Explaining soil moisture variability as a function of mean soil moisture: A stochastic unsaturated flow perspective

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Received 24 August 2007; revised 5 October 2007; accepted 15 October 2007; published 21 November 2007.

[1] Understanding soil moisture variability and its relationship with water content at various scales is a key issue in hydrological research. In this paper we predict this relationship by stochastic analysis of the unsaturated Brooks-Corey flow in heterogeneous soils. Using sensitivity analysis, we show that parameters of the moisture retention characteristic and their spatial variability determine to a large extent the shape of the soil moisture variance-mean water content function. We demonstrate that soil hydraulic properties and their variability can be inversely estimated from spatially distributed measurements of soil moisture content. Predicting this relationship for eleven textural classes we found that the standard deviation of soil moisture peaked between 0.17 and 0.23 for most textural classes. It was found that the β parameter, which describes the pore-size distribution of soils, controls the maximum value of the soil moisture standard deviation. **Citation:** Vereecken, H., T. Kamai, T. Harter, R. Kasteel, J. Hopmans, and J. Vanderborght (2007), Explaining soil moisture variability as a function of mean soil moisture: A stochastic unsaturated flow perspective, *Geophys. Res. Lett.*, *34*, L22402, doi:10.1029/2007GL031813.

1. Introduction

[2] Soil moisture is a key variable controlling hydrological and energy fluxes in soils. Due to the heterogeneity of soils, atmospheric forcing, vegetation, and topography, soil moisture is spatially variable. Understanding and characterizing this spatial variability is one of the major challenges within hydrological sciences. Especially the relationship $\sigma_\theta(\langle\theta\rangle)$ between mean soil moisture content, $\langle\theta\rangle$, and its standard deviation σ_θ, has received considerable attention in the hydrological community. This relationship is important to understand the contribution of soil moisture variability at smaller scales towards the effective soil moisture observed at larger scales or its role in the parametrization of, e.g., climate and watershed models (upscaling/downscaling [e.g., *Famiglietti et al.*, 1999; *Crow et al.*, 2005; *Ryu and Famiglietti*, 2005]). Some studies report an increase in σ_θ with decreasing $\langle\theta\rangle$ [e.g., *Bell et al.*, 1980; *Famiglietti et al.*, 1998; *Oldak et al.*, 2002], while others report the opposite behaviour [*Famiglietti et al.*, 1999; *Choi and Jacobs*, 2007]. Re-examination of recent experimental work [*Ryu and Famiglietti*, 2005; *Choi and Jacobs*, 2007; *Choi et al.*, 2007] and of results from simulations and stochastic analysis of water flow in heterogeneous soils [*Roth*, 1995; *Harter and Zhang*, 1999] shows that $\sigma_\theta(\langle\theta\rangle)$ increases during drying from a very wet stage, reaches a maximum value at a specific or critical mean moisture content, and then decreases during further drying (Figure 1). The observed unimodal shape of $\sigma_\theta(\langle\theta\rangle)$ has been explained mostly based on empirical [*Hu and Islam*, 1998] and/or statistical analysis of field data [e.g., *Famiglietti et al.*, 1998; *Ryu and Famiglietti*, 2005; *Choi and Jacobs*, 2007]. To date, an explicit mathematical analysis of $\sigma_\theta(\langle\theta\rangle)$ is lacking. In this letter, we use analytical stochastic work by *Zhang et al.* [1998], to show that $\sigma_\theta(\langle\theta\rangle)$ is directly related to the soil hydraulic properties and their statistical moments and that inverse modelling can be used to estimate these properties from moisture data. Our results show that the relationship between soil moisture variability and mean moisture content is controlled by soil hydraulic properties, their statistical moments and their spatial correlation. The unimodal shape of $\sigma_\theta(\langle\theta\rangle)$ observed in the field and in simulation data is well explained by existing stochastic theories.

