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Key Points:

- We study the spatial variability of soil moisture by a three-dimensional stochastic model of unsaturated flow
- The model accounts for the three relevant scales: extent, spacing among measurements, support scale of the latter
- Interplay between the scales and the correlation of the hydraulic properties rules the variability of saturation, a scale effect manifests

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Spatial Variability of Soil Moisture and the Scale Issue: A Geostatistical Approach

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Abstract We study the standard deviation of water saturation SD_S as function of the mean saturation $\langle S \rangle$ by a stochastic model of unsaturated flow, which is based on the first-order solution of the three-dimensional Richards equation. The model assumes spatially variable soil properties, following a given geostatistical description, and it explicitly accounts for the different scales involved in the determination of the spatial properties of saturation: the extent L, i.e., the domain size, the spacing Δ among measurements, and the dimension ℓ associated to the sampling measurement. It is found that the interplay between those scales and the correlation scale I of the hydraulic properties rules the spatial variability of saturation. A "scale effect" manifests for small to intermediate L/I, for which SD_S increase with the extent L. This nonergodic effect depends on the structural and hydraulic parameters as well as the scales of the problem, and it is consistent with a similar effect found in field experiments. In turn, the influence of the scale ℓ is to decrease the saturation variability and increase its spatial correlation. Although the solution focuses on the medium heterogeneity as the main driver for the spatial variability of saturation, neglecting other important components, it explicitly links the spatial variation of saturation to the hydraulic properties of the soil, their spatial variability, and the sampling schemes; it can provide a useful tool to assess the impact of scales on the saturation variability, also in view of the several applications that involve the saturation variability.

1. Introduction

The soil moisture θ is spatially variable and controlled by many factors, like, e.g., the hydraulic properties of the soil, topography, interaction with surface water systems, precipitation, and vegetation among others, in a nonlinear fashion. The water content has a deep influence on several aspects of the hydrological cycle, including rainfall-runoff processes, evapotranspiration, the partitioning of net radiation in latent and sensible fluxes, to mention some (Destouni & Verrot, 2014; Gebler et al., 2017; Grayson et al., 1997; Robinson et al., 2008; Rodriguez-Iturbe et al., 2001; Rosenbaum et al., 2012; Vereecken et al., 2008a; Western et al., 2002). A deeper understanding of the hydrological processes ruling the spatial distribution of θ is needed to address several important scientific questions, like, e.g., the uncertainty estimation of hydrological models (Heathman et al., 2003; Heuvelink & Webster, 2001) the setup of measurement networks (Heathman et al., 2009), and the calibration and validation of remote sensing products (Choi & Jacobs, 2007; Famiglietti et al., 2008a; Greifeneder et al., 2016; Rötzer et al., 2014).

The understanding of the spatial variability of soil moisture and its causes is also important for the development of suitable downscaling techniques of satellite products (Jacobs et al., 2004). In fact, aircraft and satellite products are often validated through field measurements which are typically determined at much lower support scales (for a review on water content measurements see Romano, 2014; Vereecken et al., 2008a). To this matter, Western and Blöschl (1999) suggested that a scale triplet, composed of *spacing*, *support*, and *extent*, should be considered in studies of soil moisture scaling. The mutual interactions between those scales are of crucial importance when assessing the spatial variability of θ. In particular, it is seen that the spatial variability of θ typically increases with the size of the domain where measurements are taken. The support scale of the measurements, i.e., the spatial scale of the measurement volume of the device, also impacts the spatial variability of water content, leading typically to a decrease with increasing size of the support scale.

The assessment of the spatial variability of soil moisture has been the subject of intense research in the last decades (Brocca et al., 2012, 2007; Choi & Jacobs, 2007; Famiglietti et al., 2008a; Fatichi et al., 2015; Hawley et al., 1983; Hupet & Vanclooster, 2004; Laio et al., 2001; Mohanty et al., 2000; Ojha et al., 2014; Teuling & Troch, 2005; Vereecken et al., 2014, 2007; Western & Blöschl, 1999). Many of the above studies have shown that a meaningful representation is in terms of the standard deviation (SD) of θ as function of its mean value, which usually shows an upward convex shape, with a peak in the intermediate soil moisture range (see, e.g., Famiglietti et al., 2008a; Vereecken et al., 2007). Soil moisture variations, quantified in terms of the SD, show a general increase with increasing spatial scale (Famiglietti et al., 2008a; Western & Blöschl, 1999). Contributions of the different individual physical controls on the θ variability are still debated and object of active research (e.g., Fatichi et al., 2015).

Among all the possible factors that determine the SD of θ, of interest for the present work is its relation with the spatial distribution of the hydraulic properties of the soil. The matter was investigated by Vereecken et al. (2007, 2008b) by a 1-D stochastic model of flow in unsaturated media, following similar research work carried out in the past through numerical simulations (e.g., Harter & Zhang, 1999; Roth, 1995). Their solution was developed originally by Zhang et al. (1998) along a stochastic approach to unsaturated flow in heterogeneous porous media which has been started to develop some three decades ago (e.g., Bresler & Dagan, 1983; Indelman & Dagan, 1993a, 1993b; Mantoglou & Gelhar, 1987; Russo, 1998, 1995, 1993; Russo & Bresler, 1980a; Severino et al., 2010, 2009; Yeh et al., 1985a, 1985b; Zhang et al., 1998).

Although soil variability is clearly not the only driver of water content variability (Famiglietti et al., 2008b) nevertheless it may represent a significant source for determining meaningful quantities, like the standard deviation of water content (e.g., Chen et al., 2014; Clapp et al., 1983; Fatichi et al., 2015), and hence it is worth to be further investigated.

Scope of the present work is to investigate the standard deviation of water saturation by a stochastic model of unsaturated flow, which is based on the first-order solution of Russo (1998). The model aims at linking the spatial variation of saturation to the hydraulic properties of the soil, their spatial variability and the sampling schemes. Although approximated and with limitations, we believe that mathematical models can provide insight and help in formulating and testing suitable conceptualizations of the physical systems.

