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Four Decades of Progress in Monitoring and Modeling of Processes in the Soil-Plant-Atmosphere System: Applications and Challenges

# Using HydroGeoSphere in a forested catchment: How does spatial resolution influence the simulation of spatio-temporal soil moisture variability?

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# Abstract

Soil moisture is a key variable in the soil-plant-atmosphere system because it interacts with various system components. Both the measurement and the simulation of the soil moisture pattern and its spatio-temporal variability are current challenges in hydrology. This study applies the model HydroGeoSphere in a natural forest ecosystem to assess whether the model can simulate the spatio-temporal variability and pattern of soil moisture. The assessment is performed by comparing the simulation results with soil moisture measurements. The model is used at two different model resolutions to reveal the scale dependency of the calibrated model parameters, the water balance, the discharge components, and the spatial distribution of soil moisture and its variogram parameters. Discharge simulation results show that the model is capable of reproducing the discharge characteristics. A weak correlation is found between simulated and measured soil moisture dynamics in the topsoil, but the correlation is stronger in 20 cm depth. In 50 cm depth, the model is able to simulate the seasonal trend but not the short-term dynamics because preferential flow is not simulated. Furthermore, a decrease in soil moisture variance during continued drying is observed for both simulations and the measurements at both resolutions. In addition, the pattern of measured soil moisture shows a patchy character that does not show in the simulated pattern indicating that using uniform soil properties in the topsoil makes the soil moisture simulation inaccurate.

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## 1. Introduction

Soil moisture is a key variable in the soil-plant-atmosphere system because it interacts with various system components. Climatic conditions [1], vegetation type [2], topography [3], antecedent soil moisture [4] and soil properties [5] determine the spatio-temporal soil moisture variability and pattern, which in turn affect discharge generation mechanisms and transpiration. The spatial variability of soil moisture and its interactions have been studied using geostatistical analyses [6] or the time stability method [7], from the plot scale [8] to study areas of several 1000 km<sup>2</sup> [9] and for agricultural land [10], a grassland and pasture mix [1] and forests [2].

The relationship between mean soil water content and its variance has received special attention in research because a clear pattern could be observed ([5] [11] [4] [6]). The pattern provides a framework to explore how different processes contribute to the spatial variability of soil moisture. In an idealized test case for only two soil types with contrasting soil texture, [4] found a unimodal and non-linear relationship between mean soil moisture and its variance with a peak in the intermediate soil moisture range. This relationship means that the soil moisture variability increases during wetting from dry to intermediate soil moistures and then decreases during further wetting. Based on an analysis of soil moisture data from the Wüstebach catchment, Germany, [6] observed that the influence of vertical flow and root water uptake increases but the influence of lateral flow and soil properties, such as the particle size distribution and the saturated hydraulic conductivity, decreases during continuous wetting.

Bogena et al. (2010, [12]) stressed the need for modeling to test the assumptions made about hydrologic processes influencing soil moisture distribution. In addition, [13] and [14] emphasize that both the calibration of unsaturated zone properties with spatially distributed data - such as soil moisture - and integrated values - such as discharge - would improve simulation results. Despite these encouragements, the explicit analysis and comparison of simulated soil moisture with catchment scale physically based hydrological models is rare, e.g. [15], [16], [17].

Taking these aspects into account, the physically based model HydroGeoSphere was chosen because of its ability to simulate the soil moisture redistribution three-dimensionally and because it has been successfully applied to the simulation of a broad range of processes, e.g. the simulation of the effect of different bank slopes on bank storage [18], the investigation of surface/subsurface interactions [19] and vegetation effects on surface/subsurface processes [20].

When analyzing patterns and processes, the question of their scale dependency inevitably arises. The scale dependency of soil moisture dynamics and its spatial variability is investigated by applying two scaling methods. First, the application of HydroGeoSphere provides soil moisture patterns at different spatial resolutions (process-based scaling) and second, the behavioral scaling methods variogram and kriging provide a comparison of measured and simulated soil moisture patterns at a given resolution. The aim is to analyze whether the three-dimensional simulation reproduces statistical measures of the observed soil moisture pattern.

# 2. Catchment description

The Wüstebach catchment (see Figure 1) is located in the low mountain area of the Eifel National Park (50° 30' N, 6° 19' E, WGS84) in western Germany. The Wüstebach catchment is a headwater catchment with an area of 0.27 km<sup>2</sup>, an elevation between 595 and 628 meters, a mean slope of 3.6% and a maximum slope of 10.4% [12]. Since 1950, the area has been covered with Norwegian spruce (Picea Abies (L.) H. Karst. [21]). The catchment belongs to the warm temperate climate zone with a mean annual precipitation of 1220 mm (1979-1999; [12]) and a mean annual temperature of 7°C. Soils have developed in a 1-3 meter thick periglacial solifluction layer covering Devonian shales with sporadic

sandstone inclusions. In areas with no groundwater influence, Cambisols have developed in the western part and stagnic Cambisols in the eastern part. In groundwater influenced areas, Planosols, Gleysols and half-bogs have developed (see Figure 1). The mean soil texture is silt loam.



