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Key Points:
- Derive the new closed-form expression based on VGM model
- Predict subgrid variability of soil water content
- Inversely estimate the spatial variability of hydraulic properties

Supporting Information:
- Text S1
- Figure S1
- Figure S2
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- Table S1
- Table S2

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Predicting subgrid variability of soil water content from basic soil information

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Abstract Knowledge of unresolved soil water content variability within model grid cells (i.e., subgrid variability) is important for accurate predictions of land-surface energy and hydrologic fluxes. Here we derived a closed-form expression to describe how soil water content variability depends on mean soil water content ($\sigma_\theta(<\theta>)$) using stochastic analysis of 1-D unsaturated gravitational flow based on the van Genuchten-Mualem (VGM) model. A sensitivity analysis showed that the *n* parameter strongly influenced both the shape and magnitude of the maximum of $\sigma_\theta(<\theta>)$. The closed-form expression was used to predict $\sigma_\theta(<\theta>)$ for eight data sets with varying soil texture using VGM parameters obtained from pedotransfer functions that rely on available soil information. Generally, there was good agreement between observed and predicted $\sigma_\theta(<\theta>)$ despite the obvious simplifications that were used to derive the closed-form expression. Furthermore, the novel closed-form expression was successfully used to inversely estimate the variability of hydraulic properties from observed $\sigma_\theta(<\theta>)$ data.

1. Introduction

Soil water content is known to be heterogeneously distributed in space due to variation in soil and vegetation properties, climate, and topography among other factors [*Grayson et al.*, 1997]. Part of this heterogeneity is typically not resolved by the coarse resolution of many large-scale land-surface models or remote sensing measurements. Nevertheless, it is well established that such unresolved small-scale or subgrid variability of soil water content is an important control on the magnitude of land-surface energy fluxes [*Ronda et al.*, 2002] and hydrologic fluxes such as runoff [*Gedney and Cox*, 2003]. To allow an adequate representation of small-scale soil water content variability in large-scale hydrologic, weather, and climate models, information on the relationship between subgrid soil water content variability as expressed by the standard deviation (σ_θ) and mean soil water content ($<\theta>$) would be beneficial [*Teuling and Troch*, 2005]. Improved ability to predict this relationship from basic soil data may contribute to a more efficient representation of soil water content variability in large-scale models, and consequently in more accurate predictions of land-surface processes [*Vereecken et al.*, 2008, 2014].

Reynolds [1970] was the first to derive relationships between measured σ_θ and $<\theta>$ as well as other controlling factors, i.e., insolation and rainfall. Since then, numerous field studies have been carried out to identify factors that control the $\sigma_\theta(<\theta>)$ relationship. Several studies found that σ_θ increased with increasing $<\theta>$ [*Oldak et al.*, 2002; *Takagi and Lin*, 2011], whereas *Famiglietti et al.* [1999], *Hupet and Vanclooster* [2002], and *Western et al.* [2004] observed the opposite behavior. Moreover, a convex parabolic shape of the $\sigma_\theta(<\theta>)$ relationship with a distinct maximum in the medium range of $<\theta>$ has been observed [*Choi and Jacobs*, 2007; *Garcia-Estringana et al.*, 2013; *Rosenbaum et al.*, 2012].

Widely used methods to investigate controls on the $\sigma_\theta(<\theta>)$ relationship include virtual simulation experiments [*Albertson and Montaldo*, 2003; *Montaldo and Albertson*, 2003] and stochastic analysis [*Zhang et al.*, 1998]. Virtual experiments by *Albertson and Montaldo* [2003] and *Teuling and Troch* [2005] showed that the covariances between the soil water state and land-surface fluxes (i.e., infiltration, drainage, evapotranspiration, and horizontal redistribution) act to generate or destroy spatial variability of soil water content through time. *Zhang et al.* [1998] used stochastic analysis to derive an analytical expression that describes $\sigma_\theta(<\theta>)$ for 1-D unsaturated gravitational flow using the Brooks-Corey and the Gardner-Russo models for water retention and hydraulic conductivity. Following *Zhang et al.* [1998], *Vereecken et al.* [2007] demonstrated that the shape of $\sigma_\theta(<\theta>)$ can be explained to a large extent by the spatial variance of soil hydraulic properties, although they did not provide a direct evaluation using measured $\sigma_\theta(<\theta>)$ data and information on the spatial variation of hydraulic properties. These previous stochastic studies relied on the use of the Brooks-Corey or the Gardner-Russo model because of their mathematical tractability. However, it is generally accepted that the van Genuchten-Mualem (VGM) model [*van Genuchten*, 1980] is better suited to describe experimental soil water retention data.