The model assumes spatially variable soil properties, following a given geostatistical description, in terms of second-order statistical moments. This way, we focus on the medium heterogeneity as the main driver for the spatial variability of soil moisture, neglecting other components, like vegetation (e.g., water uptake by plant roots), topography, rainfall heterogeneity among others. The basic assumptions are similar to the most of the aforementioned studies, including Vereecken et al. (2007), i.e., steady flow and statistically stationary soil properties. Our work differs from previous studies in that it explicitly accounts for the different scales involved in the determination of the spatial properties of saturation (i.e., scale of the domain, of the measurement, of the sampling scheme), as discussed in Western and Blöschl (1999), in a rational and systematic framework; the latter permits to evaluate the interplay between scales in the determination of the spatial variability of water saturation. Also, the flow dimensionality considered here is fully 3-D, which has a significant impact over simpler 1-D formulations considered in other analytical studies.

2. Mathematical Framework

2.1. Scales and Stochastic Approach

The water saturation *s* is defined, at the Darcy scale, as the ratio between the water content θ and the porosity *n*. Our aim is to investigate the impact of soil heterogeneity on the saturation variability. We derive here a probabilistic framework for the relation between the saturation standard deviation and its mean value, which is often adopted in theoretical and practical investigations. We deal in the following with steady, uniform in the mean vertical flow.

Field analysis of saturation involves different scales. The issue was discussed by Western and Blöschl (1999) who introduced three fundamental length scales, the "scale triplet" constituted by (i) the extent, i.e., the size L of the domain where the measurements are taken, (ii) the spacing Δ between measurements, and (iii) the support scale ℓ of the single measurement of water content or saturation, which depends on the sampling device (see Blöschl & Sivapalan, 1995; Western & Blöschl, 1999); we follow here their same terminology. The three scales can differ very much, and each of them is also variable: one may have a domain of the size of the plot or a bigger area at a larger regional scale, leading to different L. The support scale ℓ can be quite

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small in the case of a TDR-based sampling, or much larger, e.g., when the measure is based on a satellite product.

Because of the spatial heterogeneity of the hydraulic properties of soils, saturation is also heterogeneous and spatially variable, as function of position **x** in the three-dimensional space, even in the simple case of steady vertical flow considered here. The spatial variability of s determined by the spatial change in the hydraulic properties (most notably the hydraulic conductivity) occurs over a spatial *correlation scale* I_s; since s is a flow-controlled attribute I_s is a saturation-dependent entity. In turn, the scale I_s strictly depends on the spatial correlation scale (or integral scale) I of the hydraulic properties of the soil, like, e.g., saturated hydraulic conductivity. The interplay between the scale I and the "scale triplet" has a fundamental role in the analysis of the standard deviation of water saturation, as discussed in the sequel. We note that the same scales (with the exception of Δ) were introduced by Dagan (1986), and further elaborated in Dagan (1989).

In order to describe the spatial variability of saturation, we adopt a probabilistic approach (e.g., Russo, 1998, 1995, 1993) and consider s as a space random function. The main assumption adopted here is that s is a second-order stationary random function; this stems from the fact that in the adopted approach, it is assumed that the inherent soil properties are second-order stationary random variables and a perturbation approach is employed (e.g., Russo, 1993), in which Darcy's law is linearized. The random s is characterized by the mean $\langle s \rangle$ and the two-point covariance $C_{ss}(\mathbf{r})$ where **r** is the separation vector of the two points; the covariance embeds the integral scale I, which rule the spatial scale of s, as discussed above. The assumption of stationarity and the single-scale (I) approach are supported by the many experimental studies where standard geostatistical analysis (e.g., through variograms) was performed (Bohling et al., 2012; Russo & Bouton, 1992; Russo & Bresler, 1981; Severino et al., 2017; Sudicky, 1986; Vereecken et al., 2000, to mention a few).

2.2. Solutions

We denote with $S(\mathbf{x})$ the saturation averaged over the sampling volume v, of support scale ℓ, reflecting the averaging process performed by the sampling device

$$S(\mathbf{x})=\frac{1}{v}\int_v s(\mathbf{x}+\mathbf{x}')d\mathbf{x}' \tag{1}$$

The spatially averaged S is again a space random variable whose variability is smoothed out with respect to s because of the space-averaging; in particular, the averaging procedure leads for S to a smaller variance and larger spatial correlation scales with respect to s (see, e.g., Chapter 1.9 of Dagan, 1989) (this point will be retaken later); clearly, $S \to s$ when $v \to 0$. The saturation S is spatially variable over the domain W of characteristic scale L (e.g., a square of side L and area L^2 as considered in the example of section 3).

In the following, we shall explore two sampling scenario: (i) a continuous sampling, i.e., when the measurement spacing is very small ($\Delta = 0$), such that the domain W is fully sampled, and (ii) a discontinuous, incomplete sampling of the domain W, where a finite number N of measurements is available ($\Delta \neq 0$); the latter case is the one usually met in applications, while the first one is rather theoretical and represents an upper bound in terms of sampling.

Scope of this section is to derive the expected value of the spatial variance of S (denoted as SD_S^2 and $SD_{S,\Delta}^2$ for the above two sampling schemes) as function of the soil parameters. The derivation follows the standard methods of stochastic subsurface hydrology (e.g., Dagan, 1989), taking advantage of the linearized solution of the 3-D Richards equation by Russo (1998). For the sake of conciseness, we reproduce the detailed developments and solutions for the two sampling schemes in Appendix A.

The final solution for $SD_S(\langle S \rangle)$ is given by (A6) for the continuous sampling case $\Delta \to 0$; in turn, $SD_{S,\Delta}$ is given by (A11), that applies when a discrete number of measurement points are available (i.e., $\Delta > 0$). We remark that the two solutions model the *ensemble average* of the saturation standard deviation over the domain W, while the SD_S of a particular realization may differ from its expected value because of lack of ergodicity, typically when $I/L=O(1)$ or less. Such deviations from the mean could be modeled through the variance of SD_S or $SD_{S,\Delta}$, which calculation is formally possible after assuming multi-Gaussianity, but it leads to involved mathematical expressions which are not explored here.

The proposed formulation is able to model the mean standard deviation of S as function of the mean $\langle S \rangle$ depending on the three relevant scales L, ℓ, Δ as well as the hydraulic conductivity heterogeneity length scale I which is embedded in the covariance C_{ss}. The latter is indeed the key parameter, and the following subsection addresses the problem of its calculation.

2.3. Solution for the Saturation Covariance

The above developments show that the saturation covariance C_{ss} plays a central role in the relation $SD_S(\langle S \rangle)$. The covariance can be formally obtained by solving the 3-D Richards equation, with random soil parameters, after some simplifying assumptions. We shall adopt in the following steady flow in an unsaturated, unbounded domain with unit mean head gradient, i.e., free drainage.