Figure 1. Location of the Wüstebach River and dominant soil types. Black dots show the sites at which soil moisture is measured in three depths using the wireless sensor network "SoilNet"

#### 3. Materials and Methods

The fully coupled surface-subsurface flow model HydroGeoSphere (HGS, [22]) is a threedimensional, physically based hydrological model that describes the water balance compartments and their processes for separate domains linked by interaction terms. The subsurface domain is discretized by 3D-prisms, the 2D surface flow domain mirrors the uppermost node layer of the subsurface domain, and the 1D channel domain is superimposed on the subsurface and surface domain. The model solves the 3D Richard's equation for subsurface flow and the 2D and 1D diffusion wave approximations of the Saint Venant equation for surface and channel flow. To analyze the contribution of different runoff components to the stream discharge like overland flow, subsurface flow, return flow, and direct rainfall to the stream, HGS is extended following the approach described by [23]. Using Kristensen and Jensen's approach (1975, [24]), interception is modeled with a bucket approach, where precipitation reaches the ground when the precipitation rate exceeds the maximum interception storage and its evaporation. Evapotranspiration influences surface and subsurface nodes and depends on LAI, a root distribution function and a non-linear function describing the dependency on soil moisture. The contribution of soil moisture to transpiration is not limited between the field capacity and the oxic limit and decreases linearly to zero at the wilting point and the anoxic limits. These thresholds are subject to calibration.

The model setup and parameterization is described in detail in [25]. The model domain is discretized with 969 nodes – including 164 nodes for the channel - at the finer and 71 nodes at the coarser grid scale. In the vertical, 23 layers down to 1.5 m depth are used for both grid scales. A critical depth boundary condition is applied to the surface nodes and a no flow boundary condition is applied to all other nodes. At the finer grid resolution, soil data are taken from representative profiles for soil types defined in the soil map for the catchment with a scale of 1:2500 (Geological Survey of North-Rhine-Westphalia). For the coarser grid scale, the van Genuchten (1980, [26]) parameters and the saturated hydraulic conductivity values were upscaled by calculating the arithmetic mean (see [25]).

The model is calibrated for 2010 and validated for 2011 both with a spin-up time of six months for a 25 m and a 100 m resolution. The model is initialized with mean measured saturation values for July 1<sup>st</sup>, 2009 (calibration) and for July 1<sup>st</sup>, 2010 (validation). Climate data are taken from the TERENO station "Schöneseiffen" (50°51' N, 6°38' E) located east of the catchment and precipitation data from the meteorological station "Kalterherberg" (50°52' N, 6°22' E; operated by the German Weather Service) located about 6 km west of the catchment. Precipitation data were corrected following [27] resulting in a 13% precipitation increase in 2011 and 2010. Snowfall is simulated with the degree-day-method [28] using measured snow height data from the meteorological station "Kalterherberg" to calibrate the degree-day-factor. Potential evapotranspiration is computed externally with the FAO Penman-Monteith cropreference method [29] for daily time steps. Soil moisture data are measured by the wireless sensor network "SoilNet" at 150 locations (see Figure 1) with 3 sensors each in 5, 20 and 50 cm depth. The network is designed to support geostatistical analysis, therefore 50 sensor units are distributed following a regular 60x60 m grid and 100 sensors are randomly distributed [12]. Quality-checked, gap-filled data from 112 measurement points are used (July 1<sup>st</sup> 2009-December 31<sup>st</sup> 2011).

As this study focuses on spatio-temporal soil moisture patterns and dynamics, the first aim of the calibration is to receive a good fit between observed and modeled soil moisture dynamics. Taking into account that the van Genuchten [26] parameterization used in this study includes the influence of the skeletal fraction of the soil but the sensor probes are not installed in skeletal rich soil parts, a calibration of residual and saturated water content seemed necessary. Due to missing field data, the residual saturation values at 20 and 50 cm depth are multiplied by a calibration factor. To compute the new porosity values, the calibrated residual saturations are added to the difference between the old residual saturations and the old porosity values.

The second aim is to achieve a tradeoff between the water balance compartments. This means that the successful simulation of the amount and dynamics of discharge – measured with Nash-Sutcliffe Coefficient [30] and Coefficient of Determination – is as equally important as the simulation of the amount of interception and the proportion between interception evaporation and transpiration. These aims are achieved by altering the canopy storage parameter, the transpiration limiting saturation and the prorosity values, which all considerably influence the transpiration amount.

