Operational Hydrology and Water Management, H SAF, H113, and the SCATSAR-SWI product derived from the fusion of ASCAT and S1-SAR measurements (Bauer-Marschallinger et al., 2018b). The study aims at shedding light on the ability of these new products to improve discharge simulations at scales commensurable with flash flood forecasting applications. To our knowledge, these issues are explored for the first time with the new generation of products (i.e. SMAP and SCATSAR-SWI) and therefore can provide useful insights for the future literature in the topic.

2. Study area and datasets

2.1. Ground meteorological network, ancillary datasets and basin description

The study area is part of the Upper Tiber River and is located in the Umbria region in Central Italy (Fig. 1). The landscape is mainly hilly, with a mountainous area in the eastern sector and a flood plain that stretches along the north–south direction.

The Umbria region meteorological network currently consists of 90 rain gauges, 77 thermometers and 43 hydrometric stations distributed throughout the territory (Fig. 1). The monitoring network provides semi-hourly data for which a quality-check step was performed to remove anomalous values and to fill any temporal gaps. Rainfall and temperature data were aggregated at catchment scale by the inverse distance weighted interpolation scheme. Streamflow data were calculated by the transformation of water levels measured at hydrometric stations via rating curves updated every 2 years.

A soil texture map based on previous studies is available for the study area (see Brocca et al., 2016). The map was obtained by analyzing more than 1600 soil surveys and by coupling this information with the regional geologic setting.

For this study, data covering the period 2004–2017 were used to force the SWAT hydrological model. Details for the data used to force the model are provided in Section 3.1.

The assimilation experiments were carried out on two catchments of the Upper Tiber River, namely Niccone at Migianella stream gauge station and Chiascio at Branca stream gauge station.

Niccone covers an area of 137 km² and the elevation ranges between 249 and 887 m a.s.l. with a mean catchment slope of 25%. The catchment is characterized by a Mediterranean climate, with precipitation occurring mostly in the autumn–spring period when floods generally occur. Based on the period 2000–2017 the average annual precipitation is about 850 mm equally distributed over the whole catchment while mean temperature is 13.0 °C. Major land use in this basin is forests (66%) followed by agriculture (33%), urban (0.5%) and pastures (0.5%). Also, there is a unique soil type (loam) in Niccone.

Chiascio covers an area of 165 km². As Niccone, the basin is mainly characterized by a Mediterranean climate with topography between 320 and 1550 m a.s.l. and mean slope of 24%. Mean annual precipitation is 1050 mm and the mean annual temperature is 13.0 °C. Higher monthly precipitation values generally occur during the autumn–winter period and are associated with floods. Major land use in this basin is forests (50%), followed by agriculture (46%), urban (3%) and pastures (1%). The basin is constituted mainly by marly formations (obtained from the same local soil texture dataset). The baseflow component of this catchment is much larger than that of Niccone suggesting a more significant influence of subsurface flow derived from the more permeable and fractured rock formation of the Apennines Chain on the east side of the catchment.

2.2. Remote sensing data

2.2.1. ASCAT soil moisture product—ASCAT is a scatterometer that operates in C-band (5.255 GHz) at VV polarization and scans the Earth's surface in descending and ascending overpasses (Bartalis et al., 2007). It was installed onboard of the Meteorological Operation-A (Metop-A, launched in 2006) satellite, and then on the two successors: Metop-B (launched in 2012), and Metop-C (launched in 2018), which are expected to provide an uninterrupted stream of ASCAT backscatter observations well into the 2020 s (Wagner et al., 2013). In this study, one of the soil moisture data products applied for developing data

assimilation into SWAT is derived from the H SAF “H113” product which is obtained from the combination of Metop-A and -B satellites and distributed within the “EUMETSAT Satellite Application Facility on Support to Operational Hydrology and Water Management (H SAF, <http://hsaf.meteoam.it/>)”. H113 is globally available since 2007 with a spatial sampling of 12.5 km and a nearly daily temporal resolution. ASCAT observations were chosen because they (1) support the periods where discharge observations are available, (2) are available in near-real time and (3) are characterized by a relatively good performance in the Mediterranean region (e.g., Paulik et al., 2014).

2.2.2. SCATSAR-SWI soil moisture product—The SCATSAR-SWI (Scatterometer-Synthetic Aperture Radar Soil Water Index, SCATSAR hereafter for simplicity) is a pre-operational data product describing soil water content at fine spatio-temporal sampling (daily at 1 km, the effective resolution varies between 5 km and 10 km) by merging two radar data sets. Radar measurements from Metop ASCAT (high temporal frequency, coarse spatial scale) and Sentinel-1 CSAR (lower temporal frequency, fine spatial scale) are individually used for the estimation of soil moisture, which are combined to the SCATSAR through data fusion (see Bauer-Marschallinger et al., 2018b for further details). During the data fusion, a S1-SAR-based parametrization substantially improves the spatial fidelity of the ASCAT signal. The Copernicus Global Land Service (CGLS, <https://land.copernicus.eu/global/>) disseminates freely the SCATSAR under the name SWI1km, featuring data from 2015 ongoing in an initial phase over Europe, and subsequently on a global scale.

2.2.3. SMAP soil moisture products—This enhanced Level-3 (L3) soil moisture product provides a composite of daily estimates of global land surface conditions retrieved by the Soil Moisture Active Passive (SMAP) radiometer. This product is a daily composite of SMAP Level-2 (L2) soil moisture which is derived from SMAP Level-1C (L1C) interpolated brightness temperatures. Backus-Gilbert optimal interpolation techniques are used to extract information from SMAP antenna temperatures and convert them to brightness temperatures, which are posted to a 9 km Equal-Area Scalable Earth Grid, Version 2.0 (EASE-Grid 2.0) in a global cylindrical projection.