The approach followed here involves a sort of "equivalent" steady state (or ESS, see Russo & Fiori, 2008, and references therein) that mimics the transient flows of the natural systems, i.e., cycles of rainfall and redistribution; similar approaches have been employed in the past. Such approximation has been adopted in the past by Russo and Fiori (2009) for modeling contaminant transport in a combined vadose zone-groundwater system, that is very much sensitive on spatial variability of water content and hydraulic properties, and found that the ESS approach is quite effective in reproducing the Breakthrough Curves at suitable control planes. Hence, we are confident that our solution, although approximated, is anyway able to capture realistic trends.

The required functional relationships between the unsaturated hydraulic conductivity K, the capillary pressure head ψ, and the water saturation s is assumed as the Gardner-Russo model (Gardner, 1958; Russo, 1988)

$$K(\psi, \mathbf{x}) = K_s \exp\left[-\alpha(\mathbf{x})\psi\right] \tag{2}$$

$$s(\psi, \mathbf{x}) = \{\exp\left[-1/2\alpha(\mathbf{x})\psi\right]\left[1+1/2\alpha(\mathbf{x})\psi\right]\}^{2/(m+2)} \tag{3}$$

where m is a parameter that accounts for the dependence of tortuosity and the correlation between pores at two different cross sections of the porous medium on water content. Based on Russo and Bresler (1980b) and Russo (1998), we assumed $m=0$, and the Gardner-Russo model depends on the formation parameters K_s, the saturated hydraulic conductivity, and α; the latter can be interpreted as the reciprocal of the macroscopic capillarity length scale. Thus, an increasing α determines a decrease in the macroscopic capillary length scale, i.e., a transition from a fine-textured soil material, associated with significant capillary forces, to a coarse-textured soil material, associated with negligible capillary forces. We remark that adopting a constant m in (3) reduces part of the nonlinear variability in the retention curves (see, e.g., Qu et al., 2015). However, we believe that the assumption leads to small differences in the results, as also shown by the analysis of Zhang et al. (1998) who compared the water content covariance after assuming the Gardner-Russo and the Brooks Corey models for 1-D flow (see, e.g., their Figure 3c); such differences are acceptable in view of the approximations employed in the model.

All the variables and parameters involved in the governing equations are stationary random variables. Hydraulic properties of heterogeneous medium (the saturated hydraulic conductivity K_s and the parameter α (see equation (3)) are second-order stationary space random variables lognormally distributed $f = \ln(K_s) \in N[\ln K_G, \sigma_f^2]$ and $a = \ln(\alpha) \in N[\ln \Gamma, \sigma_a^2]$, with K_G and Γ the geometric means of K_s and α, respectively. Their spatial patterns are described by an axisymmetric covariance structure with the same directional integral scales I and $I_v = eI$, horizontal and vertical, respectively. In the following developments, we shall adopt a constant porosity n; the assumption is justified in view of the relatively small variability in saturated water content as compared with the variability in K_s and α (see, e.g., Nielsen et al., 1973; Russo, 1998; Russo & Bouton, 1992; Russo & Bresler, 1981). In section 4, we shall provide a simplified method to consider the spatial variability of porosity in our solution.

Even with the above simplifying assumptions the analytical derivation of C_{ss} is a formidable task; it can be considerably alleviated by adopting a first-order approximation in the soil parameters (Russo, 1998). The random variables are perturbed around their mean values, and the Richards equations is solved, leading to the required $\langle s \rangle$ and C_{ss}. The approach follows closely the one of Russo (1998), with some modifications, and the details of the derivations are given in Appendix B. The resulting expressions for the mean $\langle S \rangle$ and the covariance C_{ss} are rather involved and reproduced in Appendix B (equations (B1) and (B3)), which are function of the following dimensionless parameters: the soil texture parameter $\Gamma'=\Gamma I$, the variances σ_f^2, σ_a^2 of saturated log conductivity f and texture parameter a, the correlation ρ_{af} between f and a and the anisotropy ratio $e=I_v/I$ of the hydraulic properties, which reflects the geological macroscopic structure.

3. Illustration Examples and Discussion

We show here the results of the above methodology through a few exemplifying cases. We start from the case of continuous sampling, i.e., when the spacing between adjacent measurements is $\Delta=0$, which is described by solution (A6). In the following, we assume for the sake of discussion that the domain W is a square of area A and size L, i.e., $W=A=L\times L$; similarly, the sampling size v is a square of size ℓ. This way, the expressions for σ_S^2 (A7) and R_S (A8), i.e., the variance of the sampling mean, appearing in (A6) can be written as follows (the mathematical passages are omitted for brevity)

$$\sigma_S^2=\frac{4}{\ell^4}\int_0^\ell\int_0^\ell(\ell-x)(\ell-y)C_{ss}(x,y,0)dxdy \tag{4}$$

$$\begin{aligned}R_S=&\frac{4}{L^4\ell^4}\int_0^L\int_0^L\int_0^\ell\int_0^\ell(L-x)(L-y)(\ell-x')(\ell-y')\cdot\\&\{2C_{ss}(x+x',y+y',0)+C_{ss}(x-x',y-y',0)+C_{ss}(-x+x',-y+y',0)\}]dxdydx'dy'\end{aligned} \tag{5}$$

The above expressions, inserted in (A6), permit to evaluate the standard deviation of saturation, as function of the scales L, ℓ, I and the soil related parameters σ_f^2, σ_a^2, ρ_{af}, Γ, and e.

We illustrate first the ergodic case $L\to\infty$, for which $R_S=0$ and consequently $SD_S=\sigma_S$; we neglect for now the impact of the sampling volume, assuming $\ell=v=0$. Figure 1 displays the ratio σ_S/σ_f as function of the mean saturation $\langle S\rangle$ for a few values of the dimensionless $\Gamma'=\Gamma I$, corresponding to different soil textures, and two values of the ratio σ_a^2/σ_f^2; the anisotropy ratio is kept constant as $e=0.1$, and the cross correlation $\rho_{af}=0.3$. The latter choice is justified by considering that K_s and α should be positively cross correlated. Since in field soils K_s is controlled by structural voids rather than by the entire continuum of pore sizes that controls α (Russo et al., 1997), one can expect only weak to moderate (positive) cross correlation between the two soil parameters; this is also suggested by experimental evidence (Russo & Bouton, 1992; Russo et al., 1997; Wierenga et al., 1991).