In this paper, we first derive a closed-form expression for $\sigma_\theta(<\theta>)$ using stochastic analysis of 1-D unsaturated gravitational flow based on the VGM model. A sensitivity analysis is presented to identify the effect of VGM parameters on $\sigma_\theta(<\theta>)$. Next, the predictions of the novel closed-form expression for $\sigma_\theta(<\theta>)$ are evaluated using eight data sets of observed $\sigma_\theta(<\theta>)$ relationships obtained at test sites with a wide range of VGM parameters as determined from pedotransfer functions that rely on available basic soil data. Finally, we inversely estimate the variability of hydraulic properties from observed $\sigma_\theta(<\theta>)$ data.

2. Model Development

The stochastic approach of *Zhang et al*. [1998] to describe 1-D unsaturated gravitational flow in a heterogeneous flow domain was used to derive a closed-form expression that describes $\sigma_\theta(<\theta>)$ as a function of the mean and standard deviation of the soil hydraulic parameters of the VGM model. The starting point of this derivation is the steady state simplification of the Richards equation:

$$\frac{\partial}{\partial x}\left[K(h)\left(\frac{\partial h}{\partial x}+1\right)\right]=0 \tag{1}$$

where $K(h)$ (cm d^{-1}) is the unsaturated soil hydraulic conductivity, h (cm) is the pressure head, and x (cm) is the vertical coordinate. The VGM model to describe the soil water retention and hydraulic conductivity curves is given by

$$S_e(h)=\frac{\theta-\theta_r}{\theta_s-\theta_r}=\frac{1}{\left(1+(\alpha|h|)^n\right)^m},\quad h<0 \qquad m=1-\frac{1}{n} \tag{2}$$

$$K(S_e)=K_sS_e^{0.5}\left[1-\left(1-S_e^{1/m}\right)^m\right]^2,\quad h<0 \tag{3}$$

For mathematical convenience, the log-transformed saturated hydraulic conductivity ($\ln(K_s)$) is used in our study. In our analysis, residual soil water content (θ_r) is assumed to be constant. All other variables and parameters, i.e., pressure head (h), soil water content (θ), hydraulic conductivity (K), effective saturation degree (S_e), saturated soil water content (θ_s), saturated hydraulic conductivity (K_s), and the fitting parameters α and n of the VGM model are considered to be realizations of a second-order stationary stochastic process, which can be decomposed into their mean and perturbations. Following the stochastic analysis of *Zhang et al*. [1998], we derived the expressions of the mean and covariance of soil water content for 1-D unsaturated gravitational flow in an infinitely long vertical profile using first-order Taylor expansions. In particular, we related the covariance of soil water content and pressure head to the variance and covariance of VGM parameters (K_s, θ_s, α, and n) using equations (1)–(3). For a detailed derivation we refer to the supporting information (Text S1). The closed-form expression for $\sigma_\theta(<h>)$ is

$$\begin{aligned}\sigma_\theta^2={b_0}^2\Bigg\{&{b_1}^2\sigma_\alpha^2+{b_2}^2\left[\frac{\sigma_f^2\rho_f}{(1+a_2\rho_f)a_2}+\frac{a_1\sigma_\alpha^2\rho_\alpha}{(1+a_2\rho_\alpha)a_2}+\frac{a_3\sigma_n^2\rho_n}{(1+a_2\rho_n)a_2}\right]\\&+{b_3}^2\sigma_n^2+{b_4}^2\sigma_{\theta_s}^2+2b_1b_2\left(-\frac{a_1\sigma_\alpha^2\rho_\alpha}{1+a_2\rho_\alpha}\right)+2b_2b_3\left(-\frac{a_3\sigma_n^2\rho_n}{1+a_2\rho_n}\right)\Bigg\}\end{aligned} \tag{4}$$