3. Methodology

3.1. The soil and water assessment tool (SWAT) model

The SWAT model is a long-term simulation watershed model developed by Arnold et al. (1998) for the United States Department of Agriculture (USDA). The model is process-based and has the ability of simulating the hydrological components in fine spatial details. SWAT divides the basin into sub-basins and each sub-basin is further divided into Hydrological Responses Units (HRU) that consist of homogenous land use, soil type and slope. The input variables for each sub-basin are: climate data (precipitation, air temperature, solar radiation, wind speed and relative humidity) and spatial data (soil type, land use and slope maps). The model has been widely applied by various researchers for hydrological parameter estimation (e.g. Muttiah and Wurbs, 2002; Gasman et al., 2007; Li et al., 2010; Shiferaw et al., 2016). The hydrological process simulated by SWAT model is based on the water balance equation (Neitsch et al., 2011):

$$SW_t = SW_0 + \sum_{i=1}^t (R_i - Q_i - E_i - w_{seepi} - Q_{gwi}) \quad (1)$$

where, SW_t and SW_0 are the final and initial soil moisture in day t (mm H₂O); R_i is the amount of rainfall on day i (mm H₂O); Q_i is the amount of surface discharge on day i (mm H₂O); w_{seepi} is the amount of water entering the vadose zone from the soil profile (mm H₂O); Q_{gwi} is the amount of return flow on day i (mm H₂O) and E_i is amount of Evapotranspiration on day i (mm H₂O).

SWAT applies the SCS curve number procedure (SCS, 1972) and the Green and Ampt method (1911) to estimate surface runoff. In this study, the partitioning of rainfall into surface and sub-surface runoff is carried out by SCS Curve Number method. The method was developed to provide a basis for estimating the runoff under different land use and soil type (Rallison and Miller, 1981). The SCS curve number equation is as follows:

$$Q_{surf,i} = \frac{(R_i - I_a)^2}{(R_i - I_a - S_i)} \quad (2)$$

where, $Q_{surf,i}$ is the accumulated runoff on day i (mm H₂O), I_a is the initial abstraction which includes surface storage, interception and infiltration prior to runoff (mm H₂O), and S_i is the retention parameter (mm H₂O).

The soil moisture in each sub surface layer is updated by using the following equation in the model:

$$sol_{sti} = sol_{stinit} - sepdai - latlyr_i - lyrtile_i \quad (3)$$

where sol_{sti} (mm) is the amount of water stored in the soil layer on the i th day; sol_{stinit} (mm) is the initial amount of water stored in the soil layer on the i th day; $sepdai$ (mm) is the percolation from the soil layer on the i th day; $latlyr_i$ is the lateral subsurface flow in the layer on the i th day; and $lyrtile_i$ (mm) is tile drainage in the soil layer on the i th day. The water balance equation used by the model is well explained in the SWAT manual (Neitsch et al., 2011; Arnold et al., 1998).

Based on the mentioned input datasets (see section 3.3) the SWAT model is set up for Chiascio and Niccone basins.

3.2. Ensemble Kalman filter

The ensemble Kalman filter (EnKF, Evensen, 2003) is a data assimilation technique originated from the integration of Kalman filter theory and Monte Carlo estimation method. The goal of this sequential data assimilation approach is to update the model predictions by optimum merging of the observations. The EnKF uses the traditional update equation of the classical Kalman filter methods with the difference that, in the gain calculation, the error covariance is evaluated by using an ensemble of model states. The main equation of EnKF is as follows:

$$Y_k^{i+} = Y_k^{i-} + K_k [Z_k + v_k^i - H_k Y_k^{i-}] \quad (4)$$

where, Y_k^{i-} is the forecasted ensemble state, Y_k^{i+} is an ensemble of model state after assimilation, H_k is the observation operator that maps the model state to the observations, v_k^i is a synthetic error added to observation Z_k and K_k is Kalman Gain:

$$K_k = P_k^- H_k^T (H_k P_k^- H_k^T + R_k)^{-1} \quad (5)$$

where, P_k^- is the covariance matrix of the forecast error calculated by propagating an ensemble of model states (obtained by Monte Carlo or other ensemble generation methods) using the updated states from the previous time step.

$$P_k^- = \frac{[Y_k^- - \langle Y_k^- \rangle][Y_k^- - \langle Y_k^- \rangle]^T}{N - 1} \quad (6)$$

where $\langle \rangle$ is the mean operator. For further details on the method the reader is referred to Evensen (2003).

3.3. SWAT model setup

Prior to the SWAT model calibration ArcSWAT, an ArcGIS interface for SWAT, was used to delineate the sub basins and stream network from 20 m-resolution Digital Elevation Map. Chiascio and Niccone basins were divided into 37 and 36 sub-basins, respectively. A further division of sub-basins into HRUs was carried out using soil and land use information. The land cover was extracted from Corine/2006 (Coordination of information on the environment, <https://www.eea.europa.eu/publications/COR0-landcover>) dataset. The Corine database is available from the European Environmental Agency and it provides 44 classes at a scale of 1:100 000. For obtaining soil type information, we used a soil texture map available for the study area (Brocca et al., 2016).

By using a 5% threshold for land use and soil type and 0% for slope, a total of 233 and 192 HRUs were generated for Chiascio and Niccone basins, respectively. The mentioned threshold levels were used to eliminate minor land uses and soil types in each sub-basin as to obtain more computational efficiency without detrimental effect on the model performance. SWAT operates at daily time step. So daily precipitation, minimum and maximum daily temperatures were applied as meteorological inputs. Solar radiation was computed by the SWAT model whereas relative humidity and wind speed, being absent in the study area were taken from the closest stations of the network outside the catchment boundaries.

The model was calibrated using daily discharge measured at the outlets of Niccone and Chiascio, which are Migianella and Branca, respectively. For Chiascio basin the first year (Jan 2009 to Dec 2009) was used as warm-up period, Jan 2010 to Dec 2013 was used for calibration and the model was validated during Jan 2014 to Dec 2017. For Niccone basin, the warm up period involved the first four years (Jan 2000 to Dec 2003) while the following eight years (Jan 2004 to Dec 2013) were used for calibration. Finally, the model was validated over the period Jan 2014 to Dec 2017. Note that, the warm-up period (which is

largely dependent on the type of model and basin) was chosen based on the data availability and after some tests, the choices made above were found the ones guaranteeing best results.