2. Stochastic Theory

[3] Over the past thirty years, various stochastic theories of unsaturated water flow have been developed to predict effective water fluxes, state variables, and hydraulic parameters for heterogeneous soils [e.g., *Yeh et al.*, 1985; *Zhang*, 2002]. Briefly, across a field site, the variability in soil hydraulic parameters leads to an ensemble of moisture retention curves, $\theta(h)$, where h is the pressure head, that typically show the largest variation of θ in the medium range of logarithmic pressure head values. Stochastic perturbation theory predicts that when soil gets drier the variance of both, pressure head and moisture content increase [*Harter and Zhang*, 1999]. Given the fact that $\theta(h)$ is bounded between θ_r, the residual moisture content and θ_s, the saturated moisture content, $\sigma_\theta(\langle\theta\rangle)$ is also bounded even when the variance of the pressure head increases to large values. This is demonstrated by numerical simulations and stochastic analysis of water flow in heterogeneous unsaturated porous media [*Roth*, 1995; *Zhang et al.*, 1998; *Harter and Zhang*, 1999]. *Zhang et al.* [1998] derived closed form equations for the variances and covariances of h and θ and the cross-covariances between h and hydraulic parameters in the Brooks-Corey (BC) and Gardner-Russo equations for the case of 1D gravity dominated unsaturated flow in mildly heterogeneous flow domains. These equations are derived assuming stationarity in saturated hydraulic conductivity and pressure

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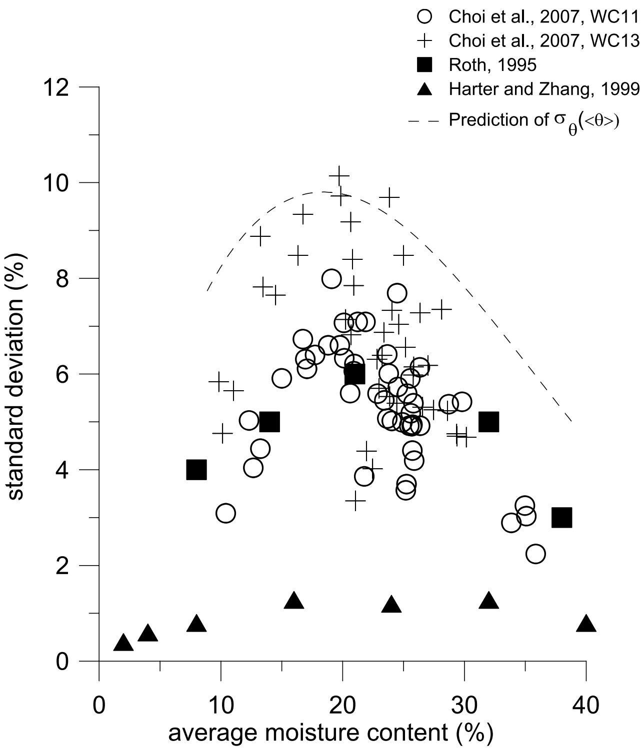

Figure 1. Soil moisture variability with respect to mean soil moisture content for the measurements made by *Choi et al.* [2007] on field sites WC11 and WC13. Symbols demonstrate results obtained with numerical simulations [*Roth*, 1995; *Harter and Zhang*, 1999]. The dashed line represents the theoretical $\sigma_\theta(\langle\theta\rangle)$ (1) based on Table 2 values for the soil of *Choi et al.* [2007]. Actual σ^2_α and σ^2_β at the field site may be smaller than estimated from Table 2 leading to the high values for the theoretical $\sigma_\theta(\langle\theta\rangle)$.

head, joint-Gaussian spatial distribution of hydraulic parameters with exponential covariance functions and negligible correlation between the hydraulic parameters. Despite these restrictions, the derived equation provides an excellent tool to analyze the relationship between $\langle\theta\rangle$ and σ_θ. Using the BC equation for $\theta(h)$ and the hydraulic conductivity function [*Zhang et al.*, 1998] the variance of effective moisture content for 1D vertical flow is written as:

$$\sigma^2_{\theta_e}(\langle\theta_e(x_3)\rangle) = b0^2\left\{\frac{b2^2\sigma^2_{\ln K_s}\lambda^2_{\ln K_s}}{\left(1+a2\lambda^2_{\ln K_s}\right)a2} + \frac{b1^2\sigma^2_\alpha}{(1+a2\lambda_\alpha)} + b3^2\sigma^2_\beta\left[1+\frac{b2\lambda_\beta(6a2+9b2)}{(1+a2\lambda_\beta)a2}\right]\right\} \quad (1)$$