To investigate the scale effect on the soil moisture pattern, a variogram and a kriging analysis are performed with MATLAB algorithms provided by Wolfgang Schwanghart (www.mathworks.com/matlabcentral/fileexchange) and the Kriging Software Package by Dezhang Chu and Woods Hole (http://globec.whoi.edu/software/kriging/ easy\_krig/easy\_krig.html). As the finer grid resolution has eight times more nodes than soil moisture measurement points, 112 nodes that are closest to the measurement points were selected with the "near" tool of the proximity toolbox of ArcGIS. The influence of this procedure on the mean soil moisture is marginal, as the soil moisture in 5 cm increases on average by 2.4% with a maximum increase of 3.6%. However, the variance increases by 22% on average in the topsoil (maximum increase is 74%). This means that an increase in sill and therefore a decrease in ranges can be expected by selecting these points. For the measured soil moisture data, an exponential model is fit to the experimental semivariogram using 30 lags, a maximum distance of 300 m and a lag tolerance of 50%. The simulated soil moisture data are fitted to a spherical model with a maximum distance of 300 m, a tolerance of 50% and 10 lags. Kriging is performed for a 10 m grid with a search radius of 300 m, a minimum number of points of 4 and a maximum of 71 for the coarser and 112 for the finer resolution and the measurements.

# 4. Results and discussion

Figure 2 shows the discharge simulation results for the 25 m grid resolution for 2010 (calibration) and 2011 (validation). In both years, a period of snowfall and snow melt is followed by a pronounced low flow period between May and mid-August, followed in 2010 by an abrupt discharge recession and a period of high discharge dynamics. In 2011, the discharge recession is postponed to the beginning of December due to low rainfall amounts between August and November.



Figure 2. Discharge simulation results at 25 m resolution for 2010 and 2011.

Figure 3 shows the difference between the discharge simulations of both resolutions. As the low differences show, the low flow period is well captured by both resolutions but peaks during the low flow period are not captured, neither is the discharge recession in August 2010. The finer resolution also shows higher discharge peaks in the summer and winter. Both resolutions simulate high groundwater contribution rates. The remaining contribution to the stream flow is at both resolutions provided by direct rainfall to the stream to a major and by overland flow and return flow to a minor extent. Both simulations produce a fast reacting groundwater flow, which corresponds to the finding of [31] that subsurface storm flow or fast groundwater flow is the dominant runoff generation process in forested headwater catchments. However, fast runoff components may be simulated for the wrong reasons. It is likely that these components are not caused by fast reacting baseflow but by preferential flow, which is known to occur in forested catchments [2].

At both resolutions, the model overestimates discharge during the calibration period, especially during winter, but produces better simulation results during the validation period (Table 1).



Figure 3. Difference in simulated discharge and baseflow between the 25 m and the 100 m resolution for 2010 and 2011.

Observed data	Calibration		Validation	
Precipitation (mm)	1230		1308	
Measured Discharge (mm)	593		605	
Potential Evapotranspiration (mm)	689		740	
Simulated data	25 m	100 m	25 m	100 m
Simulated Discharge (mm)	714	707	665	624
Fraction of Groundwater (%)	91	82	80	66
Interception (mm)	230	236	246	265
Transpiration (mm)	258	265	314	330
Actual Evapotranspiration (mm)	488	501	560	595
Coefficient of Determination	0.68	0.58	0.79	0.74
Nash-Sutcliffe Coefficient	0.66	0.56	0.78	0.74

Table 1. Water balance components and statistical measures for both resolutions for 2010 and 2011.

The scale dependency of the calibrated parameters is low as the canopy storage parameter (0.0012) and the multiplication factors remained unchanged. The multiplication factor at 20 cm depth was set to 5 leading to a mean porosity of 0.46 (originally 0.27) for the 25 m and of 0.462 (originally 0.279) for the 100 m resolution. At 50 cm depth, the multiplication factor was set to 3.3 leading to a mean porosity of

0.37 (originally 0.26) for the 25 m and of 0.367 (originally 0.265) for the 100 m resolution. Only the anoxic limit had to be increased by 0.02 (to 0.97) which is in line with the finding by [25] who found that the upscaling of HGS leads to a decrease in transpiration.

The comparison of the temporal cycle of mean catchment soil moisture shows no scale dependency due to calibration but large differences between simulation and measurements. Thus, Figure 4 only compares the measured soil moisture with the simulated soil moisture for the finer resolution. The simulation does not capture the short-term dynamics in 50 cm at all, reproduces some parts of the short-term dynamics in 20 cm depth and overestimates the dynamics in 5 cm depth. The dynamics in 20 and 50 cm depth results from the vertical flow components due to bypass flow occurring in spruce covered catchments [2] but is not simulated by the model. In addition, Figure 4 shows that a considerable amount of water is missing during the summer period in 2010 at all depths and for both resolutions. This might be due to the overestimation of the potential evapotranspiration, the lack of an aquifer in our simulation or uncertainties in the van Genuchten [26] parameters.



Figure 4. Soil moisture simulation results at 25 m resolution for 2010 and 2011.

We can state that the simulation of soil moisture dynamics is successful only for the 20 cm depth. A comparison to the findings by [17] and [15] is limited because the former only compare measured and simulated soil moisture at the event scale and the latter compare their simulation to 14 sampling locations distributed over a catchment of 1280 m<sup>2</sup>. Zhang and Wegehenkel (2006, [16]) use continuous TDR measurements for 3 depths (0-30 cm, 30-60 cm, 60-90 cm) and compare them to simulation results. They report an Index of Agreement between 0.45 and 0.80 with the best fit for the first and the worst fit for the last layer. As the TDR-technique only provides an integrated result over a certain layer, their results are hard to compare with our results providing soil moisture for a specified depth.

In the following analyses, topsoil soil moisture dynamics is described in more detail because the topsoil covers a large range of soil moisture states. The relationship between mean soil moisture and its variance clearly shows a unimodal shape for measured and simulated soil moisture as reported e.g. by [4]. The highest variances (190%) occur at soil moistures between 35 and 40% for the measurements and

between 35 and 40% for the simulations (98% for 25 m and 140% for 100 m resolution). On average, the finer grid resolution simulates lower variances (~10%) than the coarser resolution. During a drying period (21.6.10 – 2.7.10), the topsoil moisture variance linearly decreases for the simulated and measured soil moistures; however, the decrease of the measured soil moisture is higher than the decrease of both model resolutions. The decrease in variance is stronger for the finer resolution than for the coarser resolution. This can be explained by the finer resolved topography at the 25 m resolution. With further drying, areas that still have enough soil water for transpiration dry out, thus reducing the variability [32].

The variogram parameters show a pronounced scale dependency. The measured soil moisture shows a slight decrease in range with depth and no seasonal cycle. The sill shows a decrease with depth from 164% in 5 cm to 90% in 50 cm. For the finer model resolution, the mean range decreases by 76 m with depth and shows no seasonal cycle. However it increases heavily during precipitation events.

The mean sill decreases with depth by 50% and shows a seasonal cycle with higher values during the low flow period. For the coarser resolution, the range slightly decreases (12 m) with depth but the seasonal cycle is pronounced with ranges up to 260 m during the low flow period. In contrast, the sill decreases from 81% in 5 cm to 9% in 50 cm and closely follows the cycle of the range. In addition, the range decreases during or after a precipitation event and increases during drying, which is in contrast to the finer resolution showing an increase in range during a precipitation event. The reaction of the finer resolution is expected because the precipitation is applied uniformly in our simulation.



Figure 5. Soil moisture simulation results at 25 m resolution for 2010 and 2011 at 5 cm depth.

Figure 5 compares the kriging results of the measured and simulated soil moisture for the first and last day of the drying at 5 cm depth. Only the simulation results of the 25 m resolution are shown here. Figure

5 shows that the measured topsoil moisture pattern looks "patchy" but that the simulated pattern is clearly dependent on topography. This is because soil properties have no spatial variation within each soil mapping unit in the topsoil as a result of limited data availability. All variogram parameters for both the measured and the simulated soil moisture (for both resolutions) decrease during the drying period. The decrease is most pronounced for sill values with a maximum decrease of 82% for the finer resolution.

## 5. Conclusion

In this study, a three-dimensional fully coupled hydrological model was applied to a forested catchment in Germany. Discharge and soil moisture simulations compare well with measured water balance and discharge dynamics and are consistent between the two resolutions. The soil moisture simulation in 5 cm overestimates the changes in soil moisture and thus shows lower water values in the summer. Furthermore, the measured soil moisture exhibits a patchy structure that does not show up in the simulation for either of the grid sizes. In addition, the upscaling of the non-linear transpiration function of HGS does not lead to a pronounced scale dependency of transpiration fitting parameters in this study because the calibration of the porosities may account for the variation in transpiration. In addition, the lack of short-term soil moisture dynamics in 50 cm depth clearly shows that the model does not cover an important part of hydrological processes. These are all issues that will have to be investigated in future work. For example, further investigations at depths below the groundwater table would account for the patchy soil moisture structure or would improve the simulation of topsoil soil moisture dynamics.

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