$$\text{where } b_0=(\langle\theta_s\rangle-\theta_r)\left(\frac{\langle\alpha\rangle\langle h\rangle}{\left[1+(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}\right](\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}\langle n\rangle}\right);$$

$$b_1=\frac{\langle n\rangle(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}+1-\langle n\rangle}{\langle\alpha\rangle}-\frac{\left[\langle n\rangle(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}+1\right](\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}}{1+(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}}\frac{\langle n\rangle}{\langle\alpha\rangle};$$

$$b_2=\frac{\langle n\rangle(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}+1-\langle n\rangle}{\langle h\rangle}-\frac{\left[\langle n\rangle(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}+1\right](\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}}{1+(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}}\frac{\langle n\rangle}{\langle h\rangle};$$

$$b_3 = -\frac{1}{\langle n\rangle} - \ln(\langle\alpha\rangle\langle h\rangle) - \frac{\left[\langle n\rangle(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}+1\right](\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}}{1+(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}}\ln(\langle\alpha\rangle\langle h\rangle);$$

$$b_4 = \langle n\rangle(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}+1;$$

$$a_1 = \frac{\left(\frac{5}{2}-\frac{1}{2\langle n\rangle}\right)(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}}{1+(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}}\frac{\langle n\rangle}{\langle\alpha\rangle};$$

$$a_2 = \frac{\left(\frac{5}{2}-\frac{1}{2\langle n\rangle}\right)(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}}{1+(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}}\frac{\langle n\rangle}{\langle h\rangle};$$

$$a_3 = \frac{\left(\frac{5}{2}-\frac{1}{2\langle n\rangle}\right)(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}}{1+(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}}\ln(\langle\alpha\rangle\langle h\rangle) + \frac{\ln\left[1+(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}\right]}{2\langle n\rangle^2} - \frac{2}{\langle n\rangle^2-\langle n\rangle};$$

$$f = \ln(K_s).$$

This novel closed-form expression describes $\sigma_\theta(<h>)$ as a function of the mean (i.e., $<\theta_s>$, $<\ln(K_s)>$, $<\alpha>$, and $<n>$), the standard deviation (i.e., $\sigma(\theta_s)$, $\sigma(\ln(K_s))$, $\sigma(\alpha)$, and $\sigma(n)$), and the vertical correlation length (i.e., $\rho_{\ln(Ks)}$, ρ_α, and ρ_n) of the VGM model parameters. Using the following equation, $<h>$ can be transformed into $<\theta>$

$$\langle\theta\rangle = (\langle\theta_s\rangle-\theta_r)\left(\frac{\langle\alpha\rangle\langle h\rangle}{1+(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}}\right)\left(\frac{\langle n\rangle(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}+1}{\langle n\rangle(\langle\alpha\rangle\langle h\rangle)^{\langle n\rangle}}\right)+\theta_r \quad (5)$$

In order to assess the importance of the pressure head fluctuations that result from flow in the heterogeneous soil profiles, we also calculated $\sigma_\theta(<\theta>)$ for $h'=0$ (i.e., assuming that the system has the same pressure head everywhere) in the supporting information. It is important to realize that the obtained σ_θ represents variability along a deep vertical profile. Since soil water content is assumed to be an ergodic second-order stationary stochastic variable, σ_θ in vertical direction corresponds with σ_θ at a certain depth (i.e., spatial variability) if sampling points are sufficiently far from each other (i.e., sampling points are independent when separation is more than the horizontal correlation length of the soil properties). It should also be noted that the vertical water flux is assumed to be identical at every location so that the effect of lateral water redistribution and variability in surface fluxes is not considered.