Based on the results of a sensitivity analysis, 14 parameters were chosen for the calibration process. The model calibration process was performed in SWAT-CUP using the available observed discharge at the outlet of the basins. The Sequential Uncertainty Fitting Algorithm (SUFI-2, Abbaspour et al., 2004) was used to maximize the NSE value between observed and simulated discharge. Since the behavior of the models in peak flow simulations was important during calibration process, the Nash Sutcliffe efficiency index (see section 3.5) was chosen as objective function. SUFI-2 is based on the following procedure.

1. The maximum and minimum ranges of each model parameter in SWAT-Cup are assigned firstly based on past literature studies and personal experience as to have as much large as possible range of parameter values to guarantee the convergence to the optimal calibration.
2. A Latin Hypercube sampling is carried out; leading to n parameter combinations, where n is the number of desired simulations (in this case equal to 1000). The simulation program is then run 1000 times and the simulated variable (e.g. discharge) are saved.
3. For each simulation, the objective function (g) is calculated and the sensitivity matrix (J) is computed as follows:

$$J_{i,j} = \frac{\Delta g_i}{\Delta b_j} \quad i = 1, \dots, C_2^n, \quad j = 1, \dots, m \quad (7)$$

where, C_2^n , is the number of rows in sensitivity matrix (equal to all possible combinations of two simulations), and m is number of columns (number of parameters (b)).

4. Next, the Hessian matrix (H), is calculated as follows:

$$H = J^T J \quad (8)$$

and Eq. (9) is used to estimate the lower bound of the parameter covariance matrix C :

$$C = s_g^2 (J^T J)^{-1} \quad (9)$$

where, s_g^2 is the variance of the objective function values resulting from n runs.

5. The estimated standard deviation and 0.95 interval of parameter b_j is then calculated as follows:

$$\begin{aligned} s_j &= \sqrt{C_{jj}} \\ b_{j, lower} &= b_j^* - t_{v,0.025} S_j, \\ b_{j, upper} &= b_j^* + t_{v,0.025} S_j, \end{aligned} \quad (10)$$

where, b^*_j is parameter b for one of the best solutions, and ν is the degrees of freedom ($n-m$). For further sampling rounds, the parameter ranges are calculated as follows:

$$b'_{j,\min} = b_{j,\text{lower}} - \max\left(\frac{(b_{j,\text{lower}} - b_{j,\min})}{2}, \frac{(b_{j,\max} - b_{j,\text{upper}})}{2}\right) \quad (11)$$

$$b'_{j,\max} = b_{j,\text{upper}} + \max\left(\frac{(b_{j,\text{lower}} - b_{j,\min})}{2}, \frac{(b_{j,\max} - b_{j,\text{upper}})}{2}\right) \quad (12)$$

where, b' is the updated value. For more information about SUFI-2 algorithm, readers are referred to Abbaspour et al. (2004).

SWAT represents soil water content as a concept of soil water storage in mm H₂O and therefore the range of soil moisture values for each layer varies with the thickness of the soil layer. Given the similarity of the soil texture over the basins of the study, SWAT sets the depth of the layers constant and equal to 10, 290, 700 mm, for the first, the second and the third layer for both basins.

3.4. Data assimilation setup

In this section, we describe the main methodological aspects necessary for the implementation of the EnKF into the SWAT model. As model states we selected the soil moisture simulated by SWAT in the three layers.

3.4.1. Model error and EnKF implementation—The sources of uncertainty, coming from the structure and SWAT model parameterization, were simulated through perturbing only model soil moisture states as in Han et al. (2012a,b). In particular, we perturbed soil moisture by adding a normally distributed zero-mean error with standard deviations σ_{m1} , σ_{m2} and σ_{m3} equal to fraction of the simulated soil moisture (i.e. a scaling factor, see Han et al., 2012a,b, for further details). These perturbations were 1) constrained to vary between 0.5 and 3 mm, 3–7 mm and 7–12 mm for the first, second, and third layer soil moistures, respectively, as to reproduce meaningful values of appropriate ensemble scores (see below), 2) allowed to vary for each HRU and 3) perfectly vertically correlated. Note that forcing variables (e.g. precipitation) and model parameters were not perturbed explicitly to generate ensemble members as we assumed that adding model error to model states takes into account all uncertainties raised from forcing variables, parameter estimation and model physics (Zhang et al., 2015). In practice, the model error calibration was carried out in a way that two ensemble verification measures (Test #1 and Test #2 from here onward) commonly used in meteorology (De Lannoy et al., 2006) were satisfied (i.e., by varying the temporally constant scaling factors for generating σ_{m1} , σ_{m2} and σ_{m3}). For the verification of the ensemble we used discharge observations as in Brocca et al. (2012). In other words, we propagated each state member Y^i to a discharge simulation Q^i to have N discharge simulations, and verifying that:

$$Test \# 1 \frac{\langle sp \rangle}{\langle sk \rangle} = 1 \quad (13)$$

$$Test \# 2 \frac{\langle sk \rangle}{\langle mse \rangle} = \sqrt{\frac{N+1}{2N}} \quad (14)$$

where:

$$\langle sp \rangle = \frac{1}{T_p} \sum_{k=1}^T \left\{ \frac{1}{N} \sum_{i=1}^N (Q_k^i - \langle Q \rangle_k)^2 \right\} \quad (15)$$

$$\langle sk \rangle = \frac{1}{T_p} \sum_{k=1}^T \left\{ (\langle Q \rangle_k - Q_{obs,k})^2 \right\} \quad (16)$$

$$\langle mse \rangle = \frac{1}{T_p} \sum_{k=1}^T \left\{ \frac{1}{N} \sum_{i=1}^N (Q_k^i - Q_{obs,k})^2 \right\} \quad (17)$$

where, Q_k^i is the simulated discharge of the i^{th} member at assimilation time t_k , $Q_{obs,k}$ is the observed discharge at time t_k , T_p is the length of the time period, while $\langle . \rangle$ is the mean operator. N is the size of ensemble.