The parameters $a1$, $a2$, $a3$, $b0$, $b1$, $b2$, $b3$ are functions of $\ln K_s(x3)$, $\alpha(x_3)$, $\beta(x_3)$, $h(x_3)$. $\alpha(x_3)$ is the air entry value, $\beta(x_3)$ is the pore size distribution index characterizing the shape of the moisture retention characteristic, $K_s(x_3)$ is the saturated hydraulic conductivity, and x_3 the vertical coordinate. $\theta_e(x_3)$ is the effective moisture content equal to $\theta(x_3) - \theta_r$. Further, $\sigma^2_{\ln K_s}$ is the variance of $\ln K_s(x_3)$, σ^2_β the variance of β, σ^2_α the variance of α, and λ_i, the correlation length of $\ln K_s(x_3)$, $\alpha(x_3)$, $\beta(x_3)$. In the subsequent we will drop the coordinate symbol x_3 and use $\sigma_\theta(\langle\theta\rangle)$ rather than $\sigma_{\theta e}(\langle\theta_e\rangle)$ for convenience.

3. Methods

[4] First, we use four typical soils (Table 1) to demonstrate the effect of soil texture on $\sigma_\theta(\langle\theta\rangle)$. Values of the BC parameters, $\langle\alpha\rangle$, $\langle\beta\rangle$, and $\langle\ln K_s\rangle$, for the sandy loam were obtained from *Zhang et al.* [1998]. The values for the other soils were derived from soil texture data using pedotransfer functions, PTF ("Rosetta" [*Schaap et al.*, 1998]), and then fitting the BC-equation to the Van Genuchten model obtained from Rosetta. We assumed that CV_α (CV: coefficient of variation) and CV_β were 30%, $\sigma^2_{\ln K_s} = 1$ and correlation scales were equal to 25 cm based on field data [e.g., *Russo and Bresler*, 1981; *Mallants et al.*, 1996; *Schaap et al.*, 1998]. θ_r and θ_s were assumed to be constant. Second, the sensitivity of $\sigma_\theta(\langle\theta\rangle)$ to the variability in soil hydraulic parameters in (1) was investigated. Third, we used (1) to estimate $\langle\alpha\rangle$, $\langle\beta\rangle$, σ^2_α, σ^2_β and $\sigma^2_{\ln K_s}$ from an artificial, computer-generated $\sigma_\theta(\langle\theta\rangle)$ data via inverse modelling. The inverse model was based on least-squares optimization with the Levenberg-Marquardt algorithm (MATLAB, 2007). Assumptions about θ_r, θ_s, λ_α, λ_β and $\lambda_{\ln K_s}$ were as above. The inverse modelling was performed using the loamy sand (Table 1) and by generating synthetic datasets of $\sigma_\theta(\langle\theta\rangle)$. White noise ($N(0, 1)$) was added to the computed value of $\sigma_\theta(\langle\theta\rangle)$. Six noise levels were used: 0%, 1%, 2%, 3%, 4% and 5%. For each level, ten realizations were obtained, inverse modelling was performed, and average parameter estimates and estimation variances were calculated. The 0% noise case was used to test the algorithm. Fourth, we calculate $\sigma_\theta(\langle\theta\rangle)$ using BC-data for eleven textural classes (Table 2) according to *Rawls et al.* [1982] and *Cosby et al.* [1984] to find the relation between moisture content and σ_{max}, the max. standard deviation. Fifth, we show an application to field data of $\sigma_\theta(\langle\theta\rangle)$ [*Choi et al.*, 2007]. Again, θ_r and θ_s were obtained based on available soil texture data using PTF. Values of $\langle\alpha\rangle$, $\langle\beta\rangle$, σ^2_α, σ^2_β and $\sigma^2_{\ln Ks}$ were estimated by applying field texture data to Table 2.

4. Results and Conclusions

4.1. Effect of Soil Texture on $\sigma_\theta(\langle\theta\rangle)$

[5] Finer textured soils (silt loam, clay loam) have a clear peak in $\sigma_\theta(\langle\theta\rangle)$ whereas the sandy loam soil and the loamy

Table 1. Brooks-Corey Parameters of the Example Soils[a]

	Sandy Loam	Loamy Sand	Silt Loam	Clay Loam
θ_r [cm^3 cm^{-3}]	0	0.057	0.067	0.095
θ_s [cm^3 cm^{-3}]	0.5	0.41	0.45	0.41
α [cm^{-1}]	0.022	0.177	0.026	0.025
β	1.738	1.07	0.394	0.292
$\sigma^2_{\ln K_s}$	1 (0.1, 0.5, 1)			
λ_α, λ_β, $\lambda_{\ln K_s}$ [cm]	25 (10, 40, 80)			

[a]The variance of α and β was calculated for a CV of 0.3. Values used for the sensitivity analysis are given in parentheses.

Table 2. Brooks-Corey Parameter for Different Textural Classes[a]

	θ_s	θ_r	α, cm^{-1}	$\sigma_\alpha{}^2$	β	$\sigma_\beta{}^2$	$\sigma^2_{\ln K_s}$
Sand	0.437	0.02	0.5599	8.7071	0.694	0.163	0.152
loamy sand	0.437	0.035	0.3966	3.5986	0.553	0.102	0.260
sandy loam	0.453	0.041	0.0886	0.0330	0.378	0.057	0.449
Loam	0.463	0.027	0.1425	0.1379	0.252	0.028	0.397
silt loam	0.501	0.015	0.0709	0.0282	0.234	0.017	0.303
Sandyclayloam	0.398	0.068	0.0494	0.0123	0.319	0.058	0.292
clay loam	0.464	0.075	0.0511	0.0117	0.242	0.029	0.348
siltyclayloam	0.471	0.04	0.0463	0.0085	0.177	0.019	0.372
sandy clay	0.43	0.109	0.0508	0.0152	0.223	0.031	0.109
silty clay	0.479	0.056	0.0400	0.0078	0.15	0.012	0.476
clay loam	0.475	0.09	0.0371	0.0069	0.165	0.016	0.384

[a]Parameters as given by *Rawls et al.* [1982]. The variance of $\ln K_s$ is obtained from *Crosby et al.* [1984]. The α values given by *Rawls et al.* [1982] were statistically transformed to represent its inverse value used in equation (1).

sand soil show a steady decrease in $\sigma_\theta(\langle\theta\rangle)$ from wet to dry (Figure 2). Therefore, we may observe different behavior in $\sigma_\theta(\langle\theta\rangle)$ depending on mean soil moisture status and on soil hydraulic properties. The $CV_\theta(\langle\theta\rangle)$ of the sandy soil increases as the soil dries and reaches its maximum value near the residual moisture content (Figure 2). The other soils show a more unimodal shape in $CV_\theta(\langle\theta\rangle)$.

4.2. Sensitivity of $\sigma_\theta(\langle\theta\rangle)$ to Soil Hydraulic Properties

[6] Variability in α affects $\sigma_\theta(\langle\theta\rangle)$ mainly at high soil moisture regardless of soil type (Figures 3a, 3d and 3g). However, the sensitivity is smaller for the finer textured clay loam soil. The pronounced sensitivity of σ^2_α at high soil moisture suggests that soil moisture data under a wet regime are important for estimating this parameter. All three soils show that $\sigma_\theta(\langle\theta\rangle)$ is very sensitive to σ^2_β at moderate soil moisture content, with the largest sensitivity found for the silt loam soil (Figures 3b, 3e and 3h). The effect can be explained by the fact that β is a measure of the pore size distribution of the soil. It therefore affects the shape of the entire moisture retention characteristic, particularly in the moisture range where most variation in soil

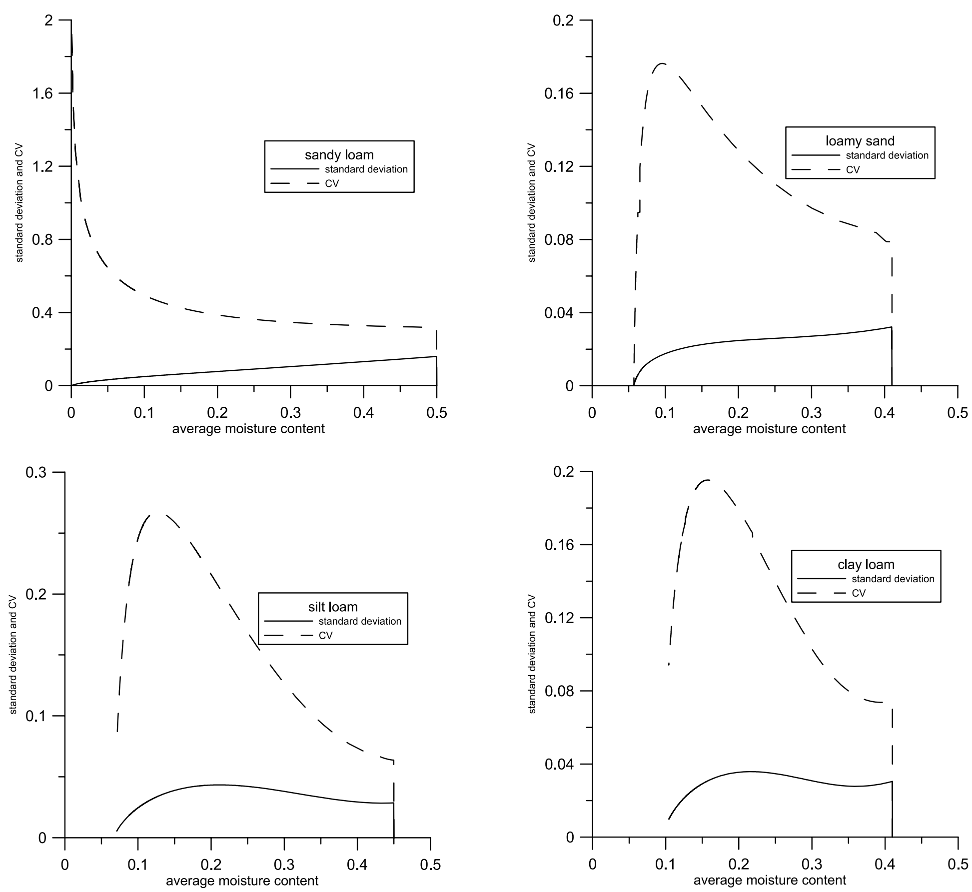

Figure 2. The $\sigma_\theta(\langle\theta\rangle)$ and the corresponding CV for four different textural classes using equation (1). Parameter specifications are given in Table 1.

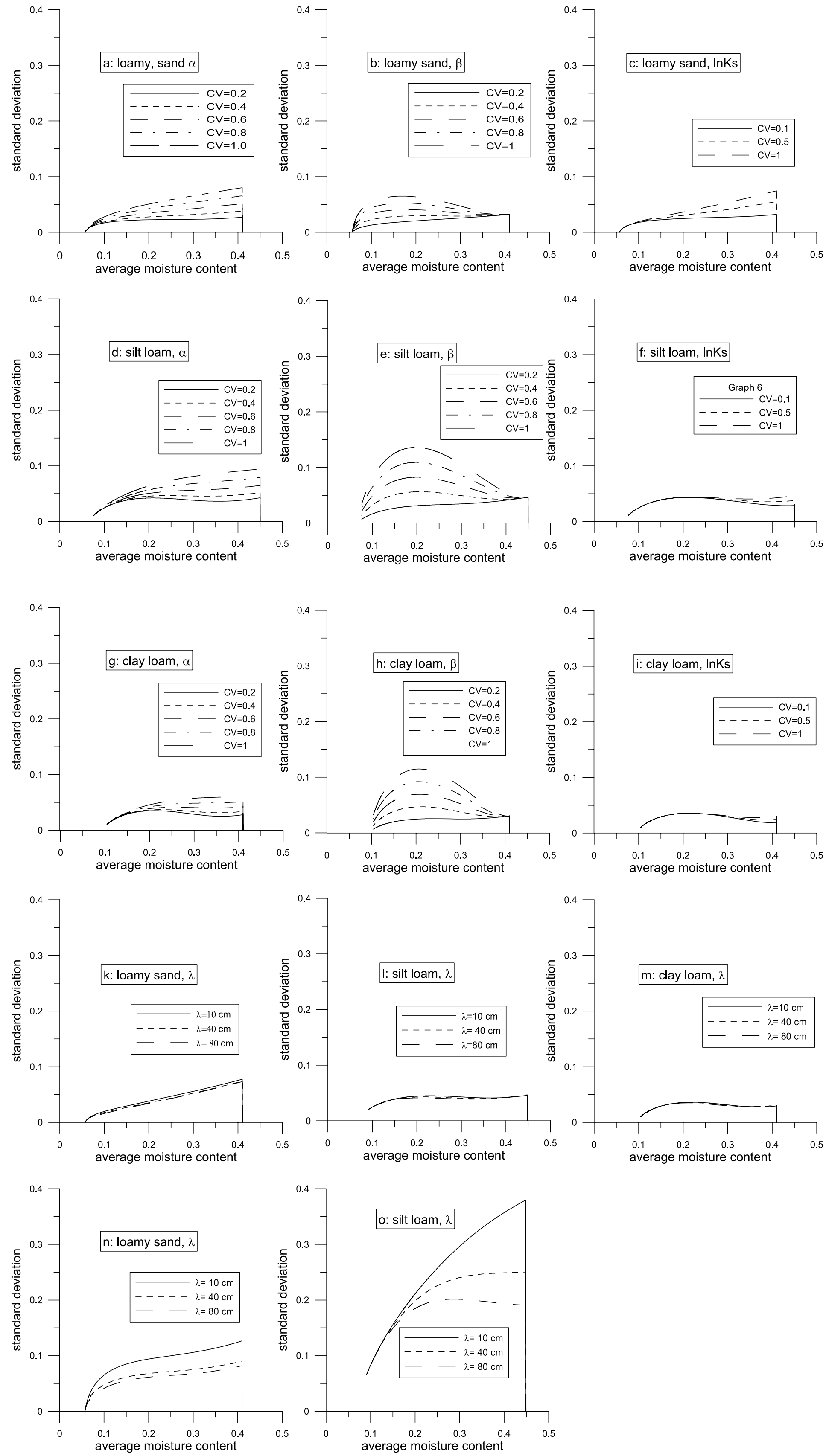

Figure 3. (a, d, g) The effect of variability in α on soil moisture variability for the loamy sand, silt loam, and clay loam soil using five different values for the CV. Similar analysis is shown for the parameter (b, e, h) β, (c, f, i) lnK_s, and (k, l, m) vertical correlation length of the Brooks-Corey parameters. (n, o) The effect of an increased coefficient of variation for $\sigma_\alpha{}^2$ and σ_β^2 (CV = 0.9) on the sensitivity of $\sigma_\theta(\langle\theta\rangle)$ for the correlation scale.

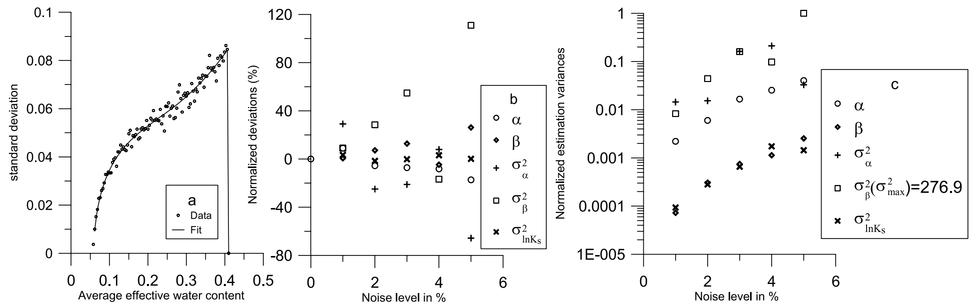

Figure 4. (a) Fit to the data with 5% measurement noise. (b) Normalized deviations from optimal parameter values. (c) Normalized estimation values with respect to σ_β^2.

moisture occurs. The impact of β on $\sigma_\theta(\langle\theta\rangle)$ at moderate soil moisture was indirectly observed by *Famiglietti et al.* [1998] who found a strong correlation between the variability in surface soil moisture content and clay content under dry conditions. *Cosby et al.* [1984] also showed that clay content and β are strongly correlated. The sensitivities of $\sigma_\theta(\langle\theta\rangle)$ to σ_α^2 and σ_β^2 are complementary: Near saturation, the sensitivity to σ_α^2 is larger and diminishes as the soil dries out whereas the sensitivity of $\sigma_\theta(\langle\theta\rangle)$ to σ_β^2 is small near saturation and increases as the soil dries out (e.g., Figures 3d and 3e). Upon further drying, however, the effect of σ_β^2 decreases as soil moisture is approaching residual moisture content. Variability in $\sigma_{\ln K_s}^2$ mainly affects the wet part of $\sigma_\theta(\langle\theta\rangle)$ (Figures 3c, 3f and 3i). This effect was also observed by *Famiglietti et al.* [1998] who found that variability in soil moisture content is controlled strongly by porosity and hydraulic conductivity under wet conditions but not under drier conditions. This is supported by our calculations, which show a decrease in the sensitivity of $\sigma_\theta(\langle\theta\rangle)$ to variability in $\sigma_{\ln K_s}^2$ as the soil is drying. In general, the sensitivity of $\sigma_\theta(\langle\theta\rangle)$ to variability in $\ln K_s$ seems smaller compared to its sensitivity to σ_α^2 and σ_β^2. The sensitivity of $\sigma_\theta(\langle\theta\rangle)$ with respect to the correlation scale is low (Figures 3k, 3l and 3m). Moreover, the sensitivity of $\sigma_\theta(\langle\theta\rangle)$ to correlation scale seems to be related to the magnitude of σ_α^2 and σ_β^2 (Figures 3n and 3o). The larger σ_α^2 and σ_β^2, the more pronounced is the effect of correlation scale on the soil moisture variability. The largest effect is observed in the wet part of the soil moisture range.

4.3. Inverse Estimation of Soil Hydraulic Parameters From $\sigma_\theta(\langle\theta\rangle)$

[7] For zero noise, the estimated soil hydraulic parameters from the synthetic $\sigma_\theta(\langle\theta\rangle)$ were in perfect agreement with their "true" values (not shown). Excellent agreement of estimated with "true" parameters was also found for low noise levels (Figure 4a). At all noise levels, good estimates of α, β and $\sigma_{\ln K_s}^2$ were obtained from the synthetic $\sigma_\theta(\langle\theta\rangle)$ data. Maximum deviations from "true" values range between 10% and 25% (Figures 4b and 4c). Higher order moments σ_α^2 and σ_β^2 show deviations larger than 30% at 2% noise and quickly increase with noise level. Estimation variances of the parameters also rapidly increase with noise level (Figure 4c).

4.4. Relation Between Mean Moisture Content and σ_{max}

[8] The largest observed moisture variability is a function of soil texture (Table 3). $\sigma_\theta(\langle\theta\rangle)$ is typically largest in the mid-range of soil moisture content for all textural classes except "sand", for which the maximum of σ_θ, σ_{max}, value is at air entry. For the finer textured soils, σ_{max} occurs at mean soil moisture values ranging from 0.18 to 0.23 (Table 3). This theoretical result based on mechanistic soil-physical analysis corresponds well with *Ryu and Famiglietti* [2005] who experimentally found that $\sigma_\theta(\langle\theta\rangle)$ tends to peak around a value of 0.2.

4.5. Comparison of Predicted and Measured $\sigma_\theta(\langle\theta\rangle)$

[9] An application of this approach to field data shows good agreement between measured $\sigma_\theta(\langle\theta\rangle)$ and the theoretical $\sigma_\theta(\langle\theta\rangle)$ curve (Figure 1) obtained by applying field texture data to Table 2. These results demonstrate that measured $\sigma_\theta(\langle\theta\rangle)$ may be used to derive soil hydraulic parameters. Further in-depth analysis and field testing is needed to evaluate the full potential of this approach, particularly when including the forcing through precipitation and vegetation. Also, it is generally accepted that the BC model has limited value in the field, particularly near saturation. Improved stochastic theories based on the Van Genuchten model or similar more realistic descriptions of the soil moisture characteristic might be valuable in improving estimation of hydraulic parameters from measured $\sigma_\theta(\langle\theta\rangle)$ curves.

Table 3. Maximum Standard Deviation in Function of Soil Type and Moisture Content[a]

	σ_{max}	θ at σ_{max}	σ at Air Entry, $1/\alpha$
Sand	0.203	0.41	0.191
loamy sand	0.056	0.153	0.041
sandy loam	0.089	0.168	0.042
Loam	0.103	0.172	0.032
silt loam	0.098	0.196	0.029
Sandy clay loam	0.089	0.179	0.024
clay loam	0.100	0.210	0.025
Silty clay loam	0.123	0.200	0.022
sandy clay	0.092	0.223	0.011
silty clay	0.114	0.211	0.021
clay loam	0.108	0.231	0.018

[a]Maximum standard deviation, σ_{max}; moisture content, θ.

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