3. Materials and Methods

3.1. Site Descriptions

We used eight different data sets from five test sites to evaluate the ability of the closed-form expression (equation (4)) to describe observed $\sigma_\theta(<\theta>)$ data. Detailed information about the test sites are given in Table S1 in the supporting information. Three data sets were obtained using wireless sensor networks deployed at the Terrestrial Environmental Observatories (TERENO) test sites Rollesbroich, Wüstebach, and Scheyern [*Terrestrial Environmental Observatories*, 2012]. For these three sites, hourly aggregated soil water content data measured at three depths (5, 20, and 50 cm for Rollesbroich and Wüstebach, and 10, 30, and 50 cm for Scheyern) were used. In addition, we used data sets that originated from the *Inner Mongolia Grassland Ecosystem Research Station* [1979]. Here water content of the top soil (0–6 cm) was measured in four experimental plots subjected to different grazing intensity, i.e., ungrazed since 1999 (ug99), ungrazed since 1979 (ug79), continuous grazing (cg), and heavy grazing (hg) [*Schneider et al.*, 2008, 2011]. Finally, we used soil water content measurements (0–30 cm) from the Tarrawarra grassland test site (Australia) that were presented in detail by *Western and Grayson* [1998].

3.2. Soil Hydraulic Parameter Prediction

We used Rosetta [*Schaap et al.*, 2001] to estimate the mean and standard deviation of VGM parameters (Table 1) from measured sand, silt, clay content, and bulk density obtained from in situ samples taken at all test sites. Although these soil samples were not always taken at the exact position where soil water content was measured, we assume that the ensemble mean and standard deviation adequately represent

Table 1. Mean and Standard Deviations of VGM Parameters Predicted by Rosetta for the TERENO, IMGERS, and Tarrawarra Test Sites

			$<\theta_r>$	$<\theta_s>$	$<\alpha>$	$<n>$	$<\ln(K_s)>$				
			(cm^3 cm^{-3})		(cm^{-1})	(—)	(cm d^{-1})	$\sigma(\theta_s)$	$\sigma(\alpha)$	$\sigma(n)$	$\sigma(\ln(K_s))$
Rollesbroich		5 cm	0.06	0.54	0.006	1.65	3.70	0.05	0.002	0.08	1.21
		20 cm	0.06	0.44	0.005	1.67	3.50	0.04	0.001	0.04	0.70
		50 cm	0.05	0.38	0.007	1.58	2.52	0.04	0.003	0.10	0.70
Wüstebach		5 cm	0.12	0.77	0.010	1.40	4.14	0.08	0.003	0.16	0.70
		20 cm	0.10	0.70	0.010	1.40	4.17	0.10	0.003	0.16	0.70
		50 cm	0.10	0.66	0.010	1.40	4.14	0.20	0.003	0.16	0.70
Scheyern		5 cm	0.04	0.52	0.029	1.46	4.68	0.06	0.005	0.14	0.59
		20 cm	0.05	0.44	0.028	1.48	3.69	0.04	0.006	0.16	0.67
		50 cm	0.05	0.42	0.028	1.55	3.34	0.04	0.009	0.42	1.25
IMGERS	ug99	0–6 cm	0.00	0.48	0.010	1.53	4.50	0.04	0.003	0.04	0.40
	ug79		0.00	0.52	0.010	1.51	5.06	0.04	0.003	0.04	0.35
	cg		0.00	0.45	0.010	1.50	3.96	0.02	0.003	0.03	0.19
	hg		0.00	0.44	0.013	1.50	4.00	0.04	0.003	0.03	0.20
Tarrawarra		0–30 cm	0.10	0.50	0.010	1.48	2.51	0.02	0.004	0.13	0.31

each test site. As $\sigma_\theta(<\theta>)$ is typically not sensitive to the correlation length of $\ln(K_s)$, α, and n [*Vereecken et al.*, 2007], we assumed a fixed correlation length of 10 cm in our study.

4. Results and Discussion

4.1. Sensitivity of $\sigma_\theta(<\theta>)$ Relationship to Soil Hydraulic Parameters

Figure 1 presents the sensitivity of the $\sigma_\theta(<\theta>)$ relationship to changes in the variability of $\ln(K_s)$, θ_s, α, and n as expressed by the coefficient of variation (CV). The mean VGM parameters were taken from the Rollesbroich