The general behavior of σ_S follows a common convex upward shape, with a peak proportional to σ_f correspondent to mean saturations $\langle S\rangle$ that decrease with the soil texture Γ, and null values in correspondence to $\langle S\rangle=0$ (residual saturation) and $\langle S\rangle=1$ (full saturation). It is seen that the effect of the heterogeneity of the Garner-Russo parameter Γ is important, especially for coarse soils, and the correlation scale I, which appears through $\Gamma'=\Gamma I$, has a significant impact on result. The important role of the dimensionless parameter Γ' can be explained as follows (Russo, 2005). An increase of I expresses an increase in the size of the

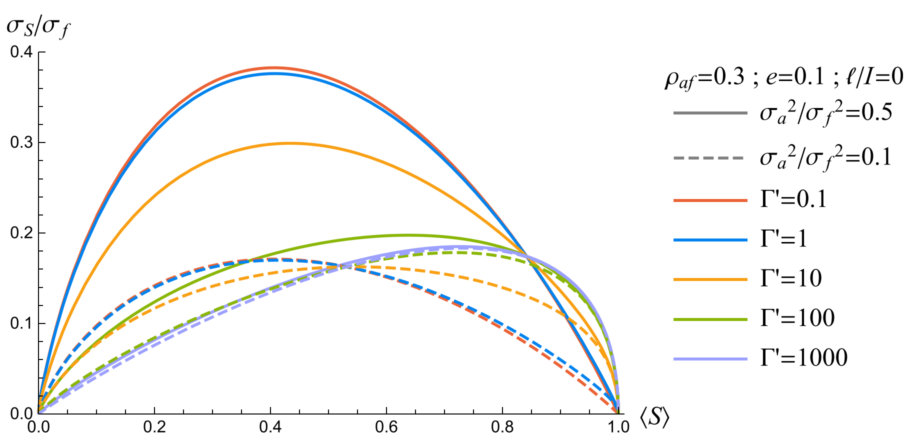

Figure 1. Saturation standard deviation versus average saturation, for two different heterogeneity degrees and five selected values of $\Gamma'=\Gamma I$; other parameters are kept as constant.

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typical flow barriers in a direction normal to the mean flow (i.e., vertical), and as a consequence streamlines are deflected less easily. On the other hand, a decreasing Γ expresses an increase in the macroscopic capillary length scale (i.e., a transition from a coarse-textured soil material, associated with negligible capillary forces, to a fine-textured soil material, associated with significant capillary forces) that leads to increasing lateral head perturbation gradients which facilitate the lateral deflection of streamlines. Thus, the two effects may compensate, and hence the relevance of the factor ΓI in the dynamics of unsaturated flow. We remark that the effect discussed here is due to the 3-D nature of flow, and it cannot be captured in 1-D analyses of flow.

It is worth noting that the present 3-D approach converges to a 1-D approach when $\Gamma I \to \infty$, i.e., when in presence of extremely coarse-textured soils and extremely large integral scales (e.g., $\Gamma = 10\,\mathrm{m}^{-1}$ and $I = 100$ m). Such circumstance, however, is quite unrealistic.