From here onward Eqs. (13 and 14) will be referred as Test#1 and Test#2, respectively. Test#1, indicates that if the ensemble spread is large enough, the temporal mean of the ensemble $\langle sk \rangle$ should be similar to the temporal average of the ensemble spread $\langle sp \rangle$ and their ratio should be close to one. That is, Test#1 < 1 indicates an under-dispersed ensemble whereas Test#1 > 1 indicates an over-dispersed ensemble. Similarly, Test#2 indicates that if an ensemble is a correct representation of analysis uncertainty, the observed or true condition should look like one of the realizations of the ensemble. Note that due to model non-linearity this procedure does not guarantee that an equally optimal ensemble of model states is derived, however, given that relatively high uncertainty of satellite soil moisture observations (i.e., it is difficult to consider it as a true condition) with respect to observed discharge data (Coccia and Todini, 2011) this procedure is one of the few alternatives existing to model uncertainty derivation in hydrological data assimilation of soil moisture. In this respect, it must be said that other model uncertainty derivation tests can be considered (e.g., Abbaszadeh, et al. 2019, Moradkhani et al., 2018; Pathiraja, et al., 2018) but all of them are still subjected to the same issue with satellite soil moisture observations. Note also that here we used the procedure of Han et al. (2012a,b) as it facilitated the calibration of Test#1 and Test#2, given that only the values of the state perturbation parameters had to be chosen. Indeed, to reach the optimal values for Test#1 and Test#2, Massari et al. (2015) demonstrated that different perturbation configurations are possible leading to a problem of equifinality (i.e., the same values for Test#1 and Test#2 can be obtained for different perturbation configurations).

In the data assimilation experiment, all vertically discrete SWAT soil moisture states of each HRU were assumed as the state vector (Y) over each sub-basin. Given that the size of HRUs is generally smaller than that of the satellite pixel, the observation operator (H) was defined as an area-weighted average operator which maps HRU surface soil moisture into each sub-basin. The Kalman gain vector, K , related to the single sub-basin (having a size equal to the number of HRUs contained in the sub-basin times the soil moisture layers simulated by the model) was then applied to project the soil moisture innovations back to individual HRU scales. No spatial correlation was assumed among the sub-basins.

The assimilation was carried out in two steps (see Fig. 2(B)) as in Crow and Ryu (2009). In the first step, EnKF was run solely to update SWAT model soil moisture states. The second run was made as a post-processing step in which the ensemble-mean of these state predictions were directly inserted into a single realization of the SWAT model for the sole purpose of predicting runoff. Note that it is also possible to neglect this post processing stage and simply average SWAT/EnKF runoff predictions across the ensemble to obtain a single EnKF runoff prediction as in Massari et al. (2015) and many other studies. However, we found the use of this alternative approach more beneficial and consequently, we retained it for all the simulations. The data assimilation runs so obtained were then compared both against the SWAT model single validation run (i.e., deterministic run) and the open loop run (OL) which was obtained by averaging the ensemble of non-up-dated model states and inserting this ensemble mean -into a single realization of SWAT to obtained runoff (Fig. 2 scheme (A)).

3.4.2. Pre-processing of observation and error calculation—At first step of preprocessing of satellite observations, because of the challenging performance of microwave soil moisture retrieval in frozen conditions data with temperature below 2 °C were removed. Since the size of HRUs is much finer than the spatial resolution of remotely sensed soil moisture retrievals, we adopted two different strategies based on the resolution of the products. For SCATSAR we aggregated the product at sub-basin scale by simple mean, for ASCAT and SMAP we used the inverse distance weighted method to interpolate the pixels on the sub-basin centroids. The resulting soil moisture product aggregated at sub-basins level was then used as “observation” within the data assimilation framework. However, prior to ingestion we performed a bias correction and observation error calculation as described below.

Satellite soil moisture retrievals and model predictions are generally biased, therefore, prior to the assimilation, this bias must be corrected. Several techniques have been used to perform these steps (see Massari et al., 2015; Chen et al. 2014 for an idea of the most used ones). Here we took advantage of the Triple Collocation (TC, Stoffelen, 1998) “difference notation” (Yilmaz and Crow 2013, Gruber et al. 2016) which provides “optimal” scaling parameters for mapping the observations (i.e., satellite soil moisture retrievals) into the model space (see Gruber et al. 2016 for further details). At the same time TC was also used to estimate the observation errors of the satellite soil moisture retrievals by applying it to triplets built among first layer SWAT soil moisture (this was assumed as the reference against which rescale observations), one active soil moisture retrieval (either ASCAT or SCATSAR) and the passive soil moisture retrieval (i.e., SMAP). In particular, two triplets

were considered: SWAT model 1st layer, ASCAT, SMAP and SWAT model 1st layer, SCATSAR, SMAP.

Table 1 shows the period and mean number of observations available for both basins and then assimilated into SWAT. Given the larger revisit time of SMAP with respect to ASCAT-based products, the number of available SMAP data for both periods are smaller than the ones of ASCAT and SCATSAR.

3.5. Evaluation scores

Different indices were used to evaluate the goodness of the simulations. The Nash-Sutcliffe efficiency index (Nash and Sutcliffe, 1970) was used as calibration score.

$$NSE = 1 - \frac{\sum_{i=1}^N (Q_{obs_i} - Q_{Sim_i})^2}{\sum_{i=1}^N (Q_{obs_i} - \bar{Q}_{Obs})^2} \quad (18)$$

where, Q_{obs} , Q_{sim} , $\bar{Q}_{Obs}$ are observed, simulated, mean observed discharge, respectively and N is the length of the time series. NSE can range from $-\infty$ to 1. NSE equal to 1 corresponds to a perfect match of modeled discharge to the observed data.

NSE gives particular relevance to high flows since the differences between the observed and predicted values are calculated as squared values (Legates and McCabe, 1999).

To evaluate the specific improvement of the assimilation in low flows, we adapted the Nash-Sutcliffe index for low flows (Hoffmann et al., 2004).

$$NS_{(\log Q)} = 1 - \frac{\sum_{i=1}^N [\log(Q_{sim_i} + \epsilon) - \log(Q_{obs_i} + \epsilon)]^2}{\sum_{i=1}^N [\log(Q_{obs_i} + \epsilon) - \log(\bar{Q}_{Obs} + \epsilon)]^2} \quad (19)$$

where, ϵ is arbitrarily chosen as a small fraction of the inter-annual mean discharge.

The Root Mean Squared Error (RMSE) was also used to have a measure of the potential benefit of the assimilation from a more conventional perspective. Note that also statistical scores could be used to assess the performance of the data assimilation runs (see Renard et al., 2010, DeChant and Moradkhani, 2012), however, because the scheme adopted here does not propagate each state vector member to a runoff member (see section 3.4) only deterministic measures were used to compare the different runoff runs.

4. Result and discussion

4.1. SWAT calibration

Table 2 shows SWAT calibrated parameters obtained for Niccone and Chiascio basins. In our case, both saturated hydraulic conductivity (SOL_K) and the recharge of deep aquifer (RCHRG_DP), which are indicative of a larger runoff/baseflow component, are larger for Chiascio than for Niccone. This is consistent with the larger baseflow component for Chiascio as evident in Fig. 3a and 3c. The Plant Evaporation Compensation factor (EPCO) is

a parameter that varies between 0.01 and 1. When EPCO approaches 1, deeper soil layers contribute to the plant water uptake, while when EPCO approaches 0, plant water uptake demands are met by the top soil layers. Due to the different land uses of two basins (especially in terms forest cover), different values of EPCO are obtained during calibration process with a higher value for Niccone, which is indicative of relatively larger forest cover. r_CN2 in the table refers to the “relative method” to calculate the Curve Number (CN2), in which the classical CN2 is reduced or augmented by a factor equal to r_CN2 for each HRU to take into account the soil moisture initial conditions. In our case, -0.09 and -0.12 (or -9% and -12%) for Niccone and Chiascio, respectively, suggest a general decrease in classical CN2 for each HRU for the basins which are then slightly more pervious compared to the default values suggested by SWAT based on the soil and land cover maps (see Abbaspour, 2015 for further details). The soil evaporation compensation factor (ESCO) controls the range of the soil depth used to meet the soil evaporative demands. The parameter varies between 0.01 and 1 and has a default value of 0.95. A decrease of the ESCO value results in a decrease of streamflow as well, as more water is extracted from lower levels of the soil layer to meet the evaporative demands. Here we obtained a much smaller value for Chiascio than for Niccone. This is likely due the smaller mean streamflow observed for Chiascio (with an area of 167 km^2) with respect to Niccone (with an area of 137 km^2). However, the value of this parameter and its impact on the stream flow simulations with respect to the other parameters (e.g., RCHRG_DP) would require an ad hoc sensitivity analysis which is out of the goal of the study. Finally, the lag between the time that water exits the soil profile and enters the shallow aquifer (GW_DELAY) which is dependent upon the depth of the water table and the hydraulic properties of the geologic formations characterizing the vadose and the groundwater zones, is much smaller for Niccone than Chiascio (2.36 days vs 111.79 days). It is likely that for Niccone the height of the water table is much higher but, as no groundwater observations are available for the area, nothing can be extrapolated from these results.

Fig. 3 displays the discharge time series obtained during the calibration period and their associated scatter plots. The NSE values obtained in calibration are 0.71 and 0.72 for Niccone and Chiascio basins, respectively. Despite the relatively good values of NSE, it can be seen that SWAT is not able to catch the peak flows during high flood conditions. Note that better performances could be obtained if a longer calibration period would have been considered as that accounts for a wider range of flow variability (i.e., dry and wet periods) (Perrin et al., 2007).

4.2. Model error calibration and observation error evaluation

The generation of the ensemble was carried out by choosing a number of ensemble members equal to $N = 100$. We tested different values and we found that results did not significantly change for values larger than 100 (the optimal value for Test#2 for $N = 100$ is 0.71 based on Eq. 14). The mean error standard deviations for the three layers that provided the optimal values of Test#1 and Test#2 were about 2, 5, 10 mm for the first, second and third layer (Test #1 = 1.12 and Test #2 = 0.8) for Chiascio and about 0.5, 4, 8 mm (Test #1 = 1.28 and Test #2 = 0.85) for Niccone. These values are in line with those obtained in previous literature (e.g., Brocca et al. 2012).

Table 3 shows the TC observation error (for triplets 1 and 3 and averaged across all the sub-catchments) re-projected both in the model space and in the SMAP space. While the errors of SMAP and ASCAT are comparable, SCATSAR shows larger values which we attributed to the detrimental effect of S1 in complex and vegetated terrain. Over the mentioned conditions the radiometric correction of the radar response and the LAI normalization are likely sub optimal and lead to more noisy data (Bauer-Marschallinger et al., 2018a). To verify this assumption, we also plotted the error distribution of SCATSAR for all the sub-catchments and compared it with the mean sub-catchment elevation range (see Fig. 4). It has to be noted that in the Umbrian landscape higher elevations are very much related to complex terrain and more vegetated surfaces, therefore this index can be considered a robust proxy of these two factors. Fig. 4 clearly shows the increase of the error of SCATSAR for sub-catchments characterized by higher elevations, which supports our previous assumption. In the context of data assimilation such an error spatial distribution will determine a smaller contribution of the satellite observations to the subsequent runoff simulations.

4.3. Validation and data assimilation runs

We examined a total of five different model configurations during the validation period. That is, the deterministic and the OL run as described in Section 3.4.1 and the data assimilation experiments that we named “A”, “B” and “C” configurations. In the first (configuration “A”) each soil moisture product was assimilated into the SWAT model using all observations available during the period 2014–2017 (see Table 4). In the second (configuration “B”) only the period March 2015–December 2016 was considered. B configuration aims at comparing the performance of the three products in a common period and all the available number of observations for each product were used. In the third (configuration “C”), we focused always on March 2015–December 2016 but we subsampled ASCAT to obtain the same number of observations of SMAP. This was done to analyze the benefit of having a higher product temporal resolution.

4.3.1. Deterministic and open loop runs—Table 4 summarizes the results obtained in validation for the deterministic and open loop SWAT runs and contains the results for the A configuration which will be discussed in section 4.3.2.

Compared to the results of the calibration period, during the validation the performance of the model (i.e., deterministic run) decreases strongly in terms of NSE thus indicating a sensible reduction of the predictive skills in terms of medium–high flows. This is likely due to the drier 2014–2017 with respect to previous years used for calibration. According to Table 4, the results of the open loop run are similar to the deterministic run for all the indices both for Chiascio and Niccone suggesting that scheme used to produce the OL run (Fig. 2(A)) does not induce significant bias and deterioration.

4.3.2. Data assimilation experiments—Herein, three configurations are discussed to specify the performance of the three products in the data assimilation process.

● **Configuration A:** As it was mentioned earlier, according to Table 1, the remotely sensed soil moisture data are not available continuously for the entire 2014–2017 period for

all three products. The SMAP product is available after March 2015, whereas (at the time of the writing) H113 (ASCAT) product spans from January 2014 to December 2016. Eventually, SCATSAR observations are available after October 2014. In this section, these observations were assimilated into SWAT model and the evaluation scores were calculated during 2014–2017 period. This means that in the score calculation there were some periods where no assimilation was performed (e.g., prior to March 2015 for SMAP, after December 2016 for ASCAT, prior to October 2014 for SCATSAR).

Table 4 summarizes the results obtained in this configuration for Chiascio and Niccone. For Chiascio basin RMSE were reduced of about $0.2 \text{ m}^3/\text{s}$ with respect to both OL and the deterministic run for all the products whereas NSE was increased up to 0.1 for ASCAT but never reached values above 0.5. For Niccone, the NSE increments and RSME reductions were lower with respect to Chiascio both with respect to deterministic and the OL runs with maximum increments for NSE of about 0.05.

Fig. 5 displays the monthly mean RMSE values obtained in the 2014–2017 period for the different runs. It can be seen that the improvements are mainly concentrated from January to April especially for Chiascio. To explore this further we calculated NSE (logQ) (see section 3.5 for details on its definition).

Fig. 6 plots the value of NSE(logQ) for both basins. It can be seen that the SWAT open loop for Chiascio has relatively low performance whereas a better score is obtained for Niccone. When remotely sensed soil moisture products are assimilated they provide a significant improvement in terms of low flows for Chiascio. For Niccone this improvement is smaller, this is also due to the relatively low baseflow component along with the impossibility to calculate the potential benefit of the assimilation due to the absence of many discharge observations during summer months (see Fig. 7b). In terms of soil moisture (not shown), we found a tendency of the assimilation to add water to soil profile especially during dry periods which (for Chiascio) translated in a generally higher and more delayed baseflow production as shown by the observed discharge time series (Fig. 7a).

● **Configuration B:** Configuration B evaluates the performance of the assimilation in the period March 2015–December 2016 where all the satellite soil moisture products are simultaneously available. Fig. 7 compares the observed daily discharge time series at the outlet of the Niccone and Chiascio basins obtained with OL and with the assimilation runs where ASCAT, SMAP and SCATSAR are assimilated ($\text{SWAT}_{\text{ASCAT}}$, $\text{SWAT}_{\text{SMAP}}$, $\text{SWAT}_{\text{SCATSAR}}$). As to reduce the figure complexity, here we only show the SWAT runoff runs relative to the soil moisture updated ensemble mean and OL (see Fig. 2 for details on how these simulations were obtained) while in the supplementary information in Fig. S1a and b we show two examples of the data assimilation experiments with uncertainty bounds obtained for Niccone with ASCAT and for Chiascio with SMAP. These bounds were produced by running runoff simulations relative to the 2.5 and 97.5 percentiles of the updated and non-updated (i.e., OL) ensemble of model states (i.e., soil moisture). It can be seen from these figures that the assimilation of soil moisture reduces the uncertainty bounds of simulated discharge particularly for high flows.

As it can be seen in Fig. 7 the performance is very variable in time. For instance, for Chiascio we can see a better agreement with observed discharge for $\text{SWAT}_{\text{ASCAT}}$ and $\text{SWAT}_{\text{SCATSAR}}$ at the beginning of April 2015. The two are very similar indicating that ASCAT contribution to SCATSAR is very high. Overall, $\text{SWAT}_{\text{SMAP}}$ simulation seems to perform better at the end of 2016 whereas $\text{SWAT}_{\text{ASCAT}}$ and $\text{SWAT}_{\text{SCATSAR}}$ improve discharge simulations during February 2016. On the whole, the performance is highly variable and none of the products suggests a consistent improvement over OL. For Niccone, there is a tendency of OL to overestimate peak flows, which is partially corrected in $\text{SWAT}_{\text{SCATSAR}}$ and $\text{SWAT}_{\text{SMAP}}$ but not in $\text{SWAT}_{\text{ASCAT}}$ which closely follows the OL. Here the different behavior of ASCAT and SCATSAR is likely due to the higher observation errors obtained for Niccone (see Fig. 4 and Table 3) that produces a substantial different gain with less ingestion of observations located in more vegetated sub basins.

As the judgment of the overall performance of the runs is not straightforward to visualize on a daily time scale, we also calculated the RMSE and NSE percentage difference (we calculated the differences in a way that values larger than zero always refer to improvements) between the data assimilation runs and OL (Fig. 8). We found that for Chiascio RMSE improvements range between 0 and 5% and NSE are larger than 10% for $\text{SWAT}_{\text{ASCAT}}$ and $\text{SWAT}_{\text{SCATSAR}}$ with the latter slightly outperforming the first in terms of NSE. The improvements obtained for $\text{SWAT}_{\text{SMAP}}$ are halved with respect to the $\text{SWAT}_{\text{ASCAT}}$ and $\text{SWAT}_{\text{SCATSAR}}$. For Niccone, we obtained a quite different situation with a range of RMSE of 0–5% for $\text{SWAT}_{\text{ASCAT}}$ and $\text{SWAT}_{\text{SCATSAR}}$ and up to 8% for $\text{SWAT}_{\text{SMAP}}$. NSE improvements are much larger for most of the simulations and reach almost 45% for $\text{SWAT}_{\text{SMAP}}$. The reasons for that can be many although a possible one could be the better ability of SMAP to penetrate vegetation (almost 70% of forests are present in the Niccone basin and 50% in the Chiascio basin, see further details in section 2.1) which is partly confirmed by its lower observation error.

● **Configuration C:** As depicted in Table 1 the number of available data during the period 2015–2016 is different from SMAP and ASCAT (and SCATSAR) given the different revisit times of the two products. In particular, SCATSAR and ASCAT are characterized by 642 against 276 values of SMAP. We expect that a more frequent correction is beneficial for small catchments and here we will test this assumption by downsampling ASCAT observations in a way that they are equal to that of SMAP. For doing that, the nearest neighbor approach was used.

Fig. 9 displays the improvement in terms of RMSE obtained after downsampling. It can be seen that the performance of $\text{SWAT}_{\text{ASCAT}}$ becomes close to the one of SMAP for Chiascio and reduces further for Niccone suggesting that the revisit time (and thus the number of available observations to be ingested) plays an important role in flood forecasting in small basins. The results for SCATSAR lead to the same overall results and are not reported for brevity.

5. Discussion and conclusions

The main objective of the study was to explore the capability of a new era of satellite soil moisture retrievals like those derived from SMAP and Sentinel-1 missions with the aim of improving SWAT daily discharge simulations for two small ($< 500 \text{ km}^2$) and hydrologically different catchments in Central Italy. The satellite soil moisture retrievals that we assimilated were a downscaled version of SMAP with a 9 km spatial resolution, a fused ASCAT-Sentinel-1 product named SCATSAR and the ASCAT H113 product released within the H SAF project.

The satellite retrievals were ingested into the SWAT first layer by using the EnKF. The error attributed to the three products were calculated via Triple Collocation. Different configurations were tested in order to test if 1) the data assimilation was able to improve discharge simulations considering also the different catchment hydrology and land use, 2) which was the best performing product considering the higher spatial resolution obtained either with Sentinel-1 for ASCAT downscaling or via the optimal interpolation of brightness temperatures as in SMAP 9 km and 3) the effect of amount of data available to be ingested which is function of the temporal resolution of the products (SMAP data were much less than ASCAT and SCATSAR observations given its less frequent revisit time).

SWAT hydrological simulations were relatively good during the calibration of the model whereas during validation a general reduction of the performance was observed. One main reason for this reduction, especially in terms of NSE was caused by the drier validation period with the respect to the calibration. The ingestion of the three products was generally successful. This confirms that in this area satellite soil moisture observations are characterized by relatively good quality (Brocca et al., 2012, Massari et al., 2015) and are generally able to improve discharge simulations. Temporally, higher improvements were observed during the winter-spring period where floods in the area normally occur (see Fig. 5). Similar results were obtained in Massari et al. (2015) where higher soil moisture variability was strictly related to the improvement of flood simulations.

In terms of the ability to improve the low flow components of the simulations, we found a relatively good behavior of both the active and the passive products especially for Chiascio where this component is significant whereas for Niccone, the lack of data and the small baseflow contribution, made the benefit of the data assimilation not clear or less effective. The ability of improving medium to low flow by data assimilation of soil moisture were also found by Alvarez-Garreton et al. (2015) and Massari et al. (2018).

In general, overall better skills of the active products were found in the Chiascio river basin, which is characterized by a lower forest coverage (50%). Conversely, for Niccone (70% forest cover), SMAP outperformed both ASCAT and SCATSAR. One possible reason for this could be the better performance of the passive product over more vegetated areas which is also confirmed by the lower observation error (see Table 3). However, this needs further investigation as this conclusion must be supported by a relatively larger sample of catchments. For both catchments we did not find strong differences in terms of data assimilation for SCATSAR over ASCAT although we must say that these are considered as

very challenging areas for S1 (see Bauer-Marschallinger et al. 2018a). This was confirmed by the higher error of SCATSAR over vegetated and hilly terrain, which reduced the overall contribution of the state correction over these areas.

With the aim of exploring the benefit of having more frequent satellite soil moisture observations, we reduced the temporal resolution of the ASCAT product to the one of SMAP by a simple downsampling via the nearest neighbor approach. We obtained a significant reduction of the performance of ASCAT suggesting that the temporal resolution of the product especially for small catchments has a non-negligible role for a proper representation of the catchment wetness conditions before flood events, likely more important than the one played by the spatial resolution.

Regarding our methodology, two important aspects must be highlighted. The first, is the model error estimation. In this study, we followed a procedure similar to the one of Han et al. (2012a,b) who used a scheme with the perturbation of only states. This choice resulted in a simplification of the model error estimation and in an easier satisfaction of two well-known ensemble verification criteria used also in De Lannoy et al. (2006) and many following studies. However, other perturbation schemes and model uncertainty evaluations could be explored to see if better absolute scores could be obtained in terms of data assimilation. In this respect, we found – on average – relatively good results in terms of ability to improve open loop run performance, but it must be noted that these improvements were not always present and systematic in time especially over the different flood peaks. In this respect, we believe that a more optimal model error estimation would lead to even better results but at the cost of a higher complexity. In any case, further investigations are required to assess the impacts of this issue in satellite soil moisture data assimilation.

A second aspect, which is strictly linked to the one before is the TC application to the complete observation period, which resulted in the bulk estimation of rescaling parameters and observation errors. This is a limitation, as a more correct approach should consider the variation of the observation errors in time (Su and Ryu, 2015). Potential effects of this way to proceed is the over- and undercorrection of model states and thus a sub optimal data assimilation. Despite some studies have tried to solve this issue (Alvarez-Garreton et al., 2015, Chen et al., 2014) further investigation is still required.

In addition, it has to be mentioned that despite our results are case specific and depend on many variables like catchment characteristics, experimental set up, meteorological network, they provide further evidence of the value of satellite soil moisture in flood forecasting and address the need of additional research in the topic especially with new products like those tested in this study.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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Fig. 1.

Study area with the location of the basins and the hydrometeorological network (a), the identification of the soil type and the grid size of the soil moisture products used (Chiascio, Panel b and Niccone, Panel d) and the land cover information (Chiascio, Panel c and Niccone, Panel e). In panels b and d, it can be seen the relatively coarse spatial sampling of ASCAT and SMAP (12.5 and 9 km, respectively) with respect to the catchment size. Conversely, SCATSAR-SWI with its 1 km spatial sampling (thanks to the contribution of the Sentinel 1 information) is theoretically able to provide the variability of soil moisture within the basins.

Fig. 2.
Data assimilation scheme used in the study. (A) Open loop run, (B) data assimilation run.

Fig. 3.

(a) Simulated discharge by SWAT model during calibration period - Chiascio (b) Scatter plot of observed and simulated discharge during calibration period – Chiascio (c) Simulated discharge by SWAT model during calibration period- Niccone (d) Scatter plot of observed and simulated discharge during calibration period – Niccone.

Fig. 4.

The SCATSAR observation error values and mean elevation of each sub-basin for (a) Niccone and (b) Chiascio basins. The increase of the SCATSAR error for sub-catchments characterized by higher elevations confirm the effect of S1 in complex and vegetated terrain.

Fig. 5.

Comparison among the monthly mean RMSE values obtained during 2014–2017 for the SWAT runs with data assimilation of soil moisture derived from ASCAT, SCATSAR and SMAP (ASCAT-SWAT, SCATSAR-SWAT, SMAP-SWAT) products, respectively and the open loop run (OL). (a) refers to Chiascio whereas (b) refers to Niccone.

Fig. 6.

Comparison of the performance in terms of adapted Nash-Sutcliffe for low flows (NSE(logQ)) for Niccone and Chiascio during validation period (2014–2017). SWAT_{ASCAT}, SWAT_{SCATSAR}, SWAT_{SMAP} refer here to the runs of SWAT with data assimilation of soil moisture derived from ASCAT, SCATSAR and SMAP, respectively.

Fig. 7.

Simulated daily discharge time series at the outlet of Chiascio (a) and Niccone (b) basins obtained by assimilating different satellite observations derived from ASCAT ($SWAT_{ASCAT}$), SMAP ($SWAT_{SMAP}$) and SCATSAR ($SWAT_{SCATSAR}$). The runs are compared against the SWAT open loop run (OL) in the legend. Period 31 Mar 2015–31 Dec 2016. The dotted lines show the period where observed data are not available.

Fig. 8. improvements in terms of Nash-Sutcliffe index (NSE) and root mean square error (RMSE) of the runs obtained by assimilating different satellite observations derived from ASCAT (SWAT_{ASCAT}), SMAP (SWAT_{SMAP}) and SCATSAR (SWAT_{SCATSAR}) with respect to the SWAT open loop for Chiascio (a) and Niccone (b).

(a)

(b)

Fig. 9. Improvement in terms for Nash-Sutcliffe index (Δ_{NSE}) and root mean square error (Δ_{RMSE}) with downsampled ASCAT at the resolution of SMAP with respect to OL for Chiascio (a) and Niccone (b).

Table 1

Availability of SMAP, ASCAT and SCATSAR soil moisture products and number of observations potentially ingestible for each product during the different study periods.

	2014			2015		2016		2017		Number of available data	
Sensors	Jan. - Sep.	Oct. - Dec	Jan. - Feb.	Mar.- Dec.	Jan.- Dec.	Jan.- Sep.	Oct.- Dec.	Jan 2014-Dec2017	Mar 2015-Dec 2016		
SMAP								582	376		
ASCAT								1096	642		
SCATSAR								1097	642		

Table 2

Details of the calibrated SWAT parameters for Chiascio and Niccone basins.

No.	Parameter	Basins		Parameter Description
		Niccone	Chiascio	
1	r_CN2	-0.09	-0.12	SCS runoff curve number relative factor
2	v_ALPHA_BF	1.07	1.06	Baseflow alpha factor (days)
3	v_GW_DELAY	2.36	111.790	Groundwater delay (days)
4	v_GWQMN	1258.30	1154.54	Threshold depth of water in the shallow aquifer required for return flow to occur (mm)
5	v_ESCO	0.94	0.01	Soil evaporation compensation factor
6	v_SOL_AWC()	0.77	0.62	Available water capacity of the soil layer (mm H ₂ O/mm soil)
7	v_SOL_K()	108.15	334.12	Saturated hydraulic conductivity (mm/hr)
8	v_GW_REVAP	0.04	0.18	Groundwater "revap" coefficient
9	v_CH_K	325.57	486.67	Effective hydraulic conductivity in main channel alluvium (mm/hr)
10	v_SURLAG	17.24	5.27	Surface runoff lag time coefficient
11	v_REVAPMN	308.73	301.89	Threshold depth of water in the shallow aquifer for "revap" to occur (mm H ₂ O)
12	v_EPCO	0.31	0.05	Plant uptake compensation factor
13	v_SLSUBBSN	164.22	83.85	Average slope length (m)
14	v_RCHRG_DP	0.02	0.53	Deep aquifer percolation fraction

r: using relative method for parameterizing.

v: using replace method for parameterizing.

Table 3

Observation error obtained by Triple Collocation for ASCAT, SMAP and SCATSAR averaged over the sub-basins. Brackets refer to the projection of this error into SMAP observation space.

Basin	Sensors		
	ASCAT	SMAP	SCATSAR
Niccone	0.48 mm (0.0235 m ³ /m ³)	0.40 mm (0.0199 m ³ /m ³)	0.64 mm (0.0389 m ³ /m ³)
Chiasco	0.16 mm (0.0112 m ³ /m ³)	0.195 mm (0.0197 m ³ /m ³)	0.22 mm (0.0321 m ³ /m ³)

Table 4

Results of deterministic and open loop SWAT runs and the data assimilation experiment A for Chiascio and Niccone basins during validation period 2014–2017. NSE and RMSE represent the Nash-Sutcliffe and the root mean square error between observed and simulated discharges.

Basin	Product	NSE	RMSE
Chiascio	SCATSAR	0.37	4.038
	ASCAT	0.41	3.910
	SMAP	0.36	4.041
	Open loop	0.31	4.210
	Deterministic SWAT	0.30	4.220
Niccone	SCATSAR	0.40	1.460
	ASCAT	0.42	1.420
	SMAP	0.39	1.480
	Open loop	0.37	1.510
	Deterministic SWAT	0.38	1.490