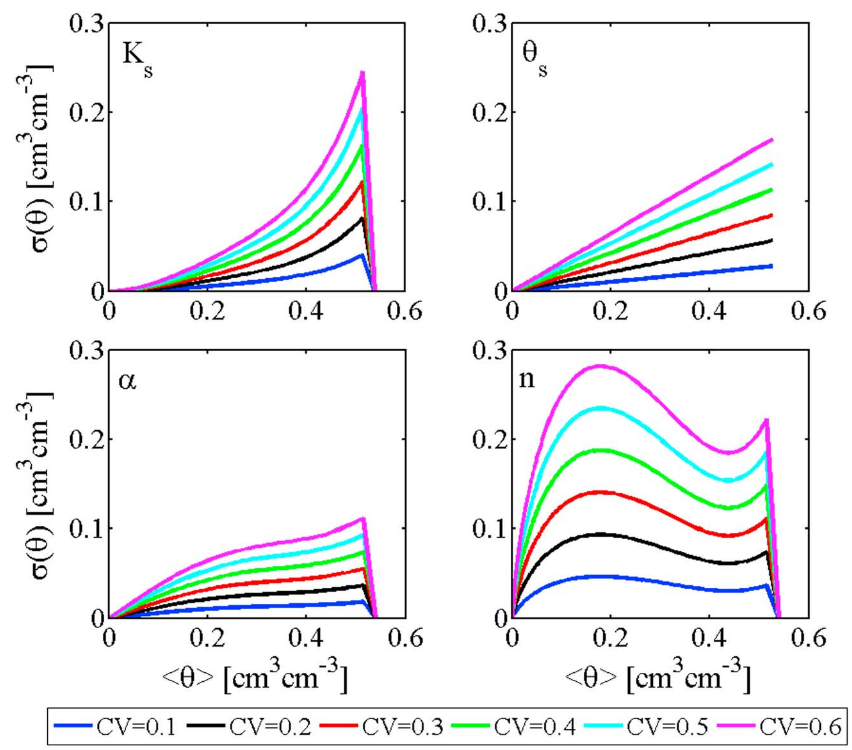

Figure 1. The effect of variability of VGM parameters ($\ln(K_s)$, θ_s, α, and n) on $\sigma_\theta(<\theta>)$ curve for silty loam soil using six different degrees of variability expressed as coefficient of variation. The sharp thresholds at the wet end are caused by setting $\sigma_\theta(<\theta>)$ to zero for fully saturated soil conditions.