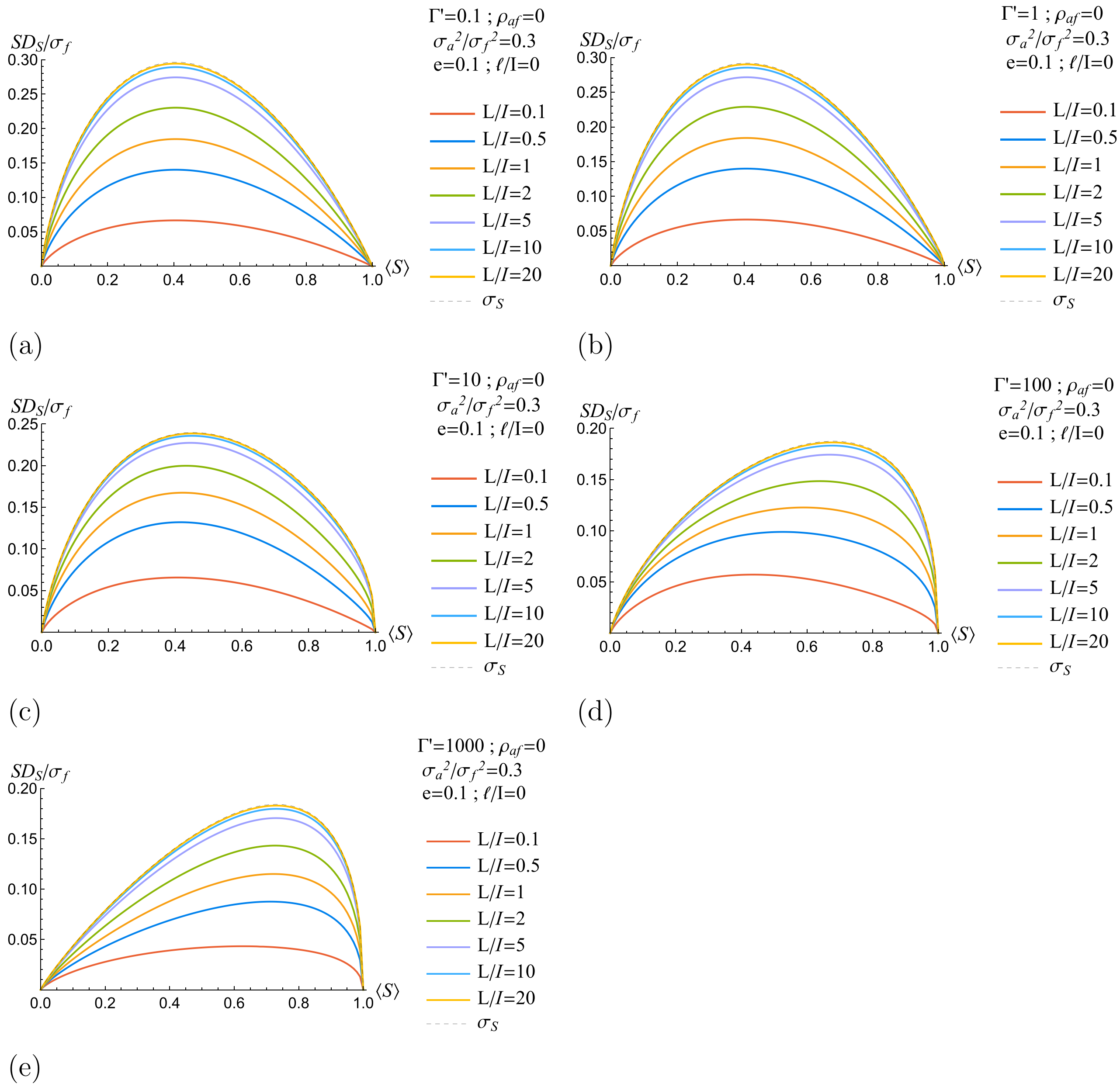

Figure 2. Saturation standard deviation versus average saturation across scales L for a continuous sampling; each plot pertains to a given soil type $\Gamma' = \Gamma I$, other parameters are kept as constant; the ergodic case is marked with dashed line.

The variance σ_a^2 of the texture parameter typically increases the saturation standard deviation, in particular for fine-textured soils (small Γ). In turn, the cross correlation ρ_{af} has a minor impact on results (not shown in the figure), although its effect might be more substantial in coarse-textured soils.

The behavior of σ_S identified here is the same found in field experiments (Brocca et al., 2012; Choi & Jacobs, 2007; Famiglietti et al., 2008a) and previous stochastic analysis of water flow in heterogeneous unsaturated porous media (Harter & Zang, 1999; Roth, 1995; Vereecken et al., 2007; Zhang et al., 1998); in particular, the above results are consistent with the analysis of Vereecken et al. (2007), although 1-D flow conditions were assumed there that may lead to different quantifications of σ_S, along the previous discussion.

We move now to the more interesting case of finite extent L, for which the present methodology is particularly suited and which represent one of the main contributions of this work. In this case, $R_S \neq 0$ and it is immediate to check from equation (A6) that the standard deviation of water saturation is always smaller than its ergodic counterpart σ_S (equation (A7)), which hence provides an upper bound for the spatial variability of S.

Figure 2 shows the ratio SD_S/σ_f as function of mean saturation for a few values of the dimensionless extent scale L/I (colored lines) and five soil textures $\Gamma'=\Gamma I$ (the five plots of Figure 2); in all cases, $e=0.1$, $\sigma_a^2/\sigma_f^2=0.3$, and $\rho_{af}=0.3$; the ergodic result σ_S/σ_f, for $L \to \infty$, is represented as dashed line.

The results clearly show the fundamental impact of the extent L on the spatial variability of water saturation, with values of the saturation variance decreasing with L. The effect is a consequence of the reduced sampling of the saturation field determined by the limit size of the area $A=L^2$. The relevant quantity for sampling is the ratio between the extent L and the correlation scale I of soil properties; in particular, the ergodic result σ_S (dashed lines) is typically achieved when $L/I \approx 20$, i.e., when roughly 20 integral scales are sampled in each dimension; when $L/I \to 0$ the saturation SD_S is identically zero for any $\langle S \rangle$, i.e., the domain size is too small for sampling the spatial distribution of water saturation. In other words, the variability of saturation can be underestimated when L is not large enough with respect to the soil variability I; the result is consistent with previous analyses (Famiglietti et al., 2008a; Oldak et al., 2002; Rodriguez-Iturbe et al., 1995) which were carried out with different methods.

We move now to the support scale ℓ. From the general relation (A7), we see that σ_S^2 varies between σ_s^2, when $\ell/I \ll 1$ and $\sigma_s^2(I/\ell)^d$ for $\ell/I \gg 1$ (Dagan, 1989); d is the space dimensionality of the averaging domain v, being $d=2$ for the case illustrated in this Section. Hence, the introduction of a finite support ℓ always leads to a decrease of the saturation variance with respect to the point value σ_s^2. Of definite interest is also the correlation scale of S, coined here as I_S; the latter is easily calculated from (A12), being for the case at hand ($v=\ell^2$) (Dagan, 1989), section 1.9.16)

$$I_S = I_s \left(\frac{\sigma_s^2}{\sigma_S^2} \right)^{1/2} \tag{6}$$

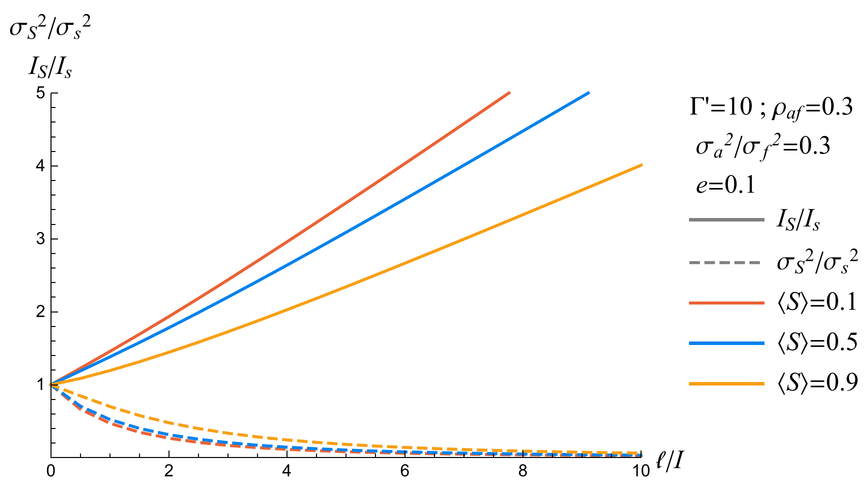

Figure 3. Relative saturation variance σ_S^2/σ_s^2 (dashed lines) and integral scale I_S^2/I_s^2 (continuous lines) as function of the sampling length ℓ, for three values of the average saturation. Other parameters are $\Gamma'=10$, $\sigma_a^2/\sigma_f^2=0.3$, $e=0.1$.

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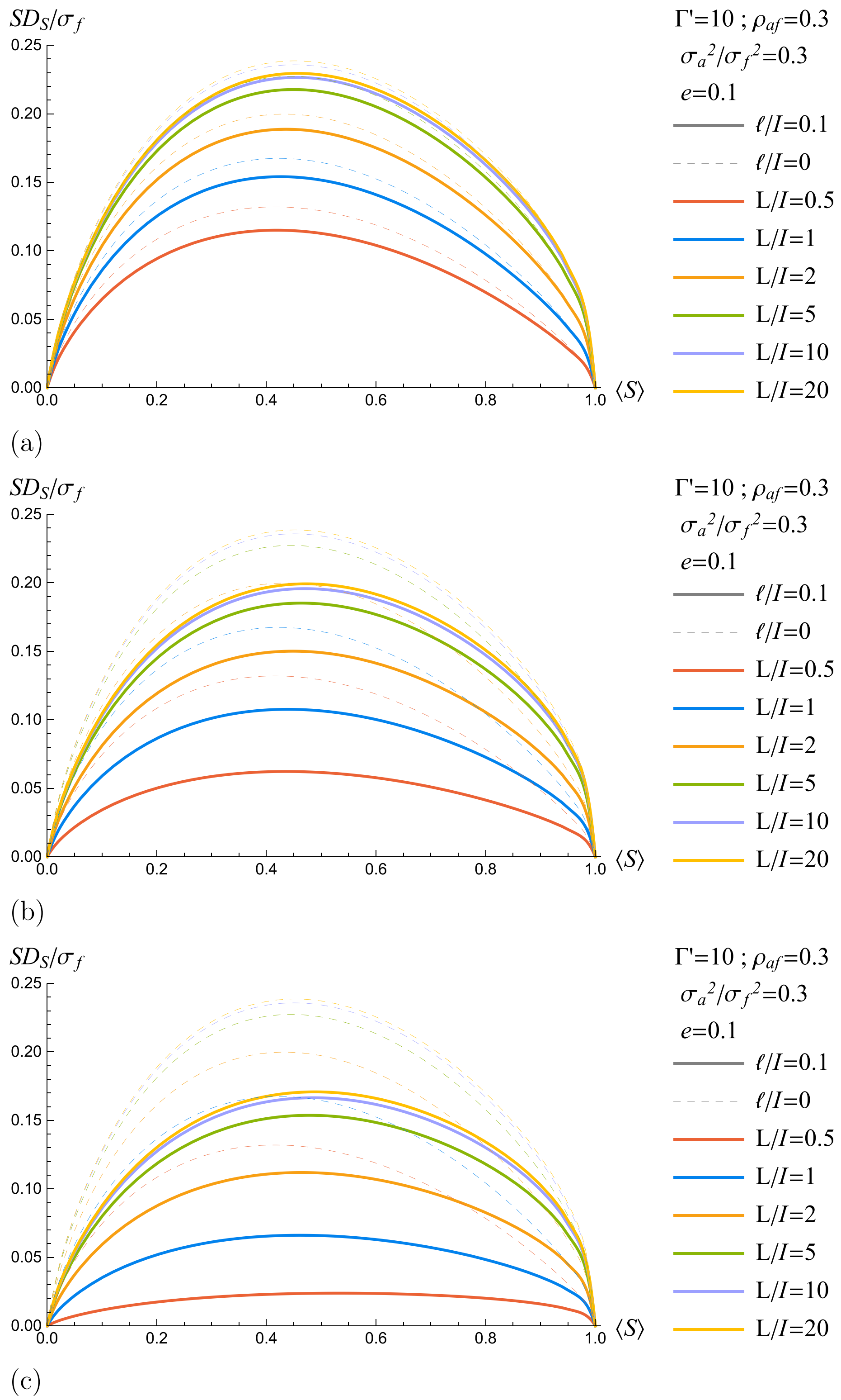

Figure 4. Saturation standard deviation versus average soil moisture for three different values of the sampling scale $\ell/I=$ 0.1; 0.5; 1 shown in different plots; different colors pertains to different domain extents. The continuous sampling cases are marked with a dashed lines.

with I_s the integral scale of s, which is proportional to I. Given the ratio σ_S^2/σ_s^2 previously discussed, it is seen that I_S changes between I_s (for $\ell \ll I_s$) and ℓ (for $\ell \gg I_s$). Summarizing, the effect of the averaging over the support ℓ is to decrease the variance of saturation and to increase its spatial correlation scale. Figure 3 illustrates the ratios σ_S^2/σ_s^2 and I_S/I_s as function of the support ℓ/I; the case is the same as Figure 2. The results reflect the aforementioned limits for small and large ℓ. Besides the decrease of the saturation variance, of definite interest is the increase of the correlation scale of saturation with the support. This reduces the number of correlations scales covered by the domain L, hence reducing the sampling and determining a further departure from the ergodic limit. The above features are illustrated in Figure 4.

The results presented so far regarding the effect of L and ℓ on SD_S are fully in line with the conclusions by Western and Blöschl (1999) that "*increasing the extent causes an increase in the apparent variance while increasing the support causes a decrease in the apparent variance*" and the framework developed here permits to quantify such effects, within the limitations of the analysis.

We move now to the effect of the spacing Δ, i.e., when the number of measurements N is finite and dictated by technical limitations and/or budget. Figure 5 shows $SD_{S,\Delta}$ as function of mean saturation for two relative domain sizes $L/I=2, 20$ and soil textures $\Gamma'=0.1, 1000$ and an increasing number of equally spaced measurements $N=1, 4, 9, 16, 25$; for all cases, $e=0.1$, $\sigma_a^2/\sigma_f^2=0.3$, and $\rho_{af}=0$; the support is set $\ell=0$ (point measurements), such that $C_{SS}=C_{ss}$. The interesting feature that emerges from the results is that a relatively small number N is typically required for getting a quite accurate estimate of SD_S, of the order of $N \gtrsim 16$ or even less for small domains; the required number of measurements is larger with increasing domain size L, as expected. The result, as well as the magnitude of N, is similar to what found by Brocca et al. (2012) by analyzing data from field experiments. However, we remark that such result pertains to the expected value of the standard deviation, and the actually observed standard deviations may vary considerably from realization to realization (the issue is briefly stated at the end of section 2.2).

The above analysis assumes equally spaced measurements, while in practice the distance between the samples may vary as function of several factors. To investigate the distribution of measurements points in the domain, we have randomized the location of $N=9$ measurements in the two domains of Figure 5 ($L/I=2, 20$) and $\Gamma'=0.1$, resulting in a series of 20 trials for which the saturation SD_S was calculated. The results are shown in Figure 6 where SD_S from the trials are represented by dotted lines. It is seen that, for a given N, the equally spaced distribution is always the most efficient way to sample S within the domain,

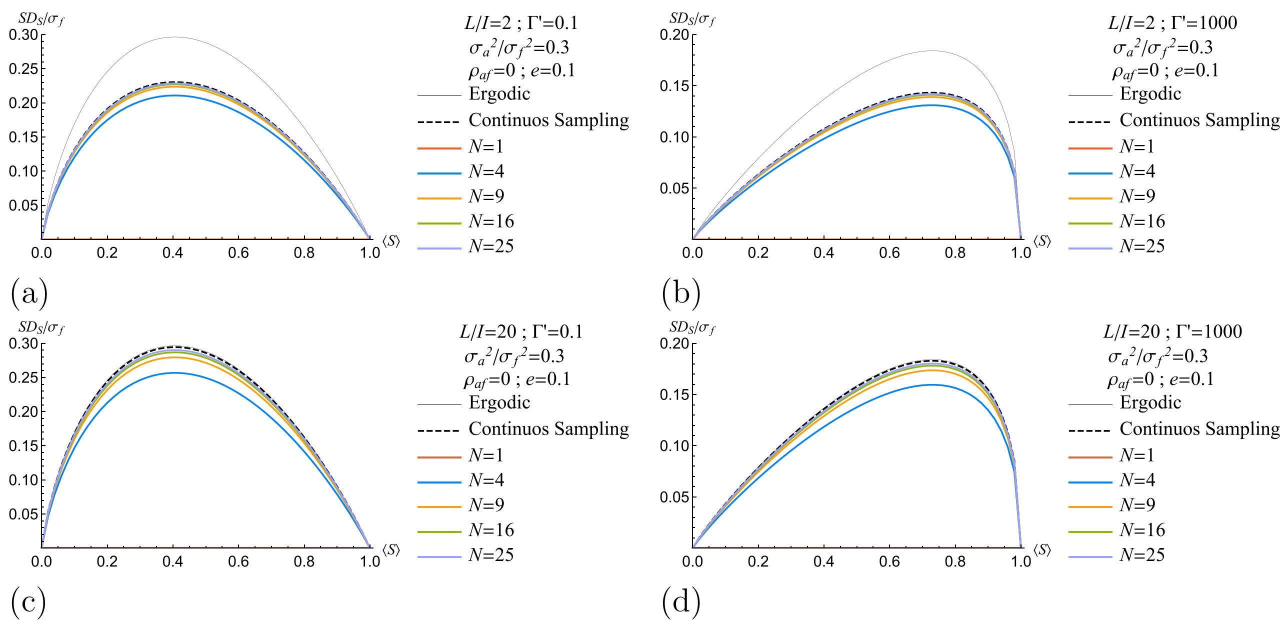

Figure 5. Saturation standard deviation versus average soil moisture content for five regular sampling spacing. Two domain extents and two values of $\Gamma'=\Gamma I$ are shown in different plots; other parameters are kept as constant. Continuous sampling is represented by a dashed line.

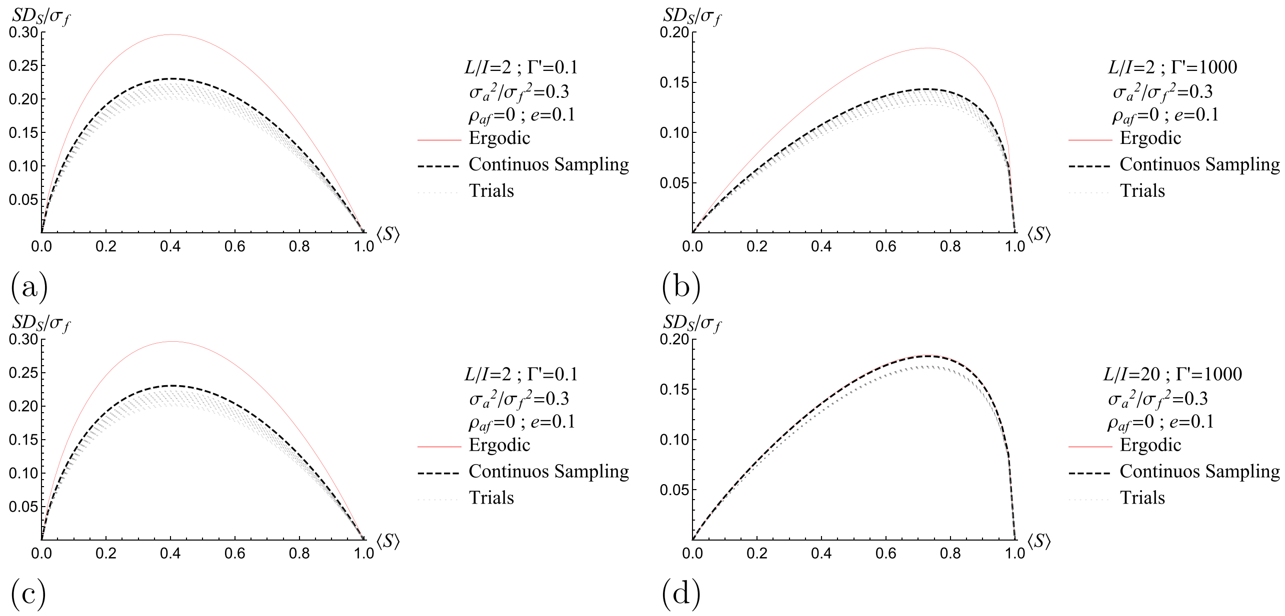

Figure 6. Saturation standard deviation versus average soil moisture content for different random sampling location. Two domain extents and two soil parameters are shown in different plots; ergodic case: thin line, continuous sampling: dashed line.

and deviations from this regular sampling scheme may lead to significant errors, especially in small domains (plot a) for which the nonergodic conditions (i.e., insufficient sampling) is often a limiting condition.

4. Application to the SGP99 Experiment

In this section, we present a simple application of the present methodology to the field data collected during the Southern Great Plains 1999 Hydrology Experiment (SGP99) in the central Oklahoma; we emphasize that our aim is to provide a simple example of the method potentiality and not to perform a deep and accurate analysis of the experimental results.

Field data were collected during the SGP99 experiment between 8 July and 19 July 1999. The multiscale data set pertains to the two adjoining sites located in the Little Washita watershed (LW21, LW22); fields were intensive winter wheat farms, with silty loam soil and flat topography. Samples were collected for a

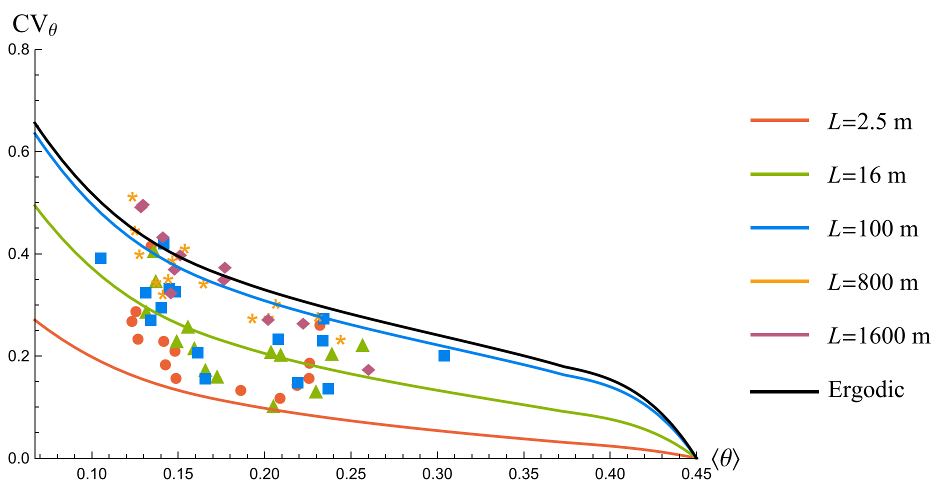

Figure 7. Coefficient of variation of the soil moisture CV_θ as function of the average soil moisture content $\langle\theta\rangle$ for the different extents L of the SGP99 experiment, represented by the different colors; continuous lines: model predictions, dots: experimental data.

Table 1
Model Parameters for the SGP99 Multiscale Experiment

Horizontal integral scale	$I=20$ m
Support scale	$\ell=0.1$ m
Anisotropy ratio	$e=0.1$
G-R parameter	$\Gamma=2$ m^{-1}
G-R parameter heterogeneity	$\sigma_a^2=0.1\sigma_f^2$
Hydraulic conductivity heterogeneity	$\sigma_f^2=0.75$
Hydraulic conductivity G-R parameter correlation	$\rho_{af}=0$
Residual soil moisture content	$\theta_r=0.067$
Maximum soil moisture content	$n=0.45$

nested grid at five different extents ranging from 2.5 m up to 1.6 km; the four larger extents, $L=16$, 100, 800, 1600 m were characterized trough 49 sampling locations placed in a regular grid, while the smaller one $L=2.5$ m was characterized though 49 randomly placed measurements. Volumetric soil moisture measurements were processed and analyzed in order to extract the major statistics of the soil moisture. Empirical relationships between the soil moisture statistics versus mean moisture content were carried out at the different scales. In the following, we analyze the soil moisture variation coefficient CV_θ versus the average values $\langle\theta\rangle$ which is often adopted instead of the soil moisture standard deviation for its fairly predictable exponential-like behavior and for displaying a more regular pattern than the standard deviation when dealing with (typically noisy) experimental data. The pattern is not as clear in the limited ranges of mean moisture content observed in SGP99 data, and the data display significant fluctuations and noise; still, an increase of variability is noticeable across scales (Famiglietti et al., 2008a). A brief description of the experiment together with the data of the reproduced here, can be found in Famiglietti et al. (2008a) (section 3.2 and Figure 7b).

Due to the lack of data, we setup our model mainly by adopting standard literature parameters; in particular, soil parameters n, θ_r are those suggested for the silty loam soil by Vereecken et al. (2007) (Table 1), $\Gamma=2$ m^{-1}, $\sigma_a^2=0.1\sigma_f^2$, $\rho_{af}=0$ while the log conductivity parameters σ_f^2, I were conveniently chosen, although no accurate fitting was carried out. The parameters are reproduced in Table 1; it is seen that the resulting medium heterogeneity is low to moderate, while the integral scale is not small but still compatible with the values reported in Rubin (2003) and the measurements by Russo and Bresler (1981). Because of the relatively large number of measurements for each extend we shall employ the continuous representation for S, along the discussion of section 3.

The empirical data and the theoretical lines predicted by the present stochastic model are represented in Figure 7. The scale effect originating from the theoretical analysis is similar to that observed in the field. The ergodic solution ($L/I \to \infty$, black line) represents a good approximation of the experimental points $L=800$ m and $L=1.6$ km, for which the data also suggest ergodic conditions. It is seen that the model provides a good estimate of the intermediate extent $L=16$ m while it overestimates the $L=100$ m one. Finally, a slight underestimation of the variability of the $L=2.5$ m extent can be noticed.

While our solution considers a constant porosity n, a simple analysis of the impact of its spatial variability on CV_θ can be done for the simple case of ergodic setup and porosity uncorrelated with saturation. Neglecting residual water content, it is $\theta=Sn$, and a simple calculation provides $CV_\theta=\left(CV_S^2+CV_n^2+CV_S^2CV_n^2\right)^{1/2}$, with CV_n the coefficient of variation of porosity. The latter is likely of the order of $CV_n=0.05\div0.1$ for the case of Figure 7 (ergodic curve), and it can be checked that the impact of CV_n on CV_θ is small. The above formula can be used for a simple assessment of the impact of porosity variability on CV_θ.

Even though the model was mainly set with the literature data without a thorough calibration, it seems to be able to capture the main scaling features of the experiment, the noise in the experimental data and the model approximations notwithstanding. We remind that our model focuses on soil heterogeneity only, neglecting other factors that may affect the variability of θ.

5. Summary and Conclusions

We have investigated the standard deviation of water saturation by a stochastic model of unsaturated flow, which is based on the first-order solution of the Richards equation by Russo (1998). The model assumes spatially variable soil properties, following a given geostatistical description, in terms of second-order statistical moments. The method explicitly accounts for the different scales involved in the determination of the spatial properties of saturation, i.e., the “scale triplet” discussed by Western and Blöschl (1999), the extent L, the spacing Δ, the support ℓ. The main scope is to provide a mathematical tool which is able to link the spatial variation of saturation to the hydraