Subgrid spatial variability of soil hydraulic functions for hydrological modelling

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Abstract. State of the art hydrological applications require a process-based spatially distributed hydrological model. Runoff characteristics are demanded to be well reproduced by the model. Despite that, the model should be able to describe the processes at a subcatchment scale in a physically credible way. The objective of this study is to present a robust procedure to generate various sets of parameterizations of soil hydraulic functions for the description of soil heterogeneity on a subgrid scale. Relations between ROSETTA generated values of saturated hydraulic conductivity (Ks) and van Genuchten's parameters of soil hydraulic functions were statistically analysed. An universal function that is valid for the complete bandwidth of Ks values could not be found. After concentrating on natural texture classes, strong correlations were identified for all parameters. The obtained regression results were used to parameterize sets of hydraulic functions for each soil class. The methodology presented in this study is applicable on a wide range of spatial scales and does not need input data from field studies. The developments were implemented into a hydrological modelling system. ~~and were used successfully in many practical applications and projects.~~

1 Introduction

One of the major challenges in hydrological process modelling is to minimize the discrepancy between model and data scale as described e.g. by Blöschl and Sivapalan (1995) or Hopmans et al. (2002).

State of the art hydrological applications require a process-based spatially distributed hydrological model. As first objective, runoff characteristics are demanded to be well reproduced by the model. Despite that and even for large scale applications, the model should be able to describe the processes at a subcatchment scale in a physically credible way. Following Blöschl and Sivapalan (1995), hydrological processes that are dominant at spatial scales larger than the smallest calculation unit (hydrological response unit respective elementary grid size) of the model are assumed to be described directly by the model. Small scale processes below the smallest spatial calculation unit are assumed to be described indirectly by the model, e.g. by calibration.

The simulation of soil water movements and storages can be particularly sensitive with respect to many model outputs (total runoff, infiltration, groundwater recharge, actual evapotranspiration etc.). Especially the water content of the soil near the surface is a decisive factor for the runoff generation (e.g. Binley et al., 1989a; Beven, 1995; de Roo et al., 1996; Coles et al., 1997; Bronstert and Bárdossy, 1999; Entin et al., 2000; Hasenauer et al., 2009). Further, the parameterization of field saturated

hydraulic conductivities (Ks values, e.g. $cm\ d^{-1}$) with proxy data is an essential factor for many physically based hydrological models (Gupta et al., 2006).

Hydrological models that rely on one "effective" (specific) parameterized set of soil hydraulic functions for each soil type may not be able to describe subgrid variation in an adequate way. Therefore it can lead to a high calibration effort and possibly to an inadequate process description. Bronstert and Bárdossy (1999), for instance, do not recommend averaged (effective) input data. Instead they suggest to use additional stochastic components to consider small scale heterogeneities. Further, Kirchner (2006) points out that *the key question is not whether models of hydrologic systems should be physically based; instead, the question is how they should be based on physics*.

Area-wide measured data of basic soil properties or even of soil hydraulic properties are not available for most hydrological model applications at the meso- and macroscale. However, in many cases rough information about the soil (e.g. soil maps) is available on a very coarse spatial resolution (1:50000 at best). Using such rough input data does not allow direct parameterization of any subgrid variability. In addition to that, soil maps are already products of regionalised input data. Consequentially, all soil hydraulic parameters based on soil maps can be interpreted (only) as effective parameters.

In this study the subgrid spatial variability for the parameterization of soil hydraulic functions will be derived indirectly from soil map information. To achieve this, three statements are formulated and will be discussed below:

1. The spatial variability of saturated hydraulic conductivity of soils on a subgrid scale can be expressed by a lognormal distribution.

2. There are relationships between the saturated hydraulic conductivity and the parameters of soil hydraulic functions.

3. These relationships are mirrored in the parameters generated by the software ROSETTA (Schaap et al., 2001). They can be used to simulate a subgrid spatial variability in a straightforward procedure, which does not require measured samples of soil properties.

The first statement was widely acknowledged in numerous studies (e.g., Law, 1944; Baker and Bouma, 1976; Sharma et al., 1980; Lauren et al., 1988; Binley et al., 1989b; Goodrich, 1990; Vauclin et al., 1994; Mallants et al., 1997; Bosch, D. D. and West, L. T., 1998; Viera et al., 2011, and many more). The second statement was investigated in several studies as well. However, compared to the first statement, the available studies are less clear. Carsel and Parrish (1988) used approx. 3000 measurements of soil textures and bulk densities, which were summarized into 12 major texture classes. They approximated van Genuchten (1980) parameters (VGP) $\Theta_S, \Theta_R, \alpha$ and n as well as Ks values utilizing the empirical regression functions of Rawls et al. (1993) to describe soil hydraulic functions. In a following step, Gaussian distributions for the VGP were approximated by using the Johnson system of transformations. This was done for every VGP independently. After the transformation, high correlations were found between VGP and Ks values. In a pursuing study de Rooij et al. (2004) used approx. 140 samples from two layers of an agricultural soil to fit VGP and Ks values each. Relationships between the VGP and the Ks values were found by means of regression analyses. However, these relationships were considered to be too weak for using the Ks values as a direct predictor for the VGP. In a next step, they used these relationships as additional information for estimating

probability distribution functions for each VGP. The assumption of Ks being lognormal distributed was considered as well. In a study of Li et al. (2007) data was measured experimentally to describe 63 pF curves as well as corresponding Ks values, texture information, bulk densities and fractions of organic matter. pF is defined as log10 values of the absolute soil pressure heads. The model of van Genuchten (1980) was adapted to fit the measured data in order to obtain pF curves. This research found high correlations between VGP, measured texture classes and bulk density as well as weak correlations between measured Ks values and bulk densities. No significant correlations were found between Ks and the texture of the soil. Regression analyses were not conducted for Ks and VGP. However, the other regressions of Li et al. (2007) indicate that there seems to be no significant relationship. Botros et al. (2009) carried out measurements to obtain pF curves for nearly 100 sediment cores. They analysed the dependence among measured Ks values and VGP, which were fitted to the measured pairs of the soil water content (Θ) and the soil pressure head (h). Significant correlations were found between Ks and α, n and Θ_S; Ks and Θ_R were also correlated, but did not yield significance. All these studies have in common that any analyse is always based on measured input data of soil properties. Aside from that, rather elaborate numerical simulations were necessary in many cases. As a general note, relationships between the VGP and Ks values were found in many studies.

Besides the lack of measured soil samples the effort of parameterization by means of sophisticated procedures that often require Monte Carlo applications is very high even for models operating on the hill slope scale. This effort is much higher for large areas and huge time scales as it is usual in e.g. climate change hydrological modelling. Consequently, the use of effective parameter sets and powerful calibration procedures is widespread. On the other hand, some kind of calibration parameters are "always" needed in hydrological modelling. Based on this, the third (innovative) statement was formulated. Premised on profound analyses of the relationship between ROSETTA generated Ks values and VGP for several texture classes, the objective of this study is to consider the subgrid spatial variability of soil hydraulic functions for hydrological modelling by using these relationships. It is worth to mention, that the methodology presented in this study is applicable for a wide range of spatial scales and does not need measured input data from field studies.

2 Methodology

In this section we shortly give the required theoretical background in soil physics and statistics. Further, the creation of a database is presented by means of the software ROSETTA. The database contains the parameters and Ks values for the description of pF-curves based on the equations of van Genuchten (1980). In a next step, correlations between the Ks values and the parameters of the soil hydraulic functions of the generated databases are analysed.

2.1 Soil hydraulic functions

Since the objective of this paper is the consideration of subgrid variability of the parameterization of soil hydraulic functions at the meso- and macroscale, the model for the description of the soil hydraulic functions has to be determined in the first place. The use of proxy information is one of very few possibilities to parameterize soil hydraulic functions extensively for large hydrological model areas. As the software ROSETTA will be used for this application (see section 2.2), the obtained

parameters are limited to the model of van Genuchten (1980). However, this model is widely used in hydrological and soil physical disciplines for describing the relation between water content and pressure head in soils:

$$\Theta(h) = \Theta_R + (\Theta_S - \Theta_R)[1 + (\alpha\,|h|)^n]^{-m} \tag{1}$$

There are synonymic designations for the relationship between water content and pressure head, see Durner and Flühler (2006) for details. In this study the designation "pF-curve" is used. In Eq. 1 $\Theta(h)$ denotes the volumetric water content ($cm^3\ cm^{-3}$), h (cm) marks the pressure head of the soil, Θ_R and Θ_S ($cm^3\ cm^{-3}$) are defined as the residual and saturated water contents of the soil, whereas α (cm^{-1}) n ($-$) and m ($-$) are shape parameters of the model. Both shape parameters have a weak physical interpretation. The inverse of α (and also n) is slightly related to the air entry pressure head (however, equation 1 has no defined air entry value). n is connected to the width of the pore size distribution of the soil between Θ_S and air entry pressure head. The product mn is related to the width of the pore size distribution of the soil between air entry pressure head and Θ_R (Durner and Flühler, 2006; Peters and Durner, 2006). Studies of Wösten and van Genuchten (1988) and van Genuchten and Nielsen (1985) analysed the influence of these parameters on the shape of the modelled pF-curve in detail. The parameter m is in most cases approximated as $1 - \frac{1}{n}$, which reduces the flexibility of the model, but enables a closed form expression for the unsaturated hydraulic conductivity by combining Eq. 1 with the pore size model of Mualem (1976):

$$K(\Theta) = K_s S_e^l \left[1 - \left(1 - S_e^{\left(m^{-1}\right)}\right)^m\right]^2 \tag{2}$$

with the effective saturation S_e ($cm^3\ cm^{-3}$) as

$$S_e = \frac{\Theta - \Theta_r}{\Theta_s - \Theta_r} \tag{3}$$

In general, the absolute values of Eq. 2 are scaled by the saturated hydraulic conductivity Ks ($cm\ d^{-1}$). The parameter l ($-$) can be approximated as 0.5 (Kutílek and Nielsen, 1994; Hillel, 1998). The unsaturated hydraulic conductivity ($K(\Theta)$ respectively $K(h)$) can either be formulated in dependency of the soil water content Θ as shown in Eq. 2, or of the pressure head h.