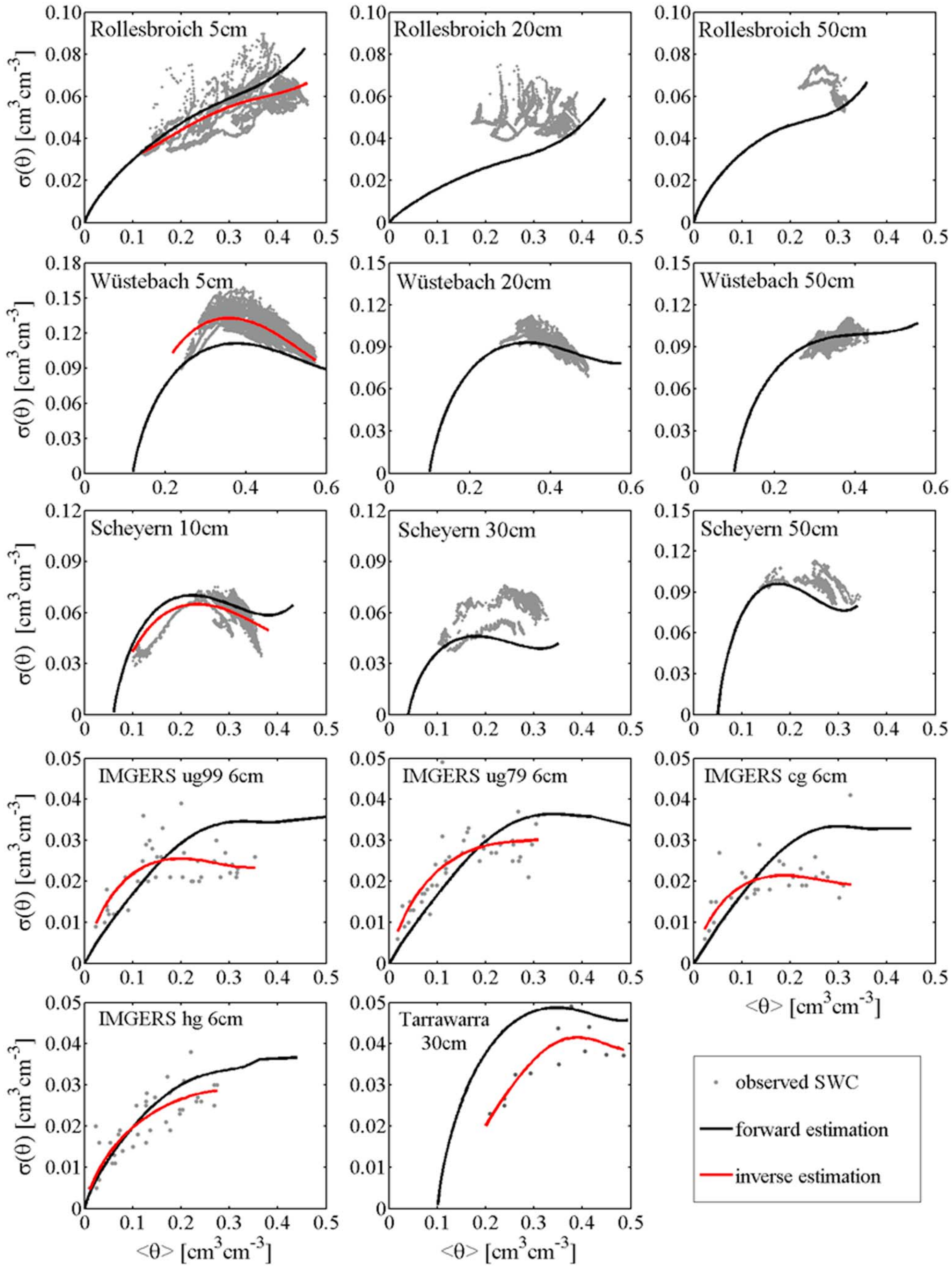

Figure 2. Field-observed $\sigma_\theta(<\theta>)$ data from the three TERENO test sites (Rollesbroich, Wüstebach, and Scheyern), the four IMGERS experiment sites (ug99, ug79, cg, and hg), and the Tarrawarra test site as well as the forward and inverse estimation results.

test site at 5 cm depth (Table 1). This sensitivity analysis suggests that $\sigma_\theta(<\theta>)$ is most sensitive to the n parameter, followed by $\ln(K_s)$, θ_s, and α, respectively. The results of the sensitivity analysis were similar for other soil textures, although the difference in sensitivity between the VGM parameters decreased with increasing sand content (results not shown). This finding is in good agreement with the results of *Vereecken et al.* [2007]. They found that $\sigma_\theta(<\theta>)$ was most sensitive to the λ parameter of the Brooks-Corey model, which is related to pore size distribution just as the n parameter of the VGM model. It has to be noted that the derived curves for different levels of variability in the n parameter show a second increase of σ_θ for $<\theta>$ larger than 0.5, which becomes more distinctive with increasing CV. Such an increase is typically not observed in actual $\sigma_\theta(<\theta>)$ data

Table 2. Correlation Coefficients (R^2) and Root-Mean-Square Errors (RMSEs) Between Observed and Forward and Inverse Estimated σ_θ Values

			Forward		Inverse	
			R^2	RMSE	R^2	RMSE
Rollesbroich		5 cm	0.76	0.007	0.79	0.007
		20 cm	0.08	0.019	-	-
		50 cm	0.22	0.021	-	-
Wüstebach		5 cm	0.55	0.020	0.77	0.014
		20 cm	0.64	0.006	-	-
		50 cm	0.56	0.011	-	-
Scheyern		10 cm	0.72	0.008	0.86	0.006
		20 cm	0.77	0.027	-	-
		50 cm	0.43	0.014	-	-
IMGERS	ug99	0–6 cm	0.55	0.007	0.72	0.006
	ug79		0.84	0.007	0.88	0.006
	cg		0.59	0.007	0.69	0.006
	hg		0.82	0.005	0.83	0.005
Tarrawarra		0–30 cm	0.80	0.017	0.83	0.005

(e.g., Figure 2). We attribute this model behavior to approximations introduced by the first-order Taylor expansions that were used to derive equation (4). Consequently, the model results will be less reliable for high values of $<\theta>$, especially in the case that the n parameter is highly variable.

4.2. Prediction of the $\sigma_\theta(<\theta>)$ Relationship From Soil Texture Data

Figure 2 shows the measured and predicted $\sigma_\theta(<\theta>)$ relationships obtained using equation (4) with the mean and standard deviation of the VGM parameters estimated from Rosetta (Table 1). Although the test sites span a wide range of climatic conditions and soil textures, the general behavior of $\sigma_\theta(<\theta>)$ was well captured by the closed-form expression despite obvious simplifications in the model derivation. Predicted $\sigma_\theta(<\theta>)$ at the Wüstebach test site was generally high because of the high values for $<\theta_s>$ and $\sigma(n)$ (see Table 1). A continuous increase of $\sigma_\theta(<\theta>)$ without an obvious maximum at intermediate soil water content was observed at the Rollesbroich test site (5 cm), and this behavior was also predicted by our closed-form expression. This is related to the high predicted value of $\sigma(\ln(K_s))$ (Table 1) for this site. At the Scheyern test site, an abrupt increase in soil water content variability was observed at 50 cm depth as compared to the shallower soil depth, and this is also nicely captured by the closed-form expression. Table 1 shows that this increase is caused by the high value of σ_n at this depth.

In order to assess the effect of the pressure head fluctuations on the predicted $\sigma_\theta(<\theta>)$, we also calculated $\sigma_\theta(<\theta>)$ neglecting variations in pressure head ($h' = 0$). We found that $\sigma_\theta(<\theta>)$ did not depend strongly on pressure head fluctuations in dry conditions (Figure S2). This implies that variability in soil hydraulic properties dominates σ_θ in this soil water content range and also explains the good fit to the observed data despite the fact that gravitational downward water flow is not likely to occur in the dry water content range. Pressure head fluctuations were more important in wet conditions, especially in soils with high sand content (Figure S3).

Noticeable deviations between observed and predicted $\sigma_\theta(<\theta>)$ can also be observed as well in Figure 2. For example, $\sigma_\theta(<\theta>)$ at 5 cm depth at the Wüstebach test site and $\sigma_\theta(<\theta>)$ at 20 and 50 cm depth in the Rollesbroich test site were clearly underestimated. This can be explained by several factors. First, both the soil hydraulic parameter estimates obtained from the pedotransfer functions and the closed-form expression are only approximations. Second, the $\sigma_\theta(<\theta>)$ relationship is not only affected by soil hydraulic parameters but also by the interplay between evapotranspiration, interception, infiltration, and lateral redistribution among other factors.

Compared to the other test sites, the Inner Mongolia Grassland Ecosystem Research Station (IMGERS) plots are considerably smaller and relatively homogeneous, which is reflected in the relatively small standard deviation of the VGM parameters (Table 1). This results in comparably small predicted $\sigma_\theta(<\theta>)$ values for the IMGERS plots, which is in good agreement with measured $\sigma_\theta(<\theta>)$ values as indicated by the R^2 values that ranged

Table 3. Results of the Best Fit Parameter Set From the Inverse $\sigma_\theta(<\theta>)$ Model Application for the TERENO, IMGERS, and Tarrawarra Test Sites

			$\sigma(\theta_s)$	$\sigma(\alpha)$	$\sigma(n)$	$\sigma(\ln(K_s))$
Rollesbroich (5 cm)			0.08	0.002	0.13	0.60
Wüstebach (5 cm)			0.05	0.004	0.21	0.41
Scheyern (10 cm)			0.02	0.013	0.15	0.10
IMGERS	ug99	0–6 cm	0.02	0.002	0.07	0.32
	ug79		0.02	0.002	0.06	0.08
	cg		0.02	0.001	0.06	0.74
	hg		0.02	0.003	0.05	0.49
Tarrawarra (0–30 cm)			0.01	0.004	0.05	0.11

between 0.55 and 0.84, and root-mean-square error values ranged between 0.005 cm^3 cm^{-3} and 0.006 cm^3 cm^{-3} (Table 2). The good match between observations and predictions at this test site is likely related to the lack of lateral water fluxes and the relatively homogeneous vegetation within each treatment, which suggests that $\sigma_\theta(<\theta>)$ is likely dominated by the variability of the soil hydraulic properties.

The soil texture at Tarrawarra covers several soil textural classes (Figure S1). However, the predicted values for the hydraulic parameters and their variability are similar to those found for the IMGERS plots despite the considerably larger area of Tarrawarra, except for $<\ln(K_s)>$ which is not included in the closed-form expression (equation (4)). Therefore, the predicted $\sigma_\theta(<\theta>)$ values at Tarrawarra are also relatively low compared to the TERENO test sites in Figure 2. Interestingly, Tarrawarra is the only test site where the closed-form expression overestimates $\sigma_\theta(<\theta>)$. This might be an indication for processes compensating soil water content variability (e.g., higher transpiration rates in wetter parts of the Tarrawarra site or lateral water redistribution during wet seasons).

4.3. Inverse Estimation of Hydraulic Parameter Variability From Observed $\sigma_\theta(<\theta>)$ Data

We tested whether it is feasible to inversely estimate the variability of hydraulic parameters in equation (4) using the observed $\sigma_\theta(<\theta>)$ data sets described above. Estimating both the mean soil hydraulic parameters and their standard deviations in equation (4) turned out not to be possible (not shown) as no unique solutions could be obtained. In order to better constrain parameter estimates, a wide range of $<\theta>$ is needed. Since the variation of $<\theta>$ was less pronounced in the subsoil, we only analyzed soil water content data measured in the topsoil. We used a Markov Chain Monte Carlo algorithm [*Vrugt et al.*, 2009] to inversely estimate the standard deviations of soil hydraulic parameters from measured $\sigma_\theta(<\theta>)$ data. We used wide parameter bounds to fully explore the parameter space (Table S2). The generally high R^2 values listed in Table 2 indicate that the inversely estimated variability of hydraulic parameters (Table 3) was able to capture the observed $\sigma_\theta(<\theta>)$ better than the forward model (Figure 2). The inverse modeling particularly captured the peak of the observed $\sigma_\theta(<\theta>)$ at 5 cm depth much better (Figure 2) than the forward estimation, leading to an increase of R^2 value from 0.55 to 0.77 at the Wüstebach test site. This is due to the higher standard deviation of n obtained in the inversion as compared to the estimate provided by the Rosetta pedotransfer function (i.e., $\sigma(n)$ increased from 0.16 to 0.21).

5. Conclusions

We presented a new closed-form expression for $\sigma_\theta(<\theta>)$ based on the VGM model to study the effect of soil hydraulic properties on $\sigma_\theta(<\theta>)$. The sensitivity analysis showed that hydraulic parameters and their spatial variability affect $\sigma_\theta(<\theta>)$ differently. The most sensitive VGM parameter is the n parameter, followed by $\ln(K_s)$, θ_s, and α, respectively. In a next step, we used basic soil properties (i.e., sand, silt, clay content, and bulk density) to predict $\sigma_\theta(<\theta>)$ relationships for eight data sets with different soil texture and climate conditions using pedotransfer functions and our closed-form expression. In most cases, predicted $\sigma_\theta(<\theta>)$ agreed well with observed $\sigma_\theta(<\theta>)$. This indicates that soil hydraulic parameter variability is an important control on $\sigma_\theta(<\theta>)$. In addition, we demonstrated that the variability of soil hydraulic parameters can be inversely estimated from observed $\sigma_\theta(<\theta>)$ data.

We propose that the closed-form expression should be used in combination with pedotransfer functions and global soil maps to estimate subgrid variability of soil water content, which is useful to further improve prediction accuracy of large-scale hydrologic, weather, and climate models. In addition, information on subgrid variability of soil water content may be useful for the estimation of the uncertainty of large-scale remote sensing measurements of soil water content provided by Advanced Scatterometer (ASCAT), Soil Moisture Ocean Salinity (SMOS), and the upcoming Soil Moisture Active Passive (SMAP) mission.

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