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# A dynamic approach for evaluating coarse scale satellite soil moisture products

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## Abstract

Validating coarse scale remote sensing soil moisture products requires a comparison of gridded data to point-like ground measurements. The necessary aggregation of in situ measurements to the footprint scale of a satellite sensor ( $>100\text{ km}^2$ ) introduces uncertainties in the validation of the satellite soil moisture product. Observed differences between the satellite product and in situ data are therefore partly attributable to these aggregation uncertainties. The present paper investigates different approaches to disentangle the error of the satellite product from the uncertainties associated to the up-scaling of the reference data. A novel approach is proposed, which allows for the quantification of the remote sensing soil moisture error using a temporally adaptive technique. It is shown that the point-to-area sampling error can be estimated within  $0.0084\text{ [m}^3/\text{m}^3\text{]}$ .

## 1 Introduction

There is ample evidence that atmospheric and climate processes are significantly conditioned by the availability of water in the soils (Fast and McCorcle, 1991; Clark and Arritt, 1995; Koster et al., 2004). Soil moisture is an essential climate variable that has importance for the interactions between the land surface and atmosphere. It is thus an essential variable in climate research and numerical weather forecast as well as land surface hydrology. Satellite remote sensing has been demonstrated to provide useful information on soil moisture dynamics at various temporal and spatial scales (Zribi and Dechambre, 2002; Bindlish and Barros, 2000; Wigneron et al., 2004, 2003; Loew et al., 2006; Schwank et al., 2005; Owe et al., 2008). Two dedicated satellite soil moisture missions have been designed to provide global information on soil moisture dynamics. The European Soil Moisture and Ocean Salinity mission (SMOS) (Kerr et al., 2001) was launched in November 2009 and is the first dedicated soil moisture mission ever built. The NASA Soil Moisture Active Passive mission (SMAP) (NRC, 2007) is planned

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to be launched in 2014. These satellite missions will provide information on soil moisture dynamics at global scale and with coarse spatial resolution ( $\gg 100 \text{ km}^2$ ). A critical aspect of the missions success is the validation of their soil moisture products to verify if they meet pre-defined accuracy requirements. This validation exercise is complicated by the scale mismatch between the satellite footprint and local in situ measurements of soil moisture which serve as a reference.

A large number of continuous soil moisture measurements would be needed to determine the soil moisture dynamics at the footprint scale (Yoo, 2002; Brocca et al., 2007; Famiglietti et al., 2008) with an accuracy better than  $0.04 \text{ [m}^3/\text{m}^3]$ , which is the typical accuracy requirement for satellite soil moisture missions (Walker and Houser, 2004). Characteristic soil moisture patterns develop that remain stable at different temporal and spatial scales (Vachaud et al., 1985; Vinnikov et al., 1996). The analysis of temporally stable soil moisture patterns has been used for the development of concepts for the upscaling of local soil moisture measurements to larger scales that could be used for the validation of satellite soil moisture products (Cosh et al., 2004, 2006). A different concept for the evaluation of the error of satellite soil moisture products has been investigated by Miralles and Crow (2010). They applied the so called triple collocation (TC) method to quantify the uncertainty of soil moisture data sets using data from three independent sources. They showed that this technique provides a useful alternative to address the satellite soil moisture validation problem and that it is possible to quantify the soil moisture error with an accuracy of  $0.0064 \text{ [m}^3/\text{m}^3]$  for their test site.

The objective of the present paper is to contrast the potential of these different techniques for the validation of coarse scale soil moisture products. The potential synergies of combining in situ soil moisture information with distributed land surface modeling for the validation of satellite products is evaluated. A temporally dynamic validation approach is proposed which applies the TC method for monthly temporal slices and provides a framework for the quantification of the uncertainties of a satellite based soil moisture product. The novelty of the approach is that it provides uncertainty estimates of soil moisture products at rather short timescales and is able to identify periods where

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either the satellite measurements or the in situ measurements don't provide reliable information on the large scale soil moisture dynamics. The method is verified on a core soil moisture validation site situated in Southern Germany using AMSR-E soil moisture products.

## 2 Methodology

A key question for the validation of remote sensing soil moisture data products is an appropriate accuracy assessment of the data products. Typically, the root mean square difference (RMSD) is used to predefine the accuracy requirements of a satellite soil moisture product (Walker and Houser, 2004; Kerr, 2007). It is defined as

$$\text{RMSD} = \sqrt{\langle (x - y)^2 \rangle} \tag{1}$$

whereas  $x$  and  $y$  correspond to vectors of collocated satellite and in-situ observations respectively. Angled brackets indicate ensemble averaging. The user requirement for global satellite soil moisture products is currently defined with  $\text{RMSD} \leq 0.04 \text{ [m}^3/\text{m}^3\text{]}$  (Walker and Houser, 2004; Kerr et al., 2001). However as by its definition, the RMSD is very sensitive to a bias between in situ reference data and the satellite product. Even if a product would perfectly reproduce the relative temporal soil moisture dynamics it would show a large RMSD if the estimates or used reference data are biased. Biases in remote sensing based soil moisture estimates might result from a variety of sources, like e.g. imperfect characterization of the land surface in the retrieval scheme of variable sensitivity of the observation system to soil moisture dynamics (van de Griend et al., 2003; Loew, 2008).

On the other hand, regular in situ soil moisture measurements are typically based on a relative small number of samples compared to the footprint scale of a satellite sensor. The monitoring of soil moisture dynamics using a very high number of observations is limited to dedicated campaigns (Famiglietti et al., 2008). Existing regular soil moisture

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networks like the Oklahoma Mesonet network ([www.mesonet.org](http://www.mesonet.org)) (Brock et al., 1995), the REMEDHUS network in Spain (Ceballos et al., 2002) or the SMOSHYD validation site (Loew et al., 2009a) provide in situ data from only a few stations  $\ll 10$  for an area corresponding to the footprint of dedicated soil moisture missions like SMOS.

Ground based soil moisture measurements are very local as soil moisture probes used for regular measurements are typically only representative for very small volumes in the order of  $10^{-4} \text{ m}^3$  (for a comparison of different measurement techniques see Walker et al., 2004). Currently, no global in situ soil moisture monitoring network exists. First efforts to collect reference data of in situ soil moisture was made by Robock et al. (2000). More recently, a research community driven in situ soil moisture network bank has been initiated to collect and distribute harmonized and quality proofed in situ soil moisture data (<http://www.ipf.tuwien.ac.at/insitu/>)

As the spatial variability in the footprint of a satellite sensor can be large, the mismatch between in situ measurements and the satellite footprint scale results in large uncertainties for the validation of satellite soil moisture products.

An appropriate validation approach therefore needs to take into account the inherent uncertainties that are associated with the upscaling of local scale soil moisture measurements to a larger scale. Two different approaches will be introduced in the following and their potential will be investigated in the further analysis of the paper.

## 2.1 Temporal stable soil moisture patterns

The concept of temporal stability was introduced by Vachaud et al. (1985) as a mean to represent large scale soil moisture dynamics using a measurement network of a few sites only. The fundamental assumption of the method is that characteristic soil moisture patterns persist, which can be used to develop time-invariant relationships between local ( $\theta$ ) and large scale ( $\bar{\theta}$ ) soil moisture dynamics in the spatial domain  $R$

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with an area  $A$  which is given by

$$\bar{\theta}_j = A^{-1} \int_R \theta_j dr \approx \frac{1}{N} \sum_{i=1}^N \theta_{ij} + \epsilon \quad (2)$$

and can be approximated by a discrete number of  $N$  measurements. The index  $i$  specifies the in situ measurements at point  $P$  with coordinates  $(x, y)$  and  $\epsilon$  is the error of Eq. (2) due to the discrete approximation. The number of required measurements to obtain a specific accuracy might vary, depending on the heterogeneity of the study area. Brocca et al. (2007) used a statistical approach to infer the number of required samples for different spatial scales and concluded that 15 to 35 measurement sites are needed to estimate  $\bar{\theta}$  with an absolute error of  $0.02 [\text{m}^3/\text{m}^3]$  for a study area with a size of  $10.000 \text{ m}^2$ . As the variability of soil moisture is also dependent on the soil moisture dynamic itself, the number of required samples might vary as a function of  $\bar{\theta}$  (Vereecken et al., 2007). Famiglietti et al. (2008) provide an analysis of a large number of soil moisture measurements from different campaigns and at various scales. They conclude that the number of measurements required to estimate  $\bar{\theta}$  with an accuracy better than  $0.04 [\text{m}^3/\text{m}^3]$  (95% confidence level) is larger than  $N = 20$  for a scale of 50 km with decreasing sample numbers for very dry or wet conditions.

A point  $i$  is considered to be temporally stable if its soil moisture dynamics is in good agreement with the spatial average. The relative soil moisture difference at time  $j$  is given as

$$\delta_{ij} = \frac{\theta_{ij} - \bar{\theta}_j}{\bar{\theta}_j} \quad (3)$$

The expected value of  $\bar{\delta}_i$  and its standard deviation is then obtained from  $M$  times as

$$\bar{\delta}_i = \frac{1}{M} \sum_{j=1}^M \delta_{ij} \quad (4)$$

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$$\sigma(\delta_i) = \sqrt{\frac{1}{M-1} \sum_{j=1}^M (\delta_{ij} - \bar{\delta}_i)^2} \quad (5)$$

A point which is representative for the large scale soil moisture dynamics therefore corresponds to small values of  $|\bar{\delta}_i|$  and  $\sigma(\delta_i)$ . If stable relationships between the local and large scale soil moisture dynamics exist, these can be used for the upscaling of local measurements to the larger scale (Brocca et al., 2010).

Spatially persistent soil moisture patterns have been analyzed using ground measurements (Vachaud et al., 1985; Grayson and Western, 1998; Cosh et al., 2004; Martinez-Fernandez and Ceballos, 2005; Teuling et al., 2006), models (Loew and Mauser, 2008) or remote sensing observations (Wagner et al., 2008). Techniques to disaggregate coarse scale remote sensing observations using prior knowledge of persistent soil moisture fields have been developed (Loew and Mauser, 2008; Wagner et al., 2008).

The temporal stability approach assumes that a specific location can be found where the relationship between local and large scale soil moisture dynamics is time-invariant. It will be evaluated in Sect. 4 if this assumption is applicable for the data used in the present study and contrasted against the triple collocation approach introduced next.

## 2.2 Triple collocation method

The triple collocation (TC) method was originally developed to estimate the errors of sea wind and wave height estimates derived from buoy, model and satellite data (Stofelen, 1998; Caires and Sterl, 2003). It estimates the uncertainties of observations of a geophysical quantity using time series of three independent data sets.

Scipal et al. (2009) was the first to apply the TC method to quantify uncertainties of surface soil moisture data, using data from two different remote sensing soil moisture products and ERA-40 reanalysis data. The method was then used for validation of remote sensing surface soil moisture observations using sparse in situ networks by Miralles and Crow (2010).

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The implementation of the TC method in the present study follows the analytical solution provided by Caires and Sterl (2003). The method and used notation is briefly introduced in the following.

It is assumed that three temporally collocated time series of  $n$  observations ( $x_i, y_i, z_i, i = 1 \dots n$ ) of an arbitrary physical quantity  $T_i, i = 1 \dots n$  exist. Their respective random errors ( $e_x, e_y, e_z$ ) are assumed to have zero mean. The true measurements ( $X, Y, Z$ ) of  $T$ , corresponding to the observations ( $x_i, y_i, z_i$ ) are related to  $T$  as

$$\begin{aligned} x &= X + e_x = \alpha_0 + \beta_0 T + e_x \\ y &= Y + e_y = \alpha_1 + \beta_1 T + e_y \\ z &= Z + e_z = \alpha_2 + \beta_2 T + e_z \end{aligned} \quad (6)$$

where the subscripts have been dropped for easier notation. Removing the mean from each of the variables and denoting the anomalies as  $x^*, y^*, z^*, T^*$ , their relationship is given by

$$\begin{aligned} x^* &= \alpha_0 + \beta_0 T^* + e_x \\ y^* &= \alpha_1 + \beta_1 T^* + e_y \\ z^* &= \alpha_2 + \beta_2 T^* + e_z \end{aligned} \quad (7)$$

If we assume that the errors of the data sets are uncorrelated,  $\langle e_x e_y \rangle = \langle e_x e_z \rangle = \langle e_y e_z \rangle = 0$ , and independent of  $T$ ,  $\langle T e_x \rangle = \langle T e_y \rangle = \langle T e_z \rangle = 0$ , we can remove the unknown deterministic variable  $T^*$  using a simple elimination procedure (see for details, Caires and Sterl, 2003) and obtain

$$\begin{aligned} \beta_1 &= \beta_0 \langle y^* z^* \rangle / \langle x^* z^* \rangle \\ \beta_2 &= \beta_0 \langle y^* z^* \rangle / \langle x^* y^* \rangle \end{aligned} \quad (8)$$

where angled brackets  $\langle \cdot \rangle$  denote ensemble averaging. The variances of the observation errors are then obtained as



$$\begin{aligned}
\text{var}(e_x) &= \langle e_x^2 \rangle = \langle (x^*)^2 \rangle - \langle x^* y^* \rangle \langle x^* z^* \rangle / \langle y^* z^* \rangle \\
&= \langle (x^*)^2 - \langle x^* y^* \rangle \frac{\beta_0}{\beta_1} \rangle \\
\text{var}(e_y) &= \langle e_y^2 \rangle = \langle (y^*)^2 \rangle - \langle x^* y^* \rangle \langle y^* z^* \rangle / \langle x^* z^* \rangle \\
&= \langle (y^*)^2 - \langle x^* y^* \rangle \frac{\beta_1}{\beta_0} \rangle \\
\text{var}(e_z) &= \langle e_z^2 \rangle = \langle (z^*)^2 \rangle - \langle x^* z^* \rangle \langle y^* z^* \rangle / \langle x^* y^* \rangle \\
&= \langle (z^*)^2 - \langle y^* z^* \rangle \frac{\beta_0}{\beta_1} \rangle
\end{aligned}
\tag{9}$$

Finally the coefficients  $\alpha_1$  and  $\alpha_2$  are estimated as

$$\begin{aligned}
\alpha_1 &= \langle y \rangle - \beta_1 (\langle x \rangle - \alpha_0) \\
\alpha_2 &= \langle z \rangle - \beta_2 (\langle x \rangle - \alpha_0)
\end{aligned}
\tag{10}$$

Note, that only four of the six coefficients can be derived using  $x, y, z$ . Defining one observation (e.g.  $x$ ) as a reference,  $\alpha_1, \alpha_2, \beta_1$  and  $\beta_2$  can be estimated. Typically it is assumed that the reference is a bias free estimator of the deterministic variable (Scipal et al., 2009; Caires and Sterl, 2003), thus  $\alpha_0 = 0$  and  $\beta_0 = 1$ . However, in a strict sense, this assumption might not be valid. In fact, it will be shown that the ground stations in the present study are not a bias free estimator of the large scale soil moisture content.

Further, modeled soil moisture as well as satellite retrievals typically exhibit their own characteristics and are therefore typically rescaled before any inter-comparison (Reichle et al., 2004; Albergel et al., 2010). In that sense, the estimation of  $\alpha$  and  $\beta$  parameters corresponds to a similar rescaling of the original data sets. However, the estimation of the errors is independent of the chosen model parameters as can be seen from Eq. (9).

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### 3 Study area and data

Three different soil moisture data sets are used in the present study. These are based on ground observations, land surface model simulations and remote sensing soil moisture estimates. The datasets and their characteristics are described after a brief introduction to the study area.

#### 3.1 Study area

The study area is located in the Upper Danube catchment area which is situated in Southern Germany (Fig. 1). A remote sensing soil moisture validation site has been established in a small sub-catchment (Vils), situated in the Northeast of the city of Munich (Loew et al., 2009a). The site is most suitable for validation of coarse resolution microwave remote sensing data as the microwave signal is not affected by open water bodies or large urban areas which might have a considerable effect on the microwave signal (Loew, 2008).

To perform a cross comparison between the different data sets, these are reprojected to a common, equal area grid. The Icosahedral Snyder Equal Area projection (ISEA4H9) is used as the reference projection (Sahr et al., 2003) which has a grid spacing of 12.5 km. The same grid is used as a reference grid for the Soil Moisture and Ocean Salinity Mission (SMOS). Each grid node has a unique identifier which will be used in the following to identify ground stations, model grid cells and satellite footprints.

#### 3.2 Soil moisture data

##### 3.2.1 Soil moisture measurements

Half-hourly measurements of soil moisture profiles are available since mid of 2007 from five stations in the test site. Soil moisture measurements are made using Time-Domain-Reflectometry (TDR) probes at depth of 5, 10, 20 and 40 cm. Surface soil

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moisture at 5 cm is measured by two different probes independently. The stations cover an area of approximately  $40 \times 40 \text{ km}^2$ .

### 3.2.2 Land surface model

The PROMET land surface model is used in the present study to simulate the surface energy and water fluxes (Mauser and Schaedlich, 1998) on an hourly basis. The model consists of a kernel model which is based on five sub-modules (radiation balance, soil model, vegetation model, aerodynamic model, snow model) to simulate the actual water and energy fluxes and a spatial data modeler, which provides and organizes the spatial input data on the field-, micro and macro-scale. Soil moisture dynamic is simulated using a modified version of the Richards equation for flow in unsaturated media (Philip, 1957). The soil water retention model of Brooks and Corey (1964) is used to relate soil moisture content to soil suction head. A detailed description of the model is given by Mauser and Bach (2009). The soil water model has been validated in different test sites using in-situ soil moisture measurements of soil moisture profiles (Pauwels et al., 2008).

PROMET model simulations are made on  $1 \text{ km}^2$  grid. The meteorological forcing is obtained from a dense network of stations which are collocated with the in situ soil moisture network. Model simulations at  $1 \text{ km}^2$  scale are made from 1st of November 2007 until end of 2009. The high resolution model simulations are then aggregated to estimate the expected large scale soil moisture dynamics at the footprint scale of a satellite sensor (see Fig. 1).

### 3.2.3 Satellite soil moisture

Remote sensing soil moisture data are obtained from a globally available data set based on the Advance Microwave Scanning Radiometer (AMSR-E), provided by the VU University Amsterdam together with NASA Goddard Space Flight Centre (Owe et al., 2008). AMSR-E is a passive microwave scanning radiometer, operating at six

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different wavelengths within the microwave spectrum (6.925, 10.65, 18.7, 23.8, 36.5, and 89 GHz). The large area coverage (swath width: 1445 km) of the sensor allows for a frequent coverage of the globe in the order of three days with increasing frequencies at higher latitudes. The spatial resolution of the different channels is varying from 5 km (89 GHz) to 56 km (6.925 GHz) (Njoku et al., 2003).

Soil moisture retrievals are based on the solution of a microwave radiative transfer model which solves simultaneously for the surface soil moisture content and vegetation optical depth without a priori information (Meesters et al., 2005). The flexible approach allows in general for the retrieval of soil moisture from a variety of frequencies. The C-band (6.925 GHz) data product is used in the present study as it is expected to have the highest sensitivity to surface soil moisture dynamics from the AMSR-E channels. The data set is available since 2002. The data product has been validated over a large range of study areas with high correlations with in situ observations in semi arid regions ( $r = 0.79$ ,  $RMSE = 0.03 \text{ [m}^3/\text{m}^3]$  for the Murrumbidgee Soil Moisture Monitoring Network in Australia, Draper et al., 2007;  $r = 0.83$ ,  $RMSE = 0.06 \text{ [m}^3/\text{m}^3]$  for the REMEDHUS soil moisture network in Spain, Wagner et al., 2007) and somewhat lower in agricultural areas ( $r = 0.78$ ,  $RMSE = 0.06 \text{ [m}^3/\text{m}^3]$  for the SMOS REX site in France, Rüdiger et al., 2009).

Only data from the daytime ascending overpass (01:30 p.m.) are used as these were found to be less noisy than the nighttime observations (Loew et al., 2009b). As the sensitivity of the AMSR-E observations to soil moisture decreases with increasing optical depth of the vegetation layer, only data with an optical depth  $\tau < 0.8$  are used for the further analysis. A single AMSR-E time series, located in the center of the test site (ISEA ID #2027099) is used in the study.

## 4 Soil moisture variability and stability

The variability of the in situ soil moisture data is analyzed in the following. The investigations are limited to the period from 01/05 to 30/10 of the years 2008 and 2009

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to cover a large variability in soil moisture and vegetation conditions, while avoiding interference by snow and frozen soil conditions.

#### 4.1 Soil moisture variability

The average soil moisture  $\bar{\theta}$  for the investigated area is calculated from the station data. As the number of stations ( $N = 5$ ) is rather small to sufficiently represent  $\bar{\theta}$  this will introduce an uncertainty in the estimation of  $\bar{\theta}$  (Famiglietti et al., 2008; Brocca et al., 2010). Figure 2 shows time series of  $\bar{\theta}$  and its standard deviation for the years 2008 and 2009. Both soil moisture curves show a dynamical range between 0.2 [m<sup>3</sup>/m<sup>3</sup>] and 0.4 [m<sup>3</sup>/m<sup>3</sup>]. The standard deviation varies between 0.025 and 0.1 [m<sup>3</sup>/m<sup>3</sup>].

#### 4.2 Temporal stability analysis

A temporal stability analysis (Sect. 2.1), is conducted for each of the stations, using  $\bar{\theta}$  as the reference. For each station and year, the statistic for  $\bar{\delta}$  is calculated using Eq. (4) and Eq. (5). Results are summarized for each station and year in Fig. 3. Considerable differences are observed between the years. The station Steinbeissen (Neusling) does best represent the large scale soil moisture dynamics in 2008 (2009) according to the  $\bar{\delta}$  metric.

The linear relationship between  $\theta_j$  and  $\bar{\theta}$  was estimated using a least square approach with  $\bar{\theta}$  as the dependent variable. The regression coefficients are given in Table 2. By removing this linear trend, we obtain the random upscaling error for each station ( $e_{\text{station}}$ ). Considerable differences are observed between the two years. The different stations do not show a consistent relationship to the large scale soil moisture dynamics. While all stations show significant correlations with the large area soil moisture dynamics over a certain time period, they might not be used to predict the spatial mean soil moisture dynamics consistently over a longer time period. The reason for these differences are small scale differences in precipitation dynamics, which are mostly related to convective events that are local.

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However at smaller timescales, a single station might be a good predictor for the large scale soil moisture dynamics. We will therefore investigate the potential of using a temporally dynamic approach to assess the soil moisture validation problem using the triple collocation technique. First, the triple collocation will be applied on an annual basis to provide comparable results with the analysis in the present section. We will then relax the method by applying it on shorter timescales to adapt it to temporally stable soil moisture patterns at shorter timescales.

## 5 Triple collocation analysis

### 5.1 Data preparation

The triple collocation method requires all data sets to be temporally collocated. They are therefore binned to daily values and spatially collocated on the ISEA grid. Satellite data which were recorded during precipitation events were not considered for the inter-comparison, as the rainfall and interception in the canopy can deteriorate the microwave signal (Saleh et al., 2007). Data from different stations were used as a reference ( $x$ ) and compared against the spatially averaged soil moisture from PROMET ( $y$ ) and AMSR-E soil moisture data ( $z$ ). The different experiments for the various stations are summarized in Table 1. It is assumed that the model and satellite data are representative for the same spatial domain, while the ground measurements are expected to provide an uncertain proxy for  $\bar{\theta}$  over the same area. We aim to obtain a robust estimate for  $e_{\text{sat}}$  to quantify the accuracy of the satellite data.

The triple collocation analysis will be either made for the entire investigation period (01/05–30/10) or for a 30 day moving window from the beginning to the end of the investigation period with steps of 15 days. As the triple collocation relies on a significant correlation between the three different data sets we first calculate the correlation between each pair of  $x, y, z$ . In case of negative correlation, the data are not analyzed. Scipal et al. (2009) further screened the data by applying a threshold of 0.2

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to the obtained correlation coefficient which corresponds to a significant correlation at the 95% level for time series with a large number of samples. However, as we restrict our analysis to much shorter timescales, we explicitly calculate the significance ( $p_{xy}, p_{xz}, p_{yz}$ ) of the correlation between the variables according to a t-test (Press et al., 1992).

## 5.2 Analysis results

The TC analysis is made in two parts. First, results from a yearly analysis are presented (static approach) and then results from the TC analysis at shorter time scales (dynamic approach) are presented.

### 5.2.1 Static approach

The static approach exploits the full time series for the estimation of the error variances, which is similar to the approach of Scipal et al. (2009). The estimated errors for the model simulated and satellite soil moisture show consistent results for the different experiments (Table 3). The model errors ( $e_{\text{model}}$ ) range between 0.0176 and 0.0285 (0.0075 and 0.0238) [ $\text{m}^3/\text{m}^3$ ] for 2008 (2009). The AMSR-E soil moisture error  $e_{\text{sat}}$  ranges between 0.047 and 0.0659 [ $\text{m}^3/\text{m}^3$ ] which is in the same order than results obtained from previous studies (Draper et al., 2007; Wagner et al., 2007). The robust results for the satellite product error for different stations indicate that the selection of a particular station seems to have minor impact on the uncertainty estimates.

All stations show significant correlations between the in situ measurements and the model simulations as well as the satellite retrievals. Further it is observed that the correlation between the station and the satellite data is in general higher than the correlation between the model and the satellite data.

As the same model and satellite data are used for all simulations, differences in the error estimates result only from differences between the ground stations. Their representativity for the large scale soil moisture dynamics changes throughout the year as was shown previously.

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The estimated gains ( $\beta_1, \beta_2$ ) vary between 0.22 and 0.86 which would have been expected due to the lower spatially aggregated soil moisture variability at larger scales compared to local measurements. Different gains are observed for the same station in different years. A comparison of the estimated error for each station ( $e_{\text{stat}}$ ) with the actual estimate of the station error ( $e_{\text{station}}$ ) shows that they are in the range between 0.0248 and 0.0356 [m<sup>3</sup>/m<sup>3</sup>] for  $e_{\text{stations}}$  and 0.0097 and 0.0489 [m<sup>3</sup>/m<sup>3</sup>] for  $e_{\text{stat}}$  (Table 3).

Considerable differences are observed between the two years for the various stations. These results indicate that data from the different stations can not be used to upscale the local soil moisture measurements in a consistent way as their representativeness for the larger area is changing with time, which is consistent with the results of the temporal stability analysis. This indicates that temporally adaptive methods are needed for the inter-comparison of the in situ soil moisture data with the footprint scale soil moisture estimates. This is at least valid for the data used in the present analysis. We will therefore investigate in the following if a dynamic collocation approach, applied on shorter timescales, might be used as an alternative for the soil moisture validation problem.

## 5.2.2 Dynamic approach

A temporal window of  $dt = 30$  days is used for the dynamic triple analysis which reduces the number of collocated data points and thus the degree of freedom for the correlation between the data tuples. The results of all different 30-day intervals are summarized in Fig. 5 – Fig. 7. These show the temporal variability of  $r$ ,  $e$  and  $\beta$ . Data sets, where the correlation for at least one out of the three data tuples ( $xy$ ,  $xz$ ,  $yz$ ) was not significant at the 95% level are marked with gray bars. Dashed lines correspond to  $e$ ,  $r$ ,  $\beta$  as estimated from the static approach and are provided for comparison.

The estimated satellite product errors are in general lower for the dynamic approach than they are for the static TC analysis. The obtained values for  $e_{\text{sat}}$  are consistent between the different stations and show a similar temporal dynamic. This indicates

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that the choice of the reference station has a minor effect on the calculation of  $e_{\text{sat}}$  and that they provide a robust estimate of the uncertainty of the satellite data product.

In a large number of sample intervals non-significant correlations are found. In general, one can differentiate between time intervals where all stations show a non-significant correlation between at least one of the data tuples and those where a single station indicates a correlation at a low significance level. As an example, Fig. 8 shows details of the analyzed time series for the stations #17 (Lochheim) and #18 (Steinbeisen) for consecutive time periods in 2008.

All three data sets capture well the decrease of soil moisture until mid of May 2008 and the increase due to the precipitation between 16th and 19th of May 2008 (a). Highly significant correlations are found between all data tuples. Frequent precipitation in the first half of June results in a couple of data gaps for the satellite data due to the precipitation masking, decreasing especially the correlation between the satellite data and model results (b). The following time period is dominated by low soil moisture dynamics until end of June (c). The satellite data capture in general this low variability, but no significant correlations with neither the PROMET model simulations nor the in situ data are found for this period for both stations. The satellite soil moisture product has large noise compared to the small soil moisture signal. The satellite data capture the increase of soil moisture after 10th of July 2008 (d) for both stations although there are data gaps during this rain period. However, no significant correlations are found between the in situ data and the satellite product for station #18 ( $p = 0.74$ ), while significant correlations are found for station #17 (e). This station is the only one that shows no significant correlations during that time period (see also Fig. 7). In this case, the lack of a significant correlation is caused by a data gap in the in situ soil moisture data from 17th to 23th of June which has been identified by the TC method.

### 5.2.3 Effect of temporal sampling

The temporal window used for the dynamic TC analysis determines how many data points are used in the analysis and thus determines the degree of freedom for the

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correlation. The previous analysis with  $dt = 30$  days did show that an analysis on short time scales is feasible and helps to make an appropriate error assessment of the satellite data. The significance of the correlations between the time series has been shown to be a useful tool for the detection of gaps and artefact's in the time series.

However, large parts of the time series show no significant correlation at the 95% level in these cases.

On the other hand, the yearly analysis did show significant correlations for all data tuples as a larger time interval results in a higher degree of freedom for the correlation threshold. A further analysis using  $dt = 60$  [days] (not shown here) did show very consistent results for the satellite error as estimated from different stations. The estimated satellite error was smaller than the one obtained from the yearly analysis, but did show less temporal variability than the one obtained using  $dt = 30$  [days]. However, the low soil moisture variability in the mid of June 2008 does still affect this analysis and non-significant correlations are identified for all stations during that time period using  $dt = 60$  [days] which provides additional information on the lack of significant information on soil moisture dynamics in the remote sensing data.

#### 5.2.4 Accuracy of error assessment

To assess the reliability of these estimates, we compare  $e_{\text{sat}}$  against the reference error  $e_{\text{station}}$ . The latter is an approximation to the actual uncertainties in representing large scale soil moisture dynamics using a single station, as has been discussed previously. In case that the TC method provides good predictive skills for the actual error of a station it should also provide reliable estimates of the error of the satellite product.

Figure 9 shows the results of the error analysis for the two years. Each point corresponds to a single triple collocation result of a 30 day period and a single station. The different number of points per station and year results from the fact that only periods with significant correlations (95% confidence) between the data sets have been used. The root mean square difference (RMSD) between the estimated and reference error is 0.00841 (0.00835) [ $\text{m}^3/\text{m}^3$ ] in 2008 (2009). These results are very close to the results

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obtained by (Miralles and Crow, 2010) who found that the triple collocation methods could provide error estimates with an accuracy between 0.00694 [m<sup>3</sup>/m<sup>3</sup>] and 0.0150 [m<sup>3</sup>/m<sup>3</sup>] using data from different test sites. It is very encouraging that the obtained error estimates are close to those estimated from the in situ data only as well as to those obtained by (Miralles and Crow, 2010) who conducted their study in completely different test sites with different soil moisture dynamics.

## 6 Discussion and conclusions

The present study did investigate different approaches for the inter-comparison of coarse scale remote sensing soil moisture data with in situ reference information on soil moisture dynamics. The TC method was successfully applied to quantify the uncertainties of AMSR-E soil moisture data in the Upper Danube catchment. While temporary persistent soil moisture patterns could be identified in the test site, no single soil moisture station was found to provide a robust proxy for the large scale soil moisture dynamics within the test site.

Combining single location in situ data with land surface model simulations and remote sensing soil moisture estimates using the (static) TC method did provide consistent estimates of the error of the satellite soil moisture product. The rescaling of the soil moisture data in the TC analysis compensates for systematic differences between the various data sets. The spatially averaged long term AMSR-E soil moisture RMSE was estimated as 0.057 [m<sup>3</sup>/m<sup>3</sup>]. The such obtained satellite product uncertainties are very valuable to provide a general estimate of the quality of the data product from a user's point of view.

The analysis of satellite soil moisture products at shorter timescales provides additional quantitative information on the temporal dynamics of its error. The proposed (dynamic) TC method compensates for the lack of representativeness of a single soil moisture station by taking into account the temporal varying relationships between in situ and satellite soil moisture dynamics.

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Consistent satellite error estimates were obtained using data from different soil moisture stations as a reference. The such obtained errors were smaller than those estimated from the long term (static) TC approach which indicates that the satellite product can have a higher accuracy in specific periods than those estimated from the annual analysis. Significant correlations between the used soil moisture data sets were found at these shorter timescales as well. The significance of these correlations provides important additional information on the quality of the error estimates. It could be shown that increasing uncertainties of the satellite soil moisture product are reflected in a decrease of the significance of the correlation. Time periods with higher errors of the satellite data product could be clearly identified when the analysis from several stations did show non-significant correlations. In case that only a single station did show a non-significant correlation, we could show that this is an indicator for a reduced quality of the reference data. Thus, there is a strong need for using multiple in situ soil moisture stations for the validation of remote sensing satellite products in a test site as these provide complementary information for the evaluation of the TC results.

In practice, periods without significant soil moisture information could not be identified without appropriate reference soil moisture information. The obtained error estimates therefore represent a lower boundary of the possible range of soil moisture errors, while the annual TC method (static) provides the upper limit. The actual soil moisture error is therefore likely to range somewhere in between these two extremes.

The dynamic TC method thus provides additional information on the accuracy of the satellite data product as well as the reference soil moisture data which is in particular useful for improving the validation and further development of remote sensing soil moisture products. The accuracy of the calculated soil moisture errors for the used soil moisture stations was estimated as  $0.0084 \text{ [m}^3/\text{m}^3]$ .

The triple collocation method provides a useful framework for the quantification of errors of satellite soil moisture products. The proposed extension to shorter timescales makes it a useful tool for a more detailed quantitative analysis of satellite soil moisture time series and their validation. The method is in general applicable to time series of

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different satellites as well as different geophysical variables. A further evaluation of the method in other test sites as well as an extension of the method to SMOS soil moisture data products is foreseen.

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**Table 1.** List of soil moisture stations, IDs of closest ISEA grid point and assigned experiment number.

Station number	ISEA	Name	lat/lon [deg]	experiment
118	2026587	Engersdorf	48.45/12.63	16
74	2026585	Lochheim	48.27/12.49	17
16	2026588	Steinbeissen	48.61/12.73	18
14	2027101	Neusling	48.69/12.88	19
49	2027611	Frieding	48.34/12.83	20

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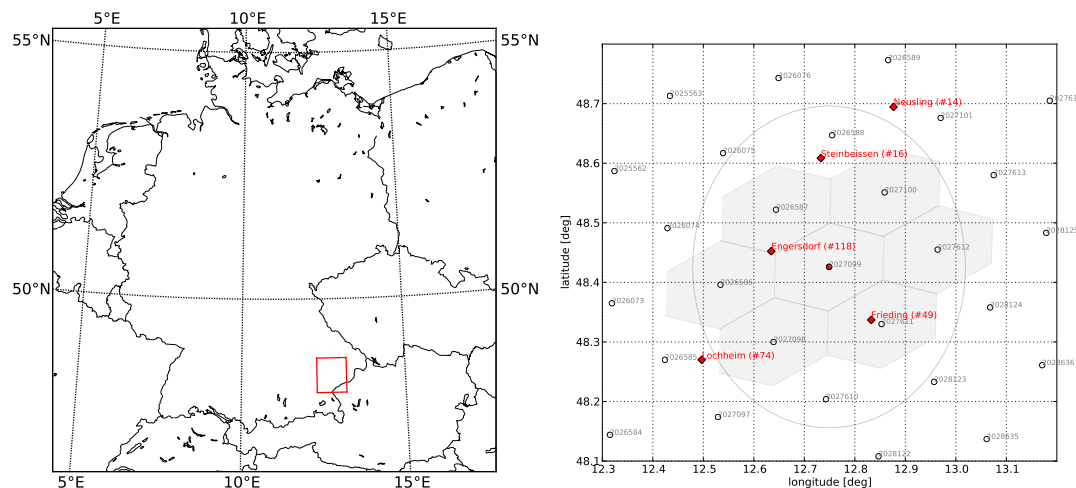


**Table 3.** Summary of soil moisture errors as estimated using triple collocation method for different stations: estimated errors  $e_{\text{sat}}$ ,  $e_{\text{model}}$ ,  $e_{\text{sat}}$ , correlation ( $r$ ), gains  $\beta$  and offsets  $\alpha$  of the relationships given by Eq. (6). Upscaling errors for the station used as variable  $x$  is shown for comparison ( $e_{\text{station}}$ ). Errors are given as  $[\text{m}^3/\text{m}^3] \times 100$ .

Year	Exp.	$e_{\text{station}}$	$e_{\text{stat}}$	$e_{\text{model}}$	$e_{\text{sat}}$	$r_{xy}$	$r_{xz}$	$r_{yz}$	$\beta_1$	$\alpha_1$	$\beta_2$	$\alpha_2$
2008	16	2.83	2.68	2.66	5.96	0.88	0.51	0.37	0.55	4.86	0.48	16.9
	17	3.23	4.49	2.85	5.80	0.85	0.53	0.35	0.34	11.6	0.32	22.0
	18	2.66	0.97	2.82	5.87	0.76	0.48	0.36	0.43	11.9	0.41	21.9
	19	3.23	1.19	2.49	5.92	0.78	0.42	0.36	0.95	−0.7	0.78	13.6
	20	3.56	4.89	1.76	5.44	0.74	0.46	0.51	0.55	9.29	0.53	21.4
2009	16	2.92	4.87	1.38	4.88	0.47	0.17	0.27	0.72	−2.7	0.51	11.7
	17	2.52	1.56	2.29	6.20	0.63	0.42	0.25	0.24	20.5	0.39	24.0
	18	2.48	2.00	2.17	5.63	0.68	0.64	0.32	0.39	12.5	0.94	−2.0
	19	2.80	2.06	2.38	4.70	0.60	0.43	0.18	0.36	16.1	0.48	19.1
	20	3.13	4.02	0.75	6.50	0.75	0.23	0.28	0.55	12.6	0.40	24.2

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**Fig. 1.** Location of test site (left) and details of used in situ stations and their mapping to the ISEA grid. The polygons correspond to ISEA grid cells used for the analysis of land surface model simulations. The circle corresponds to the AMSR-E like footprint size.

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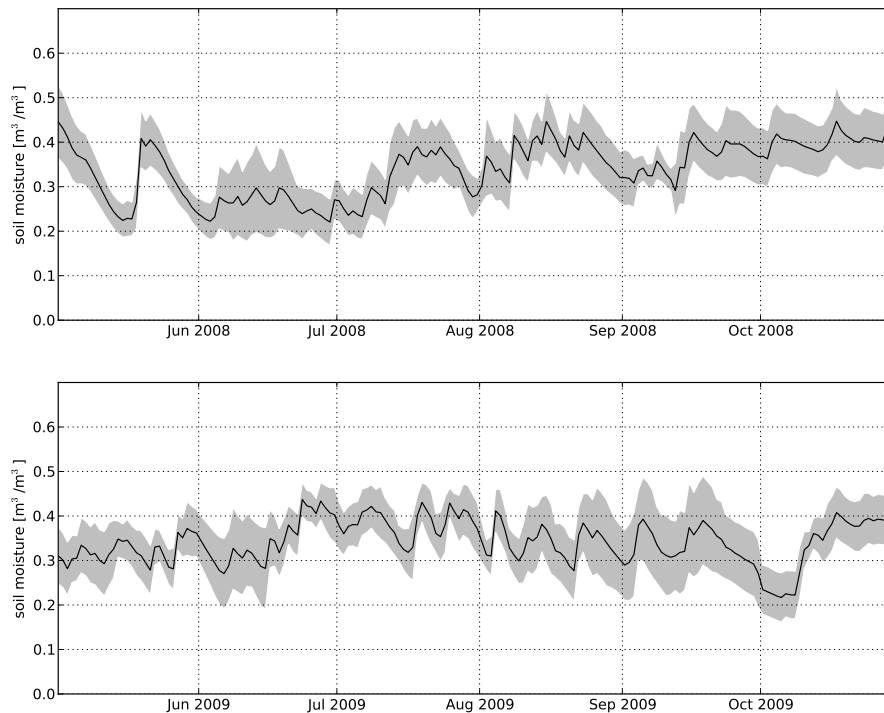
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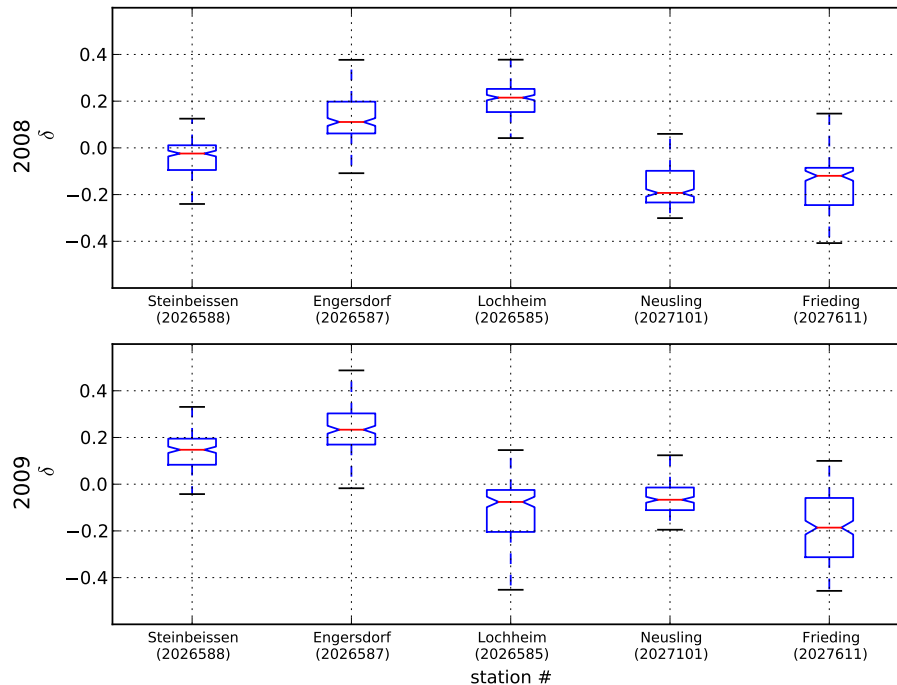
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**Fig. 2.** Temporal evolution of large scale mean soil moisture content  $\bar{\theta}$  as calculated from the average of all ground stations. Greyed area correspond to  $\pm 1\sigma_{\theta}$ .

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**Fig. 3.** Boxplot of the relative difference  $\bar{\delta}$  between soil moisture observations of a single station and the spatial mean  $\bar{\theta}$ . Boundaries of the boxes correspond to the 25% and 75% quartiles and the line indicates the median value. Whiskers indicate extreme values

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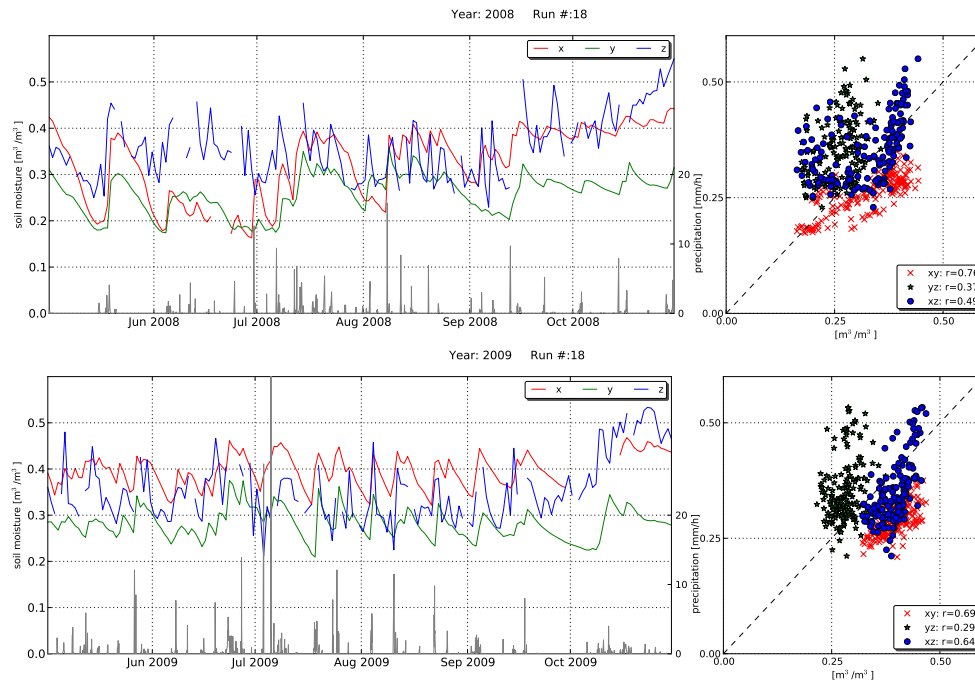
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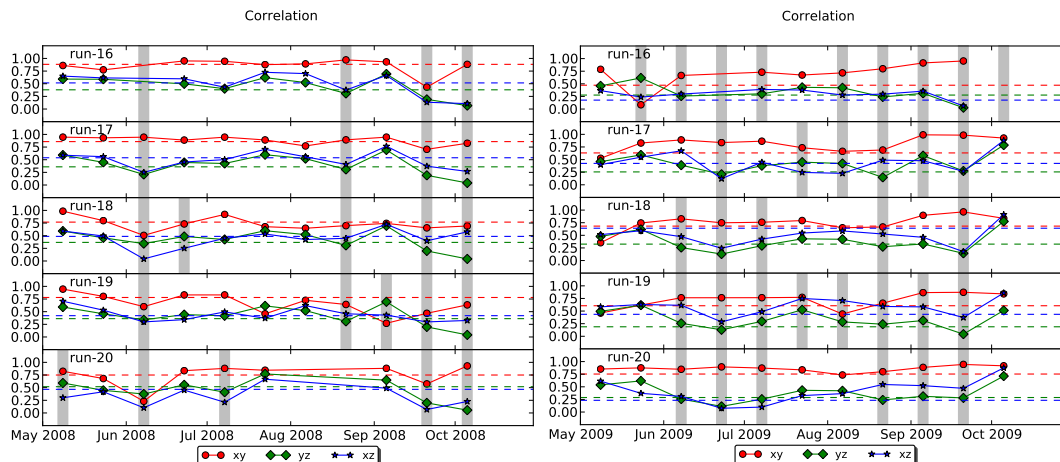


**Fig. 4.** Soil moisture time series for the station Steinbeissen #18 (red) and the corresponding model and satellite soil moisture time series. Precipitation information (grey bars). Scatterplot illustrates correlation between the different data tuples.



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**Fig. 5.** Correlation coefficients for dynamic TC analysis with  $dT = 30$  days for relationship between station and model (xy, red), model and satellite (yz, green) and station and satellite (xz, blue). Dates correspond to center of analyzed time period. Grey bars indicate cases where at least one of the correlations was not significant at the 95% level

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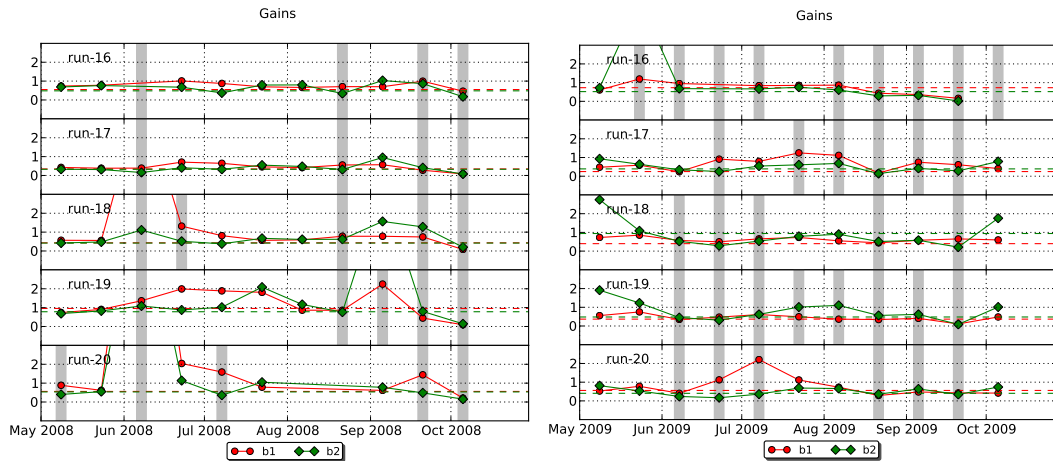
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**Fig. 6.** Same as Fig. 5 but for gains ( $\beta_1, \beta_2$ ) from Eq. (6.)

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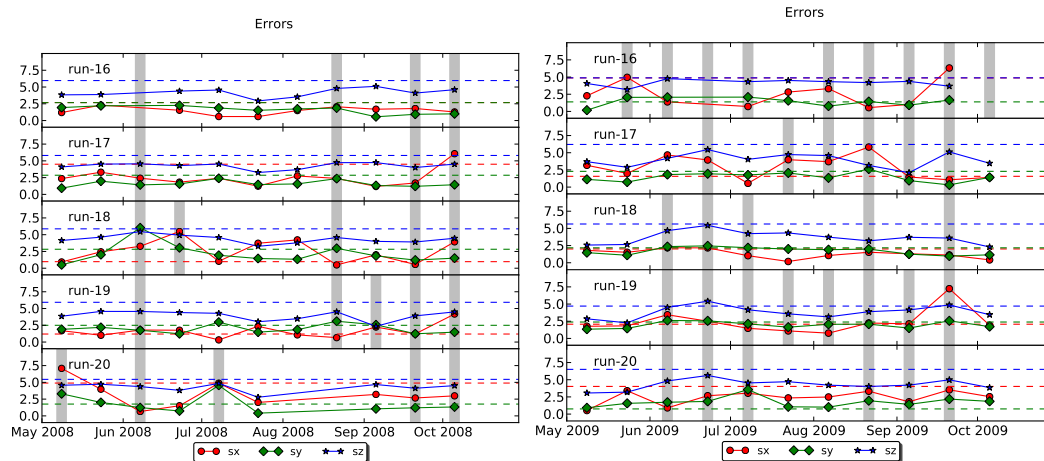
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**Fig. 7.** Same as Fig. 5 but for estimated errors of station (sx, red), model (sy, green) and satellite (sz, blue).

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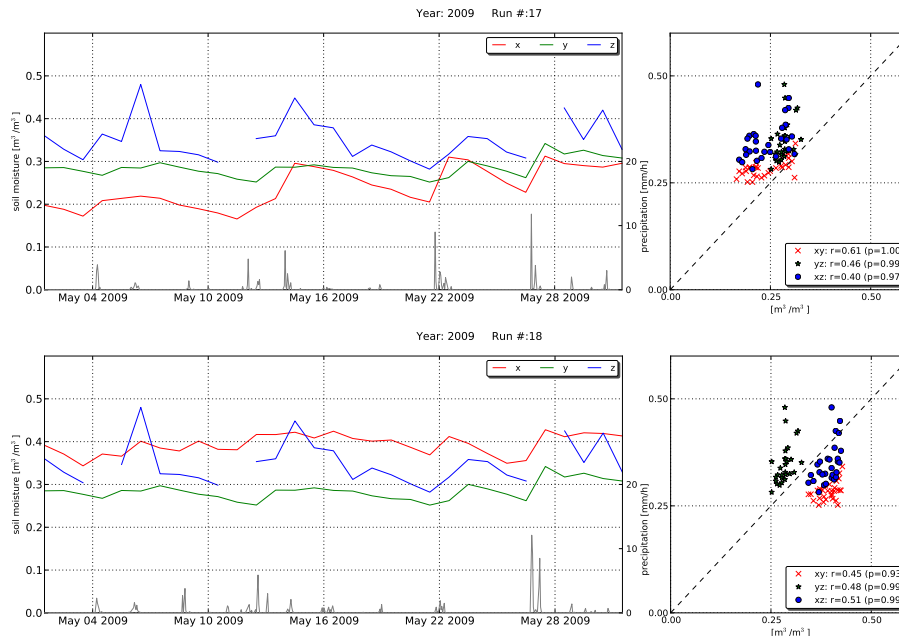
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**Fig. 8a.** Details of soil moisture time series for stations Lochheim #17 and Steinbeissen #18 (red), model (green) and satellite (blue). Correlations  $r$  between the time series and their respective significance  $p$  are provided. Information on precipitation dynamics is provided.

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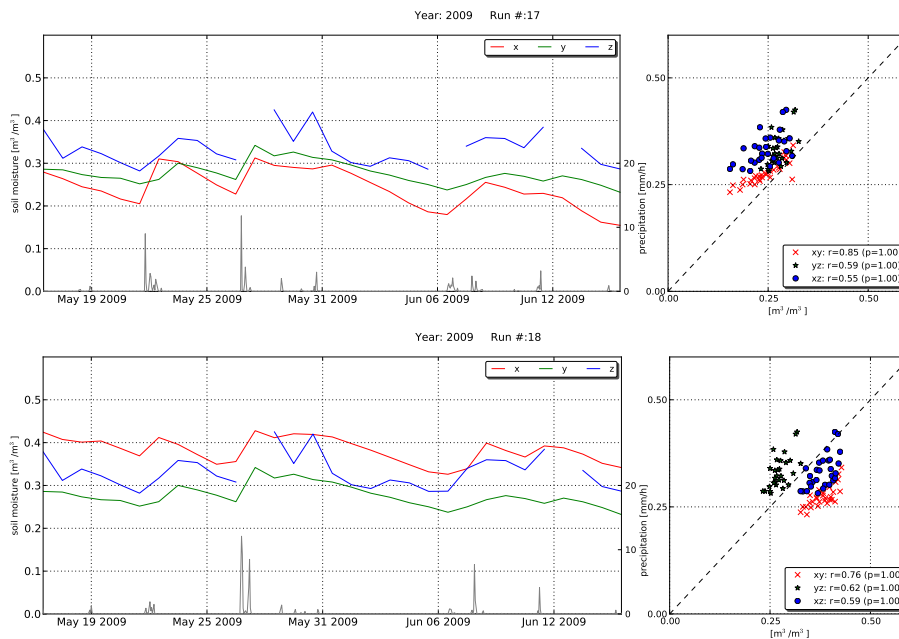


Fig. 8b. Continued.

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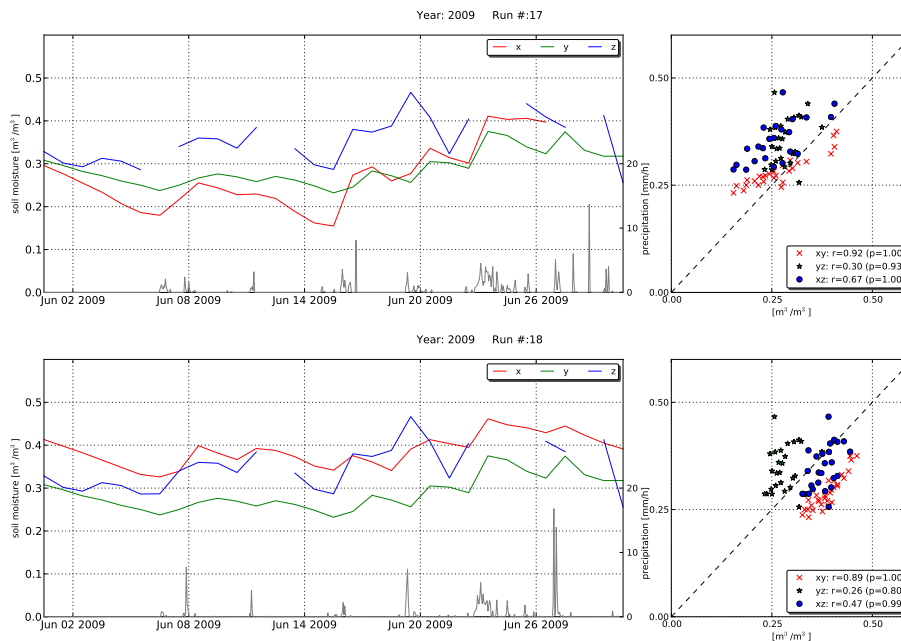


Fig. 8c. Continued.

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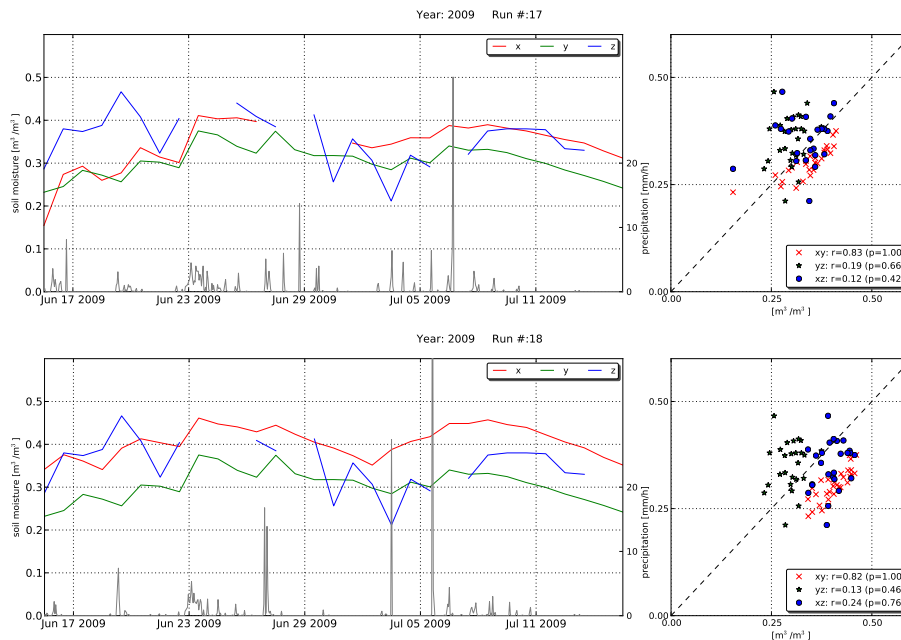


Fig. 8d. Continued.

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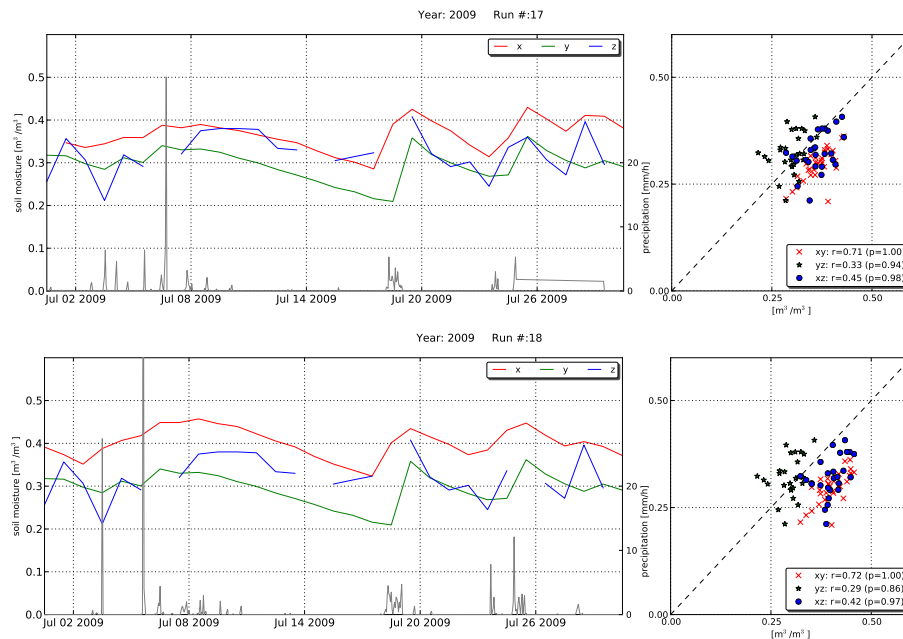


Fig. 8e. Continued.

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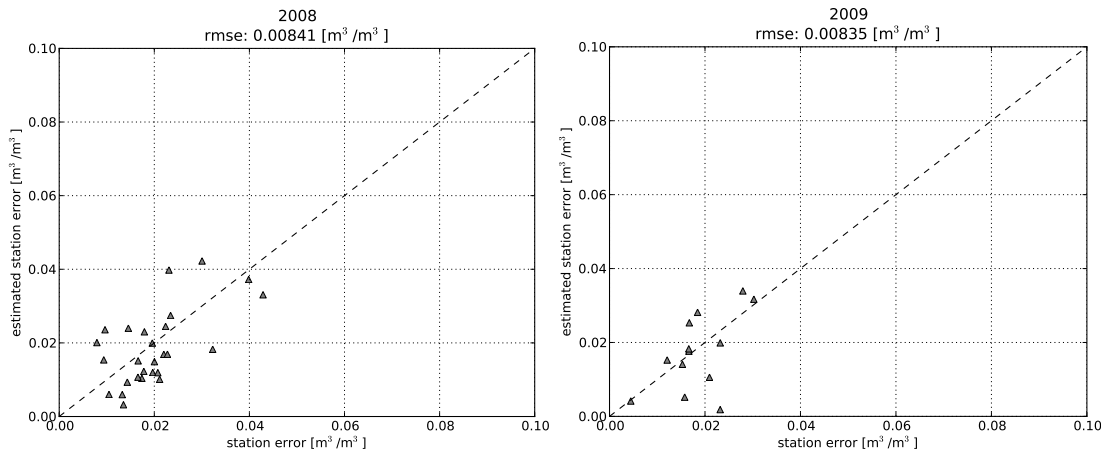
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**Fig. 9.** Comparison of the estimated station error ( $e_{\text{stat}}$ ) with the reference soil moisture error ( $e_{\text{station}}$ ) for the years 2008 and 2009 using periods with significant correlations between all soil moisture data sets.

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