2.2 Parameters for soil hydraulic functions

One objective is to investigate for correlations between ROSETTA generated VGP and Ks values. To formulate statistically significant statements, a representative population for the statistical analyses has to be considered. Therefore, a short algorithm was developed to create trios of numbers within a range of 0 to 100. These trios were randomly generated with the precondition that the sum of each trio has to be 100. The numbers of each trio are assigned to be a percentage fraction of sand, silt and clay. One million fictitious samples of possible compositions of texture fractions were obtained in this manner. All three texture fractions are characterized by the same distribution with an expected value of $33.\overline{3}$ percent sand/silt/clay. The large number of generated samples was empirically determined in order to get a representative population for the statistical analyses. The regression results were stable for populations $\geq 10^5$. The number was increased to 10^6 to safeguard validity.

The free of charge software ROSETTA (Schaap et al., 2001) was utilized to estimate the VGP Θ_R, Θ_S, α and n as well as Ks values per sample. It is based on neural network analyses and was calibrated by means of a large database comprised of 2134 soil samples that consists of more than 20000 pairs of Θ and h in total. For the saturated hydraulic conductivity 1306 soil samples were available. 235 samples also contained data for the unsaturated hydraulic conductivity function $K(\Theta)$ respectively $K(h)$ including more than 4000 data points (Schaap et al., 1998, 2001). The database UNSODA (Leij et al., 1996; Nemes et al., 2001) contributes significantly to these data points. Additional information about early neural network applications for parameterization of soil hydraulic functions can also be found in Schaap and Bouten (1996).

The VGP sets (including Ks values), obtained with ROSETTA using the randomly generated texture compositions as input, are hereafter called "database 0". In addition to this database, gradual reductions of database 0 were carried out. These reductions were a result of the evaluation of the regression analyses. Further reasons of the reduction are given in section 3. At total four different databases were generated (database 0 and three derivatives of database 0):

1. The complete **database 0**, which consists of the total of one million VGP sets including Ks values.
2. A reduced **database 1** based on the condition that $Ks < 150\ cm\ d^{-1}$. Approx. 95% of the parameter sets of database 0 are still included.
3. A reduced **database 2** based on the condition that $Ks < 150\ cm\ d^{-1}$ and $\Theta_R < 9\%$. Approx. 70.5% of the parameter sets of database 0 are still included.
4. Several selected **databases 3_x**. *Variant A*: Subdivision based on natural texture classes according to the soil map of Lower Saxony, Germany. *Variant B*: Subdivision based on soil hydraulic properties.

2.2.1 Generation of Databases 3_x, variant A: classification by soil map

The final reductions to databases 3_x were conducted for two reasons: Firstly, it is suspected that many grain size compositions in database 0 are unrealistic (e.g. 100% clay or 50% clay + 50% sand) causing the neural network of ROSETTA to extrapolate the parameters for these compositions. This may have noisy effects on possible correlations between Ks and the VGP. Secondly, the presented approach is tailored to hydrological modelling at the meso- and macroscale without employing measured data. In most cases only rough information about the soil (e.g. soil maps) is available for the model area. For that reason, the database was further reduced to obtain natural texture classes, which can be found in many soil maps. Suitable soil maps (or similar products) are widely available around the world. We used the German soil map of Lower Saxony (Edt.: J. Boess et al., 2004), see Fig. 1. Out of this, common natural compositions of grain sizes were isolated from the datasets of database 0 in order to generate databases 3_x (variant A). Abbreviations of the texture classes are defined in Table 1 and were assigned according to the German soil classification system (Sponagel, 2005). A pre-defined texture class for boggy soils (Hn) is not available. Silty clay (Tu) has similar properties as clayey loam (Lt), therefore these two texture classes (Hn, Tu) are not included in the following analyses. Instead, the texture classes for silty loam (Lu) and pure sand (Ss) were added. These texture classes are not shown in the soil map (Fig. 1). However, both are contained in other soil maps of Germany. Around each texture fraction,

a $\pm 5\%$ boundary in each direction was considered in order to get a representative number of van Genuchten datasets for the regression analyses. Note that at total more than 10^5 parameter sets of database 0 are still included in the databases 3_x (variant A). The procedure to obtain the VGP and Ks values is graphically shown in Fig 3.

2.2.2 Generation of Databases 3_x, variant B: classification by cluster analyses

Twarakavi et al. (2010) introduced a procedure to classify soils based on their hydraulic properties. To achieve this, they used the k-means clustering algorithm. The same algorithm was used in this study to subdivide database 0 by means of hydraulic properties. This algorithm is available in MATLAB. We standardized the VGP to avoid scale effects that influence the weightings in a negative way. Minimization of euclidean distance was applied as objective function. The number of resulting subdivisions (classes) is freely adjustable. We used 255 different target clases, starting with two and going up to 5680 classes.

2.3 Regression analyses for soil hydraulic parameters

A flexible exponential regression model is used, since the modalities of the relations between the Ks values and the VGP are unknown:

$$f(x) = ae^{bx} + ce^{dx} \tag{4}$$

where a, b, c and d $(-)$ are fitting parameters and e $(-)$ is Euler's number. The model is adjusted by means of the Levenberg-Marquardt algorithm (Marquardt, 1963).

In addition to the univariate regression model shown above, a multivariate regression will be performed by using a general multivariate model, which can be denoted as:

$$\boldsymbol{Y_{n\text{x}d}} = \boldsymbol{X_{n\text{x}(p+1)}}\boldsymbol{B_{(p+1)\text{x}d}} + \boldsymbol{E_{n\text{x}d}} \tag{5}$$

where the matrix $\boldsymbol{Y}$ denotes the dependent variables, which are assumed to be correlated among themselves. The matrix $\boldsymbol{X}$ includes the independent variables, the matrix $\boldsymbol{B}$ comprises the fitting coefficients and $\boldsymbol{E}$ gives the matrix of residuals. The index n denotes the number of samples, d the number of subjects and p the number of predictor variables.

To evaluate the quality of the regressions, the coefficient of determination R^2 is calculated as follows (Sachs, 2004):

$$R^2 = \frac{SSY - RSS}{SSY} = \frac{MSS}{SSY} = 1 - \frac{RSS}{SSY} = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \tag{6}$$

with

$$\bar{y} = \frac{1}{k}\sum_{i=1}^{k} y_i \tag{7}$$

SSY is the total, RSS is the residual and MSS is the regression sum of squares. By standardization of MSS with SSY the coefficient of determination R^2 is obtained. y_i denotes a data value and $\bar{y}$ describes the average of all data values, whereas $\hat{y}_i$

symbolizes a computed value of the regression model. R^2 ranges from 0 (no relation) to 1 (perfect fit).

For consideration of non-linearities, Spearman's rank correlation coefficient r_{spear} can be calculated in addition to the coefficient of determination (Sachs, 2004):

$$r_{spear} = 1 - \frac{6 \sum_{i=1}^{k} (rg(x_i) - rg(y_i))^2}{k(k-1)^2} \tag{8}$$

$rg(x_i)$ and $rg(y_i)$, which are sorted into ranks (rg), are the values of the dataset and the fitted model with the total number of k. r_{spear} has a range from -1 to 1, whereby 0 denotes no correlation and 1/-1 describe a perfect positive/negative correlation, respectively. ~~Different regression analyses were conducted based on the databases.~~

3 Results and discussion

3.1 Regression analyses

3.1.1 Complete database 0 and reduced databases 1 and 2

Regression analyses based on Eq. 4 were performed for the database 0 and for the reduced databases 1 and 2 each.

The Ks values in relation to the Θ_R values resulted in low correlations with R^2 of 0.43. A more structured $Ks - \Theta_R$ relation seems to arise for Ks values smaller than 150 $cm\ d^{-1}$ and Θ_R smaller than 9%. Consequently, database 0 was reduced to database 2 and R^2 of the regression function, that was computed out of the complete database 0, increased to 0.72. However, to obtain a function on the basis of database 2 new regression analyses were conducted leading to R^2 of 0.74. This function is shown in the first plot of Fig. 5. A similar approach was applied to evaluate Ks and Θ_S; no significant correlations were obtained. Because of the high correlations found for $Ks - \Theta_R$ in database 2, the reduction of the database 0 was also applied for Θ_S. However, only the range of the Ks values was reduced, leading to database 1. In contrast to $Ks - \Theta_R$, no significant correlations were found between Ks and Θ_S based on the reduced database, see the second plot of Fig. 5. Low correlations (R^2 = 0.41) were found for the parameter n when using database 0. An even lower fit (R^2 = 0.25) was obtained when reducing database 0 to database 1 as seen in the third plot of Fig. 5. The analysis of Ks versus α shows neither correlations for database 0 nor for database 1 (fourth plot of Fig. 5).

Generally, in some sections of the scatter diagrams there seem to be more connections between the Ks values and parameters of the soil hydraulic functions than in other sections. However, these connections are very low and too uncertain for hydrological modelling purposes. A reduction of database 0 to database 1 respectively database 2 had a positive effect on the regression of Θ_R only. Apparently, it is not possible to obtain four single regression functions, one for each parameter.

3.1.2 Databases 3_x, variant A: classification by soil map

Univariate regression analyses

Regression analyses based on Eq. 4 were performed for each of the natural texture classes. Concerning Θ_R, very high R^2 between 0.88 and 0.99 were found for 7 out of the 10 texture classes with an average R^2 of 0.96. The other three classes reached

correlations with R^2 lower than 0.5; therefore, these classes were not included in following analyses and applications. Generally, curves with a R^2 lower than 0.5 are not illustrated in the figures and tables. The regression curves of Θ_R are exponentially decreasing proportional to decreasing Ks values, which physically makes sense. However, we have to keep in mind that van Genuchten's Θ_R has no clear physical interpretation and other fitting models for the pF-curve actually have no residual water content (see e.g. Rossi and Nimmo (1994)). The high correlations between Θ_R and Ks may have to be considered as a kind of black box correlation that is valid for the ROSETTA fed van Genuchten model only. ~~On the other hand, it is unclear how much of the found correlations may also be an artefact of the ROSETTA neural network.~~

Concerning Θ_S, high R^2 between 0.68 and 0.93 were found for 5 texture classes with an average R^2 of 0.82. The behaviour of these classes can be divided into two groups. Group one includes Lu and Ls, group two includes Us, Sl and Su. The main textural difference of these two groups is the fractional higher clay and lower sand content in group one compared to group two, as seen in Table 1. This has an effect on the slopes of the fitted regression models. Group one shows decreasing values of Θ_S with increasing Ks values, group two behaves the other way round. Assuming higher sand fractions causing higher Ks values, the grain size compositions of group one are shifted in the direction to the centre of the texture triangle. This may cause smaller values of Θ_S. On the other hand, moving away from the centre of the texture triangle with higher fractions of sand (as for group two) may have the opposite effect of increasing porosity. Both effects are imaginable, however, we do not want to overinterpret the physical impact of van Genuchtens's Θ_S. ~~that is based on neural network estimates.~~

Concerning α, high R^2 values between 0.67 to 0.96 were found for four texture classes with an average R^2 of 0.75. As given in section 2.1, the parameter α is weakly related to the inverse of the air entry suction (not to forget that van Genuchten curves have no defined air entry value). In general, without specializing on van Genuchten's model, the entry suction should be higher for fine grained as for coarse grained soils. This means that the entry suction should rather decrease with increasing Ks than increase. This connection cannot be found for the texture class Lu. That's why this regression (Lu) is not considered in the subsequent analysis.

Concerning n, very high R^2 between 0.63 to 1.00 were found for 7 texture classes with an average R^2 of 0.85. Especially for the two sandy texture classes highly accurate fits were obtained. Under the assumption of n being related to the pore size distribution, many different pore sizes lead to low values of n, whereas many pores with a similar size lead to high values of n. In general, soils that are located near the borders of the texture triangle tend to have a more narrow pore size distribution than ~~as~~ soils located in the middle of the triangle. Taking into account that these soils (pure sand, pure silt~~e~~) may have higher Ks values compared to loamy soils, increasing Ks may be related to increasing values of van Genuchtens n. Again, we have to be careful not to overstretch connections of ROSETTA generated VGP to measurable physical properties of soils.

All statistical quality values from the univariate regression analyses are listed in Table 2. Additionally, p-values are included. Low p-values indicate a correlation between Ks and the parameters of the soil hydraulic functions. All p-values of Table 2 are nearly zero, yielding that all shown correlations are significant. Further, the square of r_{spear} yields approximately R^2 for most cases. This seems to validate R^2 as a quality criterion for the regression analyses.

Multivariate regression analyses

Regression analyses based on Eq. 5 were performed for each of the natural texture classes. We used $\log 10(Ks)$ ~~$\log(Ks)$~~ to fill the matrix $\boldsymbol{X}$. The matrix $\boldsymbol{Y}$ comprises Θ_R, Θ_S, n and α. These more elaborate procedures, which consider the correlations among the dependend variables, serve as references for the previous results.

Both the shape of the obtained fits of the multivariate method and the R^2 turned out to be very similar to those of the univariate method. The average R^2 both for the univariate and multivariate method equals approx. 0.835 ~~for the univariate method equals 0.84 and the average R^2 of the multivariate method is 0.83.~~. The shapes of the functions differ just slightly or are even identical. Figure 7 shows the univariate and multivariate regression results for n based on the texture class Su. It can be seen that both curves behave very similar with small differences at high Ks values. However, R^2 are equal to each other and a "better" fit cannot be pointed out. All other comparisons between the regression results of the two methods act similar to Fig. 7. The high accordance of both method's results speaks for the robustness of the less elaborate univariate method. Based on this, the results of the univariate regression analyses will be used for further applications.

3.1.3 Databases 3_x, variant B: classification based on soil hydraulic properties

Results of the subdivision

Fig 2 shows subdivisions of the soil texture based on soil hydraulic properties by means of cluster analyses for a number of 31 classes. Results of Twarakavi et al. (2010) showed that the subdivisions based on soil hydraulic properties are similar to the US texture based classification, especially for coarse textured soils (sands). These similarities were not found for fine textured soils. The results of our subdivision based on soil hydraulic properties are unlike to the texture based classification. However, this is not directly a contradiction to Twarakavi et al. (2010). They used the US texture triangle for comparison and we use the german classification. In addition to that, the rules and conditions for the algorithm of the cluster analyses have a high influence on the result.

Univariate regression analyses

In variant B we concentrate on univariate regression analyses only. In Fig. 4 the average R^2 are shown in dependency of the number of classes used for the subdivisions. As previously, regression results with R^2 lower than 0.5 are not considered. The abscissa is limited to a maximum of 200 classes. If more classes are used, the average R^2 does not increase significantly. The average R^2 ranges therefore mainly between 0.7 and 0.8. If we use 31 classes, which is the same number of subdivisions as the texture based classification of the german soil classification system, the average R^2 is 0.74 and 40% of the regression results have coeffcients of determination higher than 0.5. The maximum can be found for the number of 2128 classes (R^2=0.82 with 49% of the regression results with > 0.5). The results of the regression analyses based on databases 3_x (variant A) yielded in an total R^2 of 0.88 by using nine natural texture classes and 67% of the regression results had an $R^2 > 0.5$. In addition, the application of the univariate method is faster and less elaborative. For those reasons, we will use the results of the regression analyses based on databases 3_x (variant A) for further applications.

3.2 Applications on soil hydraulic functions

Figure 8 illustrates the impact of the regression results that were obtained by the univariate method of databases 3_x (variant A) on van Genuchten's soil hydraulic functions for the texture classes S, Su and Lu. These three texture classes are assigned to be representative for all classes that were investigated. In addition, a wide range of Ks values is covered. Ks values were selected ranging from the minimum to the maximum values that were obtained out of database 3_x (variant A). The pF curves of the texture class S are shown in Fig 8a. Van Genuchten's n was computed out of the regression function. The pF curve of the regression with the smallest Ks-value has a clearly smoother slope compared to the pF curve that was obtained for the largest Ks-value. The lower the Ks the more moves the shape of the pF curves in the direction of typical pF curves for sandy soils with a fraction of silt. The curves for low Ks values tend to have a higher usable field capacity possibly leading to higher rates of transpiration in hydrological modelling applications. The curves for the unsaturated hydraulic conductivity $K(h)$ of the texture class S are given in Fig 8d. The same parameters as for the pF curves were used. Near saturation the curves of large Ks values are above the curves of low Ks values. This relation changes after an intersection point at pF of approx. 2, caused by the variation of van Genuchten's n that is directly connected to the parameter m. From the physical point of view, the shapes of the curves can be described as reasonable. The curves with lower Ks values have a higher fraction of small pores. These fraction of small pores are able to transport water for a wider range of pF in contrast to the curve parameterizations with high Ks values. This leads to the intersection point that changes the dominating impact factor on the conductivity curves: For pF < 2 the Ks value, which simply scales the curve, is the dominating factor. For pF > 2 van Genuchten's m is the dominating impact factor. However, after the intersection point $K(h)$ is already at very low values. Therefore, the variation of m for sandy soils may have a small impact compared to the impact of variations of the Ks values.

Figure 8b shows the impact of the regression results on the pF curves of the texture class Su. Similar to Fig 8a, the curves for low Ks values have a smoother slope. In addition to that, the modifications of van Genuchten's α causes the water content dropping at higher pF values for the curves of low Ks values compared to the curves of high Ks values. This behaviour is typical for texture classes that have a slightly larger fraction of fine pores than the "standard Su". The usable field capacity is more or less the same for all pF curves. The impact on hydrological model applications might nevertheless be immense depending on the method that reduces the potential evapotranspiration to the actual one: Methods based on the actual water content of the soil within the root zone probably calculate higher rates of actual evapotranspiration using the parametrization based on low Ks values than using the ones of higher Ks values. On the other hand, methods based on pF values of the soil are expected to be less affected. The impacts on the conductivity curves for the texture class Su are plotted in Fig 8e. Here again, an intersection point can be located (at a pF of approx. 1.8). Above this pressure head, the curves of high Ks values drop below the curves of small Ks values. In contrast to the conductivity curves of the texture class S, the values of $K(h)$ at the intersection point (and close below) are still high enough to enable a water movement that is not negligible. For that reason soil water simulations are influenced, especially during dry seasons.

The pF curves for the texture class Lu are visualized in Fig 8c. Here, a shift on the ordinate can be observed, whereas the curves for low Ks values induce higher water contents than the curves for high Ks values for the same pressure head. This is

due to the relation that was found for Lu of Θ_R and Θ_S being inverse proportional to Ks. However, the variations of n cause different slopes of the curves. The impact on the reduction of the potential evapotranspiration is comparable to the impact described for the texture class Su. The impact on $K(h)$ is primary driven by the variations of the Ks values, as seen in Fig 8f. The intersection point is approximately at pF 4. At this high pF, $K(h)$ has dropped magnitudes below the saturated value.

It can be summarized that the modifications of the VGP caused by the regression results of the databases 3_x (variant A) lead to plausible pF curves. Further, the impact on the conductivity functions near saturation is primarily driven by the value of Ks. As the Ks value works as a scaling factor for the conductivity curves, this result~~s~~ is no surprise and not induced by the regression functions. For medium and low saturations however, the impact is dominated by the variations of the parameterizations of the soil hydraulic functions that were produced by the regression functions. Especially for the texture Su (and similar ones), the impact of the regression functions will have an impact on long term hydrological model applications. Taking the soil map of Lower Saxony for instance, texture classes with compositions like Su, Sl or similar occupy more than one third of the total area. For many of the texture classes, all four VGP could be fitted in dependency of Ks. However, this did not always work as seen in Table 2. Following this, the correlation matrices of the VGP, generated within the regression analyses of databases 3_x (variant A), were taken into account more deeply. It turned out that correlations were very low between VGP, which are related to Ks, and VGP, which are not related to Ks. These findings indicate the admissibility of fitting less than four VGP in dependency of Ks.

3.3 Generating subgrid spatial variability

Spatial resolutions of hydrological models mainly depend on the resolutions of the input data of soil properties and land use respectively ~~each~~. These input data are often not equally resolved in space and time (e.g. the German ATKIS database). If the model area is subdivided into polygons by the hydrological model, the spatial resolution is unequally distributed and given automatically by the input layers. If the model area is subdivided into raster cells, the spatial resolution is equally distributed and depends both on input layers as on the user's interests. For latter types of models, the spatial resolution may often induce a pseudo accuracy, because the chosen grid size can be much smaller than most of the subdivisions of the input layers. In any case, the "real" spatial resolution of a hydrological model that has to be considered for the process description is given by the spatial resolutions of the input data. In most cases these spatial resolutions are rather coarse causing that many processes are not directly resolved by the model.

To consider the spatial variability of soil water processes that are not directly resolved by the hydrological model, the following procedure is elaborated in order to generate parametrizations of soil hydraulic functions:

1. Acquisition of a soil map for the model area (or similar information). In this study: German soil map of Lower Saxony, see Fig. 1. If not already included in the soil map: Transformation of soil classifications into texture information. In this study: Usage of the German soil classification system, see Sponagel (2005).

2. Obtaining texture classes out of the soil map. Example: Sl with 65% sand, 25% silt and 10% clay (see Table 1).

3. Randomly generation of trios of numbers within a range of 0 to 100 with the precondition that the sum of each trio has to be 100. The numbers of each trio are assigned to be a percentage fraction of sand, silt and clay.

4. Consideration of a boundary in each direction (sand, silt, clay). In this study: $\pm 5\%$ boundary. Example: Sl with $65 \pm 5\%$ sand, $25 \pm 5\%$ silt and $10 \pm 5\%$ clay. Categorization of the random-number-trios into the obtained boundaries.

5. Generation of VGP sets with the software ROSETTA for the obtained texture classes (caterogies).

6. Regression analyses between Ks values and all other VGP for each texture class.

The total number of needed randomly generated numbers (point 3) may differ in dependency of the texture classes that are going to be analysed. The ROSETTA underlying databases have ~~has~~ more samples of sandy soils than of clayey soils (Leij et al., 1996; Nemes et al., 2001). Furthermore, some combinations in the texture triangle are very seldom in nature. To ensure that these disagreements do not bias the regression results, only a close range ($\pm$ boundary) near natural occurring texture classes that are obtained from soil maps should be considered for the regression analyses (here: generation of database 3_x (variant A), see section 2.2). The boundary was assigned to be $\pm 5\%$ in order to get a representative number of VGP sets for each texture class. Other values for the boundary were tested, whereby much lower values (e.g. $\pm 1\%$) lead to a very close range of the Ks values. Much higher values for the boundary (e.g. $\pm 10\%$) blurred the VGP sets of the texture classes (there was no difference left between certain texture classes). Therefore we recommend a value of $\pm 5\%$ for the boundary.

At a next step, the obtained regression functions have to be applied in a hydrological model. The following procedure is recommended:

1. Assumption of a lognormal distributions for the Ks values of each texture class. The mean values are given by the Ks values that were obtained with ROSETTA at the center of each texture class. The standard deviations are given by the user.

2. Calculation of variations of the other VGP by using the regression functions and the Ks distribution functions. The number of VGP sets is up to the user. At least three sets should be used. We recommend five sets by using the 10%, 30%, 50%, 70% and 90% percentile of the Ks distribution function. More sets are possible. ~~Calculation of percentiles out of the lognormal distribution of the Ks values (e.g. 10%, 30%, 50%, 70% and 90%).~~

3. Run the model by parallely using the VGP sets that were obtained at the previous point 2 ~~3~~.

Due to the fact that standard deviations of the Ks values are in most cases unknown for meso- and macroscale hydrological model applications, this parameter should be assumed by the user. Note that this is the only tuning parameter needed for the procedure presented in this study. The standard deviations of Ks values at field scale may vary between less than 50% and several hundred % and there seem to be no clear correlations to the texture classes of the analyzed soils, see e.g. Ciollaro and Romano (1995), Reynolds and Zebchuk (1996), Bosch, D. D. and West, L. T. (1998), Mohanty and Mousli (2000), Gupta et al. (2006) or Sobieraj et al. (2002). The range of the standard deviation that should be used is indirectly given by the minimum and

the maximum Ks values that were obtained out of database 3_x (variant A). Assuming a specific standard deviation, the 10% and 90% percentiles of the resulting Ks distribution have still to be within the range of Ks values given in database 3_x (variant A). If yes, the hydrological model is ready to start the simulation. If not, the regression function should either be restricted to the range of Ks (this is recommended) or the standard deviation should be forced to a maximum value by the model. After fulfilling this condition, the hydrological model is ready to start. A possibility to effectively process the VGP sets within the hydrological model is given in point 2 ~~3~~ of the above list. We recommend to use at least 3 different VGP sets per soil to describe the spatially variability. However, more sets can be used likewise. It is ~~easily~~ possible to simulate the soil water movement for all VGP sets parallel in one simulation run of the hydrological model. ~~The calculation time is therefore hardly affected.~~ Note that vertical information about soil profiles, if available by the soil map, can be handled with the same procedure as described so far. Hence, the spatial variability of soil hydraulic functions can either be described "horizontal" (if just texture classes without any vertical profile information is available) or "horizontal" + "vertical" (if soil profile information is available, too).

These presented developments were implemented into the hydrological modelling system PANTA RHEI (Förster et al., 2012; Förster, 2013; Kreye et al., 2010, 2012; Kreye, 2015) and were used successfully in many practical applications and projects (e.g. Hölscher et al. (2014); Wurpts et al. (2014); Kreye (2015)). PANTA RHEI has been developed by the Department of Hydrology, Water Management and Water protection, Leichtweiss Institute for Hydraulic Engineering and Water Resources, University of Braunschweig in cooperation with the Institut for water management IfW GmbH, Braunschweig (LWI-HYWAG and IFW, 2012). It is a deterministic, semi-distributed physically based hydrological model for single events or long-term simulations. The temporal discretization is adaptive, for many applications an hourly time step is used. The spatial discretization is divided into three levels: HRUs (hydrologic response units), subcatchments and gauged catchments. Watersheds are the basis for the subcatchments, which contains the HRUs. This spatial discretization makes the model very flexible to account for differences in scale of the input data, likely to the mHm model of Samaniego et al. (2010). A difference between our hydrological model PANTA RHEI compared to many other models is the low number of model parameters that are used for calibration. We work with catchment based model parameters, which have different effects on the sub-catchment scale controlled by physiographic characteristics. This leads to (only) 6-8 model parameters in total to calibrate the model for an area of a many hundred square kilometres.

The structure of the soil model of PANTA RHEI is shown in Fig. 9. Different parametrizations of VGP (e.g. 5) are established by means of lognormal distributions of Ks. After the sets of VGP are derived, we use all of them to parameterize the soil model. As mentioned, we assume that one effective set of VGP cannot express subgrid variability. Secondly, we assume that many different sets of VPG are able to do so. That is why the soil model is parameterized many times, whereby the structure and equations were not changed. These different models (domains) operate individually. However, they are connected to each other. Summarized, it can be argued that we don't have multiple model scenarios, - it is one model with multiple parameterizations solved simultaneously. The impact of the subgrid parameterization of the soil hydraulic functions are dominated by the variation of Ks in wet periods and by the variation of VGP in dry periods. Furthermore, the parameterizations have a feedback on the reduction of evapotranspiration that can be related to the pressure head of the soil (Feddes et al., 1976). The developed soil model is innovative regarding concept, interfaces, and parameterization. The model structure provides the

required interfaces for calibrations made at runoff, ~~satellite based~~soil moisture and/or groundwater level. Therefore, the demand for an automated optimisation procedure arises through the multi-variable examination of the system and its new complexity. A pioneering lexicographical strategy of optimisation was developed, using the model interfaces connected to modern data types (Gelleszun et al., 2015; Kreye, 2015). To account for the impact of the subgrid parameterization, we compared breakthrough curves (1D) with different numbers of VGP sets and with different standard deviations of the Ks distribution functions. We also compared spatially distributed simulation results of the hydrological model for soil moisture with remotely sensed satellite data (ERS1/2-ESCAT, MetOp-ASCAT, ENVISAT-ASAR). The simulated soil water contents turned out to have high accordances with the satellite based soil moisture. In addition to that, the model was able to approximate the dynamics of ground water level in a very high quality compared to measured data (Kreye, 2015). Another possibility to account for subgrid variability is to analyse the standard deviation of soil moisture as a function of the number of applied VGP sets. Further, the spatial soil moisture patterns could be compared in dependence of the number of applied VGP sets, similar to Samaniego et al. (2010). We are working on a pursuing manuscript focusing on the hydrological model and its calibration.

4 Conclusions

The objective of this study was to present a robust procedure to generate various sets of parameterizations of soil hydraulic functions for the description of soil heterogeneity on a subgrid scale. To achieve this, relations between Ks values and van Genuchten's parameters of soil hydraulic functions were investigated. The VGP were obtained with the software ROSETTA. An universal function that is valid for the complete bandwidth of Ks values could not be found. After concentrating on natural texture classes, strong correlations were identified for all parameters. The results of the numerical study presented here confirm the findings of field studies (Li et al., 2007; Botros et al., 2009). The methodology presented in this study is applicable on a wide range of spatial scales and does not need input data from field studies.

Zhu and Mohanty (2002) tried to find effective parameters for van Genuchten's soil hydraulic functions within a numerical study. They conclude that it is very difficult to define a single set of effective parameters that lead to suitable simulation results. In order to avoid effective parameters, the assumption of a parameterization of soil hydraulic functions in dependence of Ks, as presented in this study, is a promising alternative. Therefore, regression functions have to be set up a priori to the hydrological modelling. This is done in a much shorter time than the time needed for acquisition and preparation of other input data for a large scale hydrological model. Further, the procedure is robust in application and additional data (and costs) are not required. When using ROSETTA, a soil map of the modelling area is sufficient.

Our methodology ~~The procedure presented this study~~ can be connected to the work of Wösten et al. (1985), Wösten et al. (1986), Carsel and Parrish (1988) and de Rooij et al. (2004). Wösten et al. (1985) and Wösten et al. (1986) successfully elaborated a procedure to regionalize soil hydraulic properties on the total model area by using measurement point data (for different soil profiles) and soil maps. However, in contrast to our work, they needed measurement data and their modelling area is very small (a few hundred hectares) compared to meso- and macroscale hydrological model areas with several thousand square kilometres. Besides texture data, they used additional soil properties like bulk density or organic matter. The sophisticated

methods for the consideration of subgrid variability presented by Carsel and Parrish (1988) and de Rooij et al. (2004) may be difficult to implement for hydrological modelling, because of needed measurement data (again). However, for future work, it might be interesting to feed their methods with ROSETTA generated input data.

It is worth to discuss the applicability of transferring ROSETTAs results to a distributed hydrological model. An interchange of parameters between different models can be cumbersome. This was e.g. found by Koch et al. (2016) by using the model HYDRUS 1D to fit VGPs, which were passed to several hydrological models (MIKE SHE, HydroGeoSphere and ParFlow-CLM). The fitting in HYDRUS 1D was done by means of continuously measured time series of soil moisture at different locations and depths. HYDRUS 1D also incorporates a ROSETTA interface, but here inverse modelling was used to fit VGP. To parametrize the hydrological models, Koch et al. (2016) homogeneously used the same VGP at every spatial location. In a second (heterogeneous) scenario they used spatially differentiated porosity (saturated water content), but all other VGP were still homogenously distributed. Hence, they nicely concluded that *future work must focus on other possibilities to further distribute the remaining VGP parameters*. One possibility to achieve this on the mesoscale is what we introduced in our study. However, we do not use another model (like HYDRUS 1D) to estimate VGP by means of inverse modelling. Besides the need of measured input data, it is a challenge to regionalize the obtained (1D) results of a model like HYDRUS 1D to a spatial fully distributed hydrological model. As ROSETTA is based on neural network analyses, it servs as a pedotransfer function for the estimation of VGP and Ks. Data with different level of detail can be used as input, starting with texture classes and going up to more detailed (experimentally determined) information. However, ROSETTA doesn't fit VGPs and Ks by means of measured time series of e.g. soil moisture or pressure head. Hence, we again want to point out that ROSETTA has to be defined as pedotransfer function rather than using the term model. Compared to point measurements of VGP, ROSETTA is not always capable to perform a perfect fit, see e.g. Pandey et al. (2005), Li et al. (2007) or Ghorbani Dashtaki et al. (2010). However, considering the huge sizes of model areas that are common for hydrological model applications, ROSETTA is a good choice to generate parameters covering the complete area.

~~It is worth of discussion that the high correlations between ROSETTA generated Ks and the other VGP are possibly artificially caused by ROSETTA itself. The neural network establishes relations between the percentage fractions of texture classes and the VGP each. This implicitly may lead to artificial correlations between the VGP. Looking at the citet field studys on the other hand, correlations seem to exist. However, assuming that ROSETTA actually boosts the correlations to a certain extent, - the message of this study is still the same.~~

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Table 1. Definitions of the used texture classes. The fractions of sand, silt and clay is processed out of the soil map for Lower Saxony (Edt.: J. Boess et al., 2004) and the German soil classification system (Sponagel, 2005).

Abbreviation	**Definition**	**Sand [%]**	**Silt [%]**	**Clay [%]**
Lt	Clayey loam	25	40	35
Lu	Silty loam	18.5	58	23.5
Ls	Sandy loam	44	35	21
Ut	Clayey silt	9	74	17
Ul	Loamy silt	27	58	15
Us	Sandy silt	32.5	65	2.5
Sl	Loamy sand	65	25	10
Su	Silty sand	63.5	32.5	4
S	Sand	85	10	5
Ss	Pure sand	92.5	5	2.5

Table 2. Obtained coefficients of determination (R^2), Spearman correlation (r_{spear}) and belonging p-value (p) as well as the sample size (Samples) for the regressions between the Ks values and the soil hydraulic parameters for each texture class. Lu = silty loam, Ls = sandy loam, Ut = clayey silt, Ul = loamy silt, Us = sandy silt, Sl = loamy sand, Su = silty sand, S = Sand, Ss = Pure sand.

Texture	Statistic	van Genuchten parameters			
		Θ_R	Θ_S	n	α
Lu	R^2	0.94	0.82	0.78	0.73
	r_{spear}	0.97	0.91	0.86	0.88
	p	0.00	0.00	0.00	0.00
	Samples	13829			
Ls	R^2	0.88	0.90		
	r_{spear}	0.94	0.95		
	p	0.00	0.00		
	Samples	50648			
Ut	R^2	0.99		0.93	
	r_{spear}	1.00		0.96	
	p	0.00		0.00	
	Samples	6822			
Ul	R^2	0.98		0.63	
	r_{spear}	0.99		0.79	
	p	0.00		0.00	
	Samples	12995			
Us	R^2	0.99	0.78	0.56	0.96
	r_{spear}	1.00	0.89	0.74	0.98
	p	0.00	0.00	0.00	0.00
	Samples	3093			
Sl	R^2	0.92	0.68	0.88	0.67
	r_{spear}	0.95	0.83	0.96	0.80
	p	0.00	0.00	0.00	0.00
	Samples	7202			
Su	R^2	0.99	0.93	0.76	0.63
	r_{spear}	0.99	0.96	0.92	0.78
	p	0.00	0.00	0.00	0.00
	Samples	6364			
S	R^2			1.00	
	r_{spear}			1.00	
	p			0.00	
	Samples	1455			
Ss	R^2			0.98	
	r_{spear}			0.99	
	p			0.00	
	Samples	479			
	Mean R^2	0.96	0.82	0.85	0.75
	Mean r_{spear}	0.98	0.91	0.90	0.86

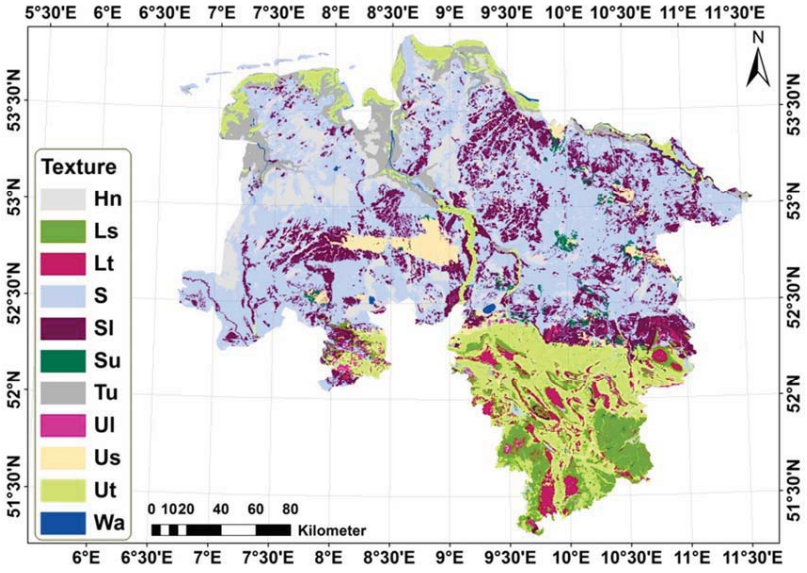

Figure 1. Soil map of Lower Saxony, Germany (Edt.: J. Boess et al., 2004). Ls = sandy loam, Lt = clayey loam, S = sand, Sl = loamy sand, Su = silty sand, Tu = silty clay, Ul = loamy silt, Us = sandy silt, Ut = clayey silt, see Table 1. In addition to that, "Hn" stands for boggy soils and "Wa" stands for water bodies (lakes, rivers).

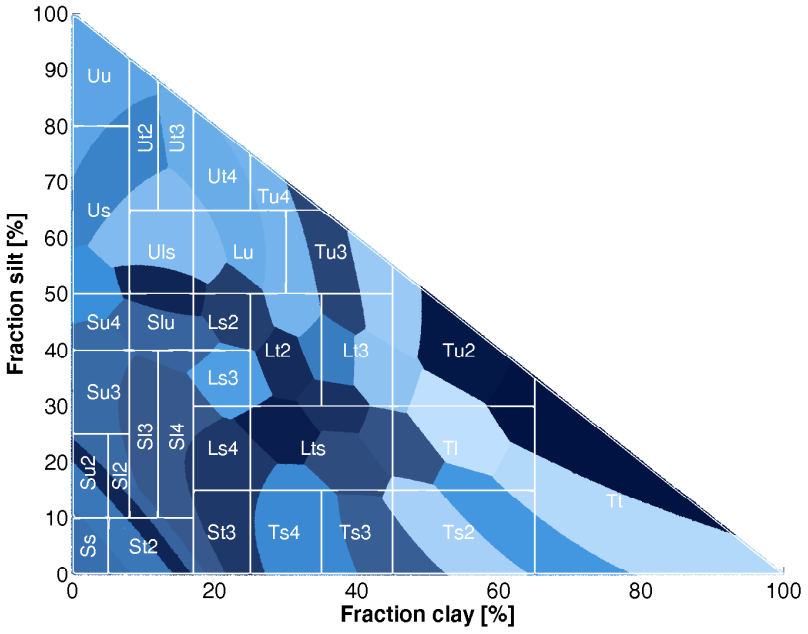

Figure 2. Subdivision of the soil texture by means of cluster analyses based on 31 classes (blue colored polygons). The classes were divided by similarity of their soil hydraulic parameters (cf. Twarakavi et al. (2010)). The subdivisions of the german soil classification system (cf. Sponagel (2005)) are overlayed with white lines.

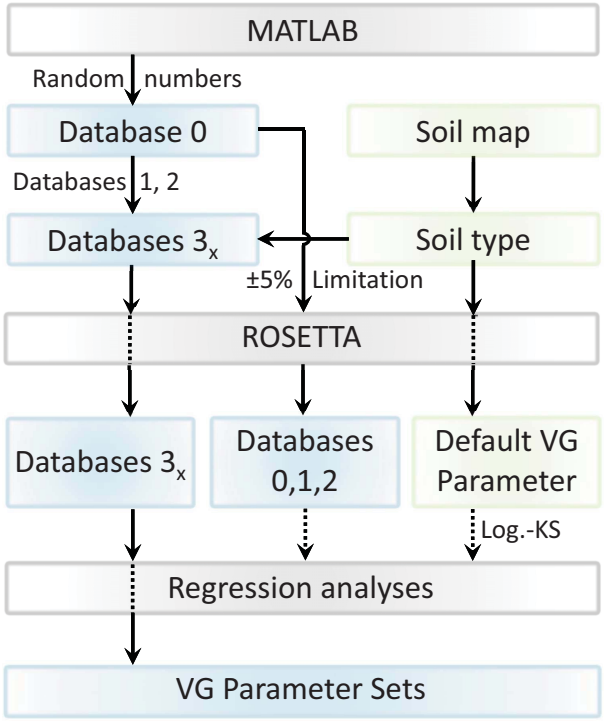

Figure 3. Procedure to obtain van Genuchten (VG) parameters and the saturated hydraulic conductivity (Ks) values based on soil map information. The Software ROSETTA is based on neural network analyses and generates van Genuchten parameters and Ks values out of soil texture information.

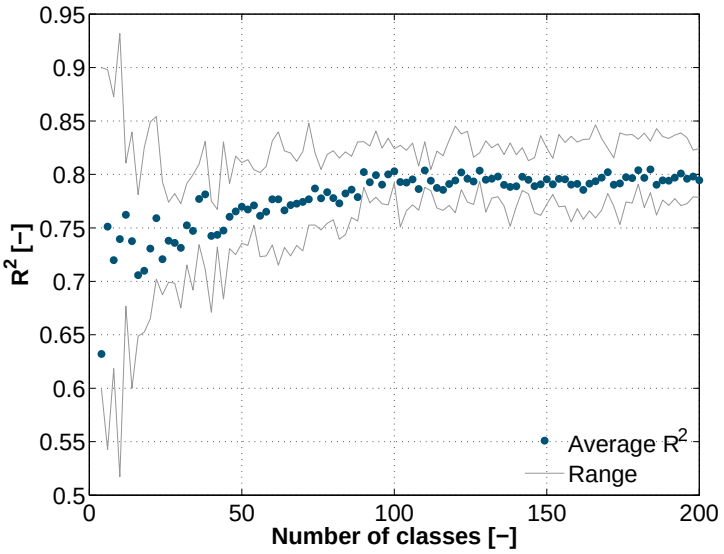

Figure 4. Average coefficient of determination (R^2) in dependency of the number of classes used for the subdivisions based on soil hydraulic properties by means of cluster analyses. The average R^2 is calculated out of the R^2 of all classes for each case. For this calculation, only classes with $R^2 > 0.5$ were considered. In addition to that, the range of R^2 is shown. The range yields out of the maximum and minimum R^2 of the individual classes.

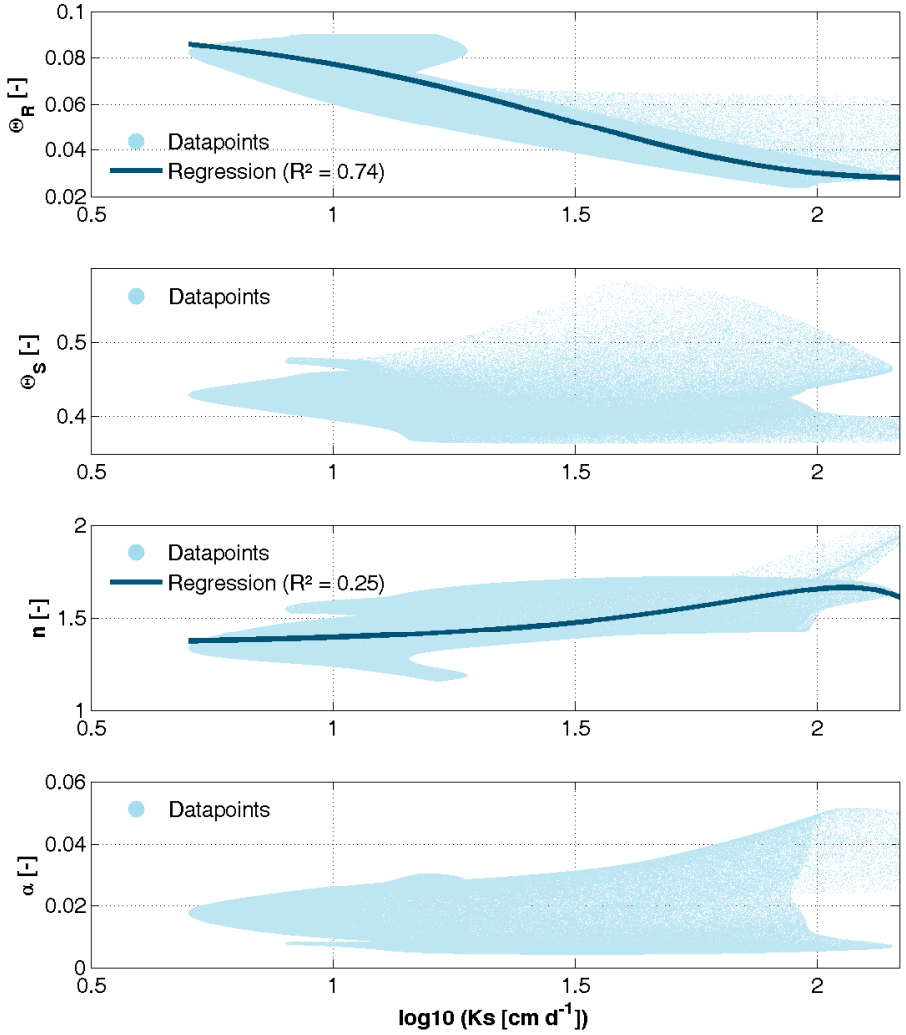

Figure 5. Scatterplots of the van Genuchten parameters (Θ_R, Θ_S, n, α) in dependency of the saturated hydraulic conductivity (Ks). Visualized is database 1 ($\Theta_R - Ks$) and database 2 ($\Theta_S - Ks, n - Ks$ and $\alpha - Ks$). A regression function with a coefficient of determination (R^2) of 0.74 was fitted between Θ_R and Ks. Furthermore, a regression function with an R^2 of 0.25 was fitted between n and Ks. $\Theta_S - Ks$ as well as $\alpha - Ks$ showed no correlation.

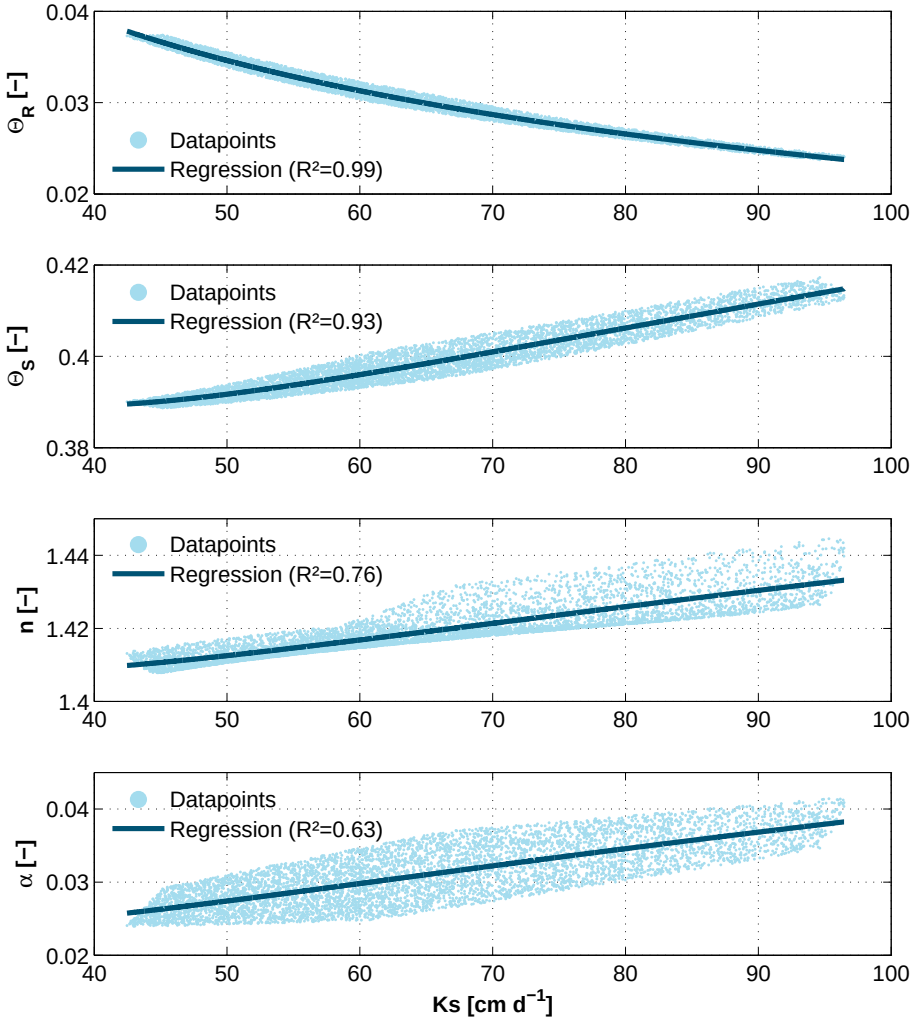

Figure 6. Scatterplots of the van Genuchten parameters VGP (Θ_R, Θ_S, n, α) in dependency of the saturated hydraulic conductivity (Ks) for the texture class Su (silty sand) out of database 3_x (variant A). Regression functions were fitted for all variants of VGP - Ks. R^2 = coefficient of determination.

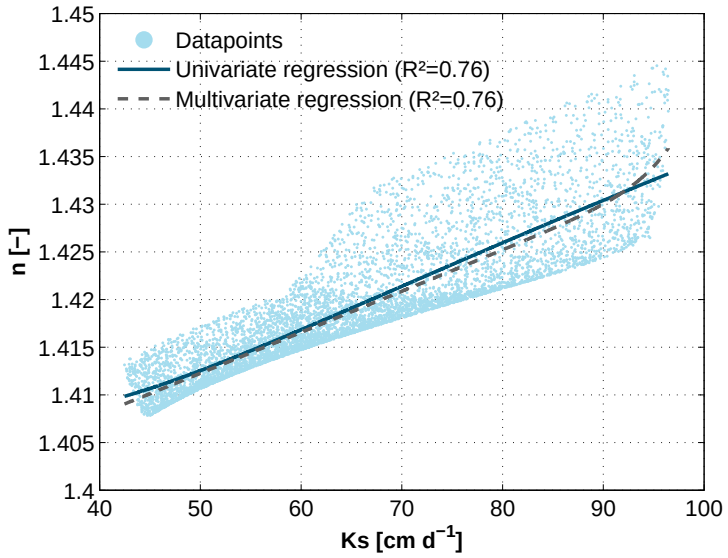

Figure 7. Scatterplot of the van Genuchten parameter n in dependency of the saturated hydraulic conductivity (Ks) for the texture class Su (silty sand) out of database 3_x (variant A). To compare the univariate and multivariate regression, both functions are shown in the graph. R^2 = coefficient of determination.

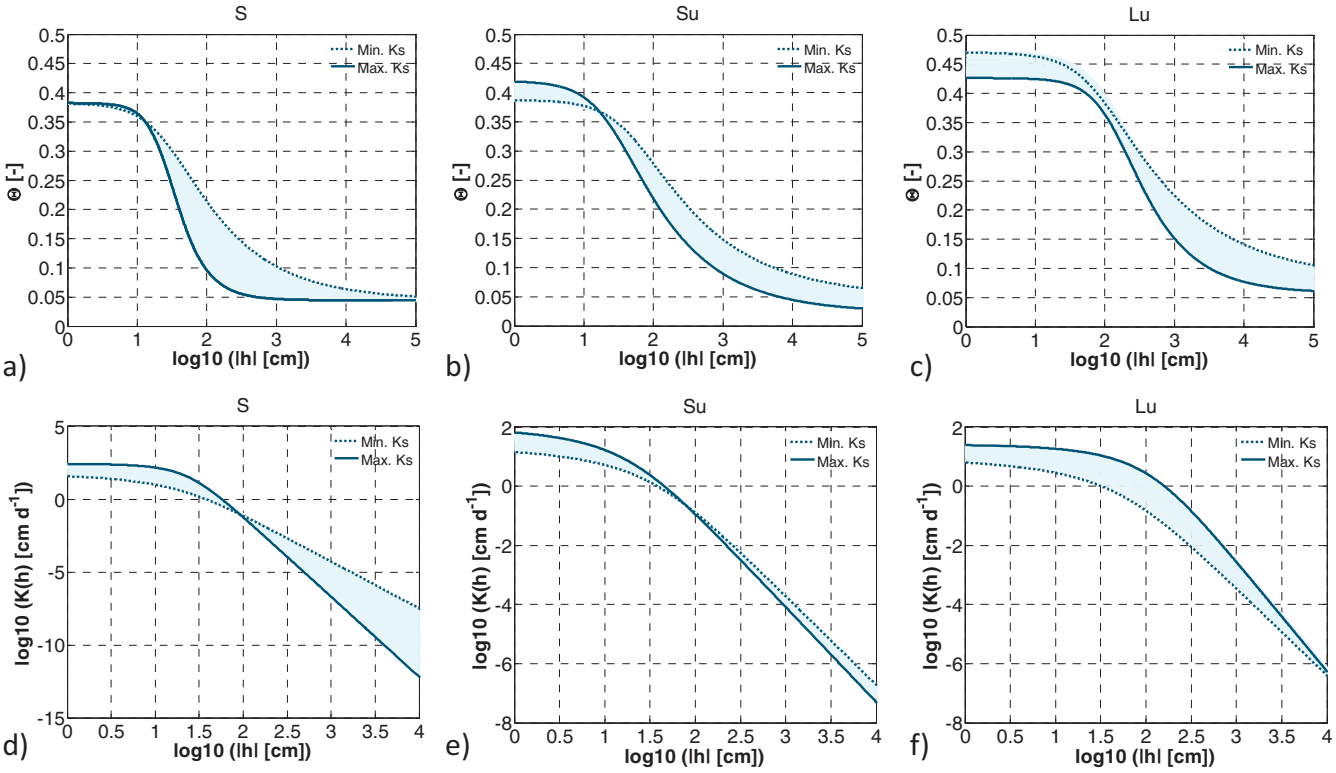

Figure 8. Impact on the pF- and $K(h)$-curves due to the univariate regression functions out of database 3_x (variant A). pF = log10 of absolute pressure head h. $K(h)$ = hydraulic conductivity in dependency of pressure head. Θ = volumetric water content. The Minimum and maximum saturated hydraulic conductivities (Ks) were given by ROSETTA. The van Genuchten parameters were changed in dependency of Ks by means of the regression functions. a: pF curves for the texture class S (sand). b and c: The same as shown in a, but for the texture classes Su (silty sand) and Lu (silty loam). d: Hydraulic ~~Unsaturated~~ conductivity curves for the texture class S. e and f: The same as shown in d, but for the texture classes Su and Lu.

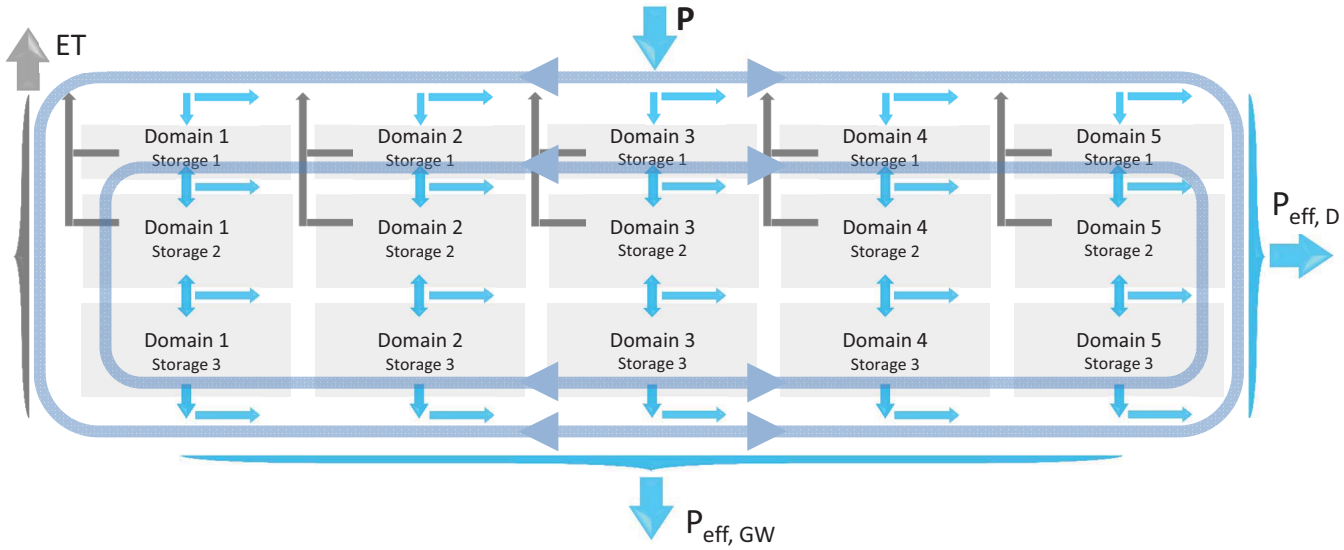

Figure 9. Application of different van Genuchten parameter sets on the soil model of the hydrological modelling system PANTA RHEI. The different parametrizations (domains) are parallel used at all spatial locations. The domains are solved simultaneously and with interaction to each other. The main input is given by the spatial precipitation (P), which was reduced in advance by vegetational interception. Results of the soil model are the direct runoff ($P_{eff,D}$), the groundwater recharge ($P_{eff,GW}$), which leads to base flow in a long term view, and actual evapotranspiration (ET).

Comment by the authors

We thank reviewer 2, Anatoly M. Zeyliger, for his detailed comments. This will help us to improve the manuscript.

Specific comments

> *The research on this article is based on a some statistical analyses of correlations between parameters linked with ROSETTA within the UNSODA soil database.*
> *In our opinion scientific significance of this research is limited by the use of the same database for analyzing relationships between saturated soil hydraulic conductivity and parameters of soil water retention curves where fitted. This limitation may be overcome by the use of another soil database like HYPRES to approve obtained results and may could provide a way for large verification of derived clusterization for any soil classes.*

As a pedotransfer function, ROSETTA works independent from its databases, which were used for its calibration. Besides UNSODA two other soil databases were used to calibrate the neural network of ROSETTA (Schaap et al., 1998). Of course you are right that our results are valid within the framework of ROSETTA only. However, parameterization of soil hydraulic functions on the hydrological meso- and macroscale are always based on one database or pedotransfer function. To have more variable van Genuchten parameter (VGP) sets, we use the method introduced in our manuscript. This methods requires many virtual sets of VGP, which can only be derived with pedotransferfunctions like ROSETTA. An inclusion of more databases (like HYPRES) is a good idea, but this demands for different methods (in our point of view).

> *In our opinion a scientific quality is also limited by the use of parameters of specific empirical models describing shapes of both unsaturated soil hydraulic properties that are "not always valid".*

We are not sure, if we understand your statement correctly. We don't use the empirical regression functions or their parameters to describe the shapes of pF and conductivity curves directly. The regression functions are only used to vary VGP. In case of low or no correlations between the saturated hydraulic conductivity and a VGP, we don't change this VGP.

> *First of all it is quite important for modeling infiltration to use adequate models for fitting and should be discussed more deeply according to some textural classes of soil and organic matter content. Thus is really important in many rainfall events for upper soil horizons with macropore structure controlling infiltration into soil profile which is not taken into account by selected Mualem-van Genuchten models.*

Yes, you are right that Mualem-van Genuchten is valid for matrix flow. However, the calculation module of infiltration and percolation within the hydrological model PANTA RHEI uses different pathways to account for preferential flow (Kreye, 2015). In addition to that, using different sets of VGP at the same spatial location has a similar effect: We don't have a "homogeneous" soil matrix. If e.g. soil moisture conditions are high, the VGP set with high saturated conductivity becomes dominant. In dry conditions, it could be the other way round.

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Comment by the authors

We thank anonymous reviewer 3 for her/his detailed comments. This will help us to improve the manuscript.

Specific comments

ROSETTA is a calibrated model which has effective parameters itself, as it is based on an imperfect model structure. This means that parameters found suitable for ROSETTA might not be very applicable in a distributed hydrological model. This was found by Koch et al. (2016) where parameters from a surrogate model (HYDRUS1D) were passed on to distributed models and it became clear that parameters are not easily interchangeable between models.
Along these lines it may be doubtful that the regression model between parameters of one model is transferable to another model. I would ask the authors to reflect on their assumption that the regression models found in ROSETTA are still valid in a more complex distributed hydrological model.

First, we would like to add some information regarding ROSETTA. This software is based on neural network analyses and servs as pedotransfer function for the estimation of van Genuchten water retention parameters (VGP) and the saturated hydraulic conductivity (Ks). Data with different level of detail can be used as input, starting with texture classes and going up to more detailed (experimentally determined) information (Schaap et al., 2001). However, ROSETTA doesn't fit VGPs and Ks by means of measured time series of e.g. soil moisture or pressure head. Hence, we prefer to define ROSETTA as "pedotransfer function" rather than using the term "model". Koch et al. (2016) used the model HYDRUS 1D to fit VGPs (thank you for this reference). This was done by means of continuously measured time series of soil moisture at different locations and depths. HYDRUS also incorporates a ROSETTA interface, but here inverse modelling was used to fit VGP. I totally agree with you, that it could be troublesome to transfer the VGP, which were determined by this manner, from HYDRUS to more complex hydrological models (but this isn't what we did). To parametrize their model, Koch et al. (2016) homogeneously used the same VGP at every spatial location for hydrological modelling. In a second (heterogeneous) scenario they used spatially differentiated porosity (saturated water content), but all other VGP are still homogenously distributed. Hence, they nicely conclude that „*future work must focus on other possibilities to further distribute the remaining VGM parameters*". One possibility to achieve this on the mesoscale is what we introduce in our study. Summary: We use ROSETTA as pedotransfer function to estimate VGP.

Section 3.3 nicely presents the workflow of the presented approach. However I would like to ask the authors to clarify how the VGP sets are incorporated in the hydrological model. Again, how can the authors support that the mean Ks value obtained from ROSETTA can be regarded as the mean Ks value for the more complex hydrological model, that may requires model dependent effective parameters (p.12,l.20). Instead a prior calibration of the hydrological model could be used to obtain suitable mean Ks values.

We feed ROSETTA with texture information based on soil maps (in our case, the soil map of Lower Saxony, 1:50.000). Therefore, the Ks values estimated by ROSETTA are effective that are values valid for the spatial resolution of the soil map. The simulations of soil water dynamics inside the hydrological model operate on the same spatial resolution as the soil map, because the spatial distribution of our hydrological model (PANTA RHEI) is based on polygons. To establish subgrid variability, we create distribution functions of Ks and VGP as described in the manuscript. But (and this is an important fact), we don't change the effective VGP/Ks set in order to calibrate the hydrological model.

How many sets of VGP sets should be used (p.12,l.24)?

The number of sets is up to the user. At least three sets should be used. In our manuscript we recommend five sets by using the 10%, 30%, 50%, 70% and 90% percentile of the Ks distribution function. Of course, more sets are possible.

Also, the authors should give guidance how the subgrid spatial variability can be quantified after all VGP sets are executed (p.12,l.20)? The standard deviation of soil moisture at each cell?

Yes, a possibility to account for subgrid variability is to analyse the standard deviation of soil moisture as a function of the number of applied VGP sets. Further, the spatial soil moisture patterns could be compared in dependence of the number of applied VGP sets, similar to Samaniego et al. (2010) (thank you for this reference). We compared breakthrough curves (1D) with different numbers of VGP sets and with different standard deviations of the Ks distribution functions. We also compared spatially distributed simulation results of the hydrological model for soil moisture with remotely sensed satellite data, but this goes beyond of this study. We are working on a pursuing manuscript focusing on the hydrological model and its calibration.

Also I did not fully understand if the authors suggest having multiple model scenarios, where each scenario is based on a different Ks value drawn from the Ks distribution for each soil class? Or if they suggest to generate stochastic fields of Ks values that are applied in the distributed model?

You are right, we have to be more precise. After the different sets of VGP (e.g. 5) are derived, we use all of them to parameterize the soil model, which is incorporated in the hydrological model (PANTA RHEI). We assume, that one effective set of VGP cannot express subgrid variability (as described in the manuscript). Secondly, we assume, that many different sets of VPG are able to do so. That's why the soil model is parameterized many times, whereby the structure and equations were not changed. These different models (domains) operate simultaneously and at the same spatial location and are connected to each other. Please take a look to the attached figure. At every spatial location (the resolution is determined by the soil map) we have different effective VGP and for every spatial location we parameterize 5 different VGP sets. The attached figure shows the idea at an abstract level, in fact our model is polygon based (and not grid based). Summary: we don't have multiple model scenarios. It is one model with multiple parameterizations.

In section 3.3 the authors address the problem of scale and that a pseudo accuracy can be created if the model is operated at smaller scales than its input. Often model input comes at various scales and in fact hydrological processes take place at various scales as well. Here, the mHm model (Samaniego et al., 2010) provides a very flexible platform at account for differences in scale in the input data and parameters. The authors should mention modelling alternatives in their manuscript.

We didn't want to focus too much on the hydrological model. However, we agree to add more information here. Thank you again for the reference, we will pick this up in our manuscript. A big difference between our hydrological model PANTA RHEI compared to many other models is the number of model parameters that are used for calibration. We work with catchment based model parameters, which have different effects on the sub-catchment scale controlled by physiographic characteristics. This leads to (only) 6-8 model parameters in total to calibrate the model for an area of a few hundred square kilometres.

The authors mention that regression between Ks and the VGP could be artificially caused by ROSETTA. If this is the case, how do the authors support their suggested approach at all? What are the "real" regression models between Ks and other VGP and how wrong is ROSETTA? Again, this should be linked to the question if the same regression model can be assumed valid in a more complex hydrological model?

Results of ROSETTA are estimations and anyhow effective values. These effective values are "never correct" if compared to experimentally derived ("real") values. However, the advantages of ROSETTA are scale equality and that no experimental measurements are necassary. For that reason, these parameters are suitable for hydrological modelling. But, if we use one VGP set it may not be possible to describe all conditions of soil water in a plausible way. For instance, soil water dynamics could be well approximated for wet situations, but provide inadequate simulations for dry situations (this was also a problem of the simulations performed in Koch et al. (2016)). Hence, we use more than on set of VGP.
Connections between (experimentally derived) Ks and VGP are found in many studies, as described in our manuscript. Using ROSETTA we find quite strong connections. That's why we discuss at which proportion this could be enhanced by the artificial

network. However, we think, that even if ROSETTA boost the connections between Ks and VGP it is admissible to generate distribution functions based on these connections as our focus is finding different "possibilities" to describe soil hydraulic behaviour within a certain framework.

100

References

Koch, J., Cornelissen, T., Fang, Z., Bogena, H., Diekkrüger, B., Kollet, S., and Stisen, S.: Inter-comparison of three distributed hydrological models with respect to seasonal variability of soil moisture patterns at a small forested catchment, Journal
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Comment by the authors

We thank Dr. Hans Thodsen for his comments. This will help us to improve the manuscript.

Specific comments

> *The text can in some sections be hard to follow for a non soil-scientist as my self (hydrological modeler) because of the large number of symbols and abbreviations.*

We could add a short appendix with a list of abbreviations, if the editor agrees.

> *Generally the figure captions needs to explain the symbols used in the figures, to comply with the "being able to stand alone" criteria.*

We totally agree and are going to improve the figure captions.

> *How is the Ks and other values included in the hydrological model? And how does the model handle the parameter-variation within each soil class (if I understand you right)? Please give an example of the difference the use of different parameter settings makes to the model outcome. Please state what the hydrological model is evaluated against.*

In the following, we partly use similar explanations as in our answer to reviewer 3, which we uploaded just shortly before you made your comment.

We use all derived sets of van Genuchten parameters (VGP) and Ks to parameterize the soil hydraulic functions of the soil model, which is incorporated in the hydrological model (PANTA RHEI). Hence, the soil model is parameterized many times with different VGP sets for the same location; the structure and equations were not changed. These "different" models (domains) operate simultaneously and are connected to each other. Summary: We have one model with multiple parameterizations (please take a look at the attached figure in our answer to reviewer 3).

We compared breakthrough curves (1D) with different numbers of VGP sets and with different standard deviations of the Ks distribution functions. Soil moisture patterns could also be compared in dependence of the number of applied VGP sets. The model is evaluated against three types of observations/data: discharge, spatial distributed soil moisture (satellite data, ERS1/2-ESCAT, MetOp-ASCAT, ENVISAT-ASAR) and groundwater level. The satellite soil moisture data accounts for the upper few cm of the soil surface. The groundwater level data accounts for the lower boundary of the soil model. Individual objective functions were used and connected to a stepwise Downhill-Simplex to calibrate the model parameters. To achieve this, a lexicographical strategy was developed, where different objectives can be defined as an order of preference (see also Gelleszun et al., 2015). At the moment, we are working on a pursuing manuscript focusing on the hydrological model and its calibration.

> *9/6 How can the multivariate method give a worse fit than the linear?*

The average R^2 are nearly the same (rounded numbers). We think that both methods achieve the same performance and the small difference in R^2 can be explained by the optimization algorithm (we used Levenberg-Marquardt, which is a local algorithm).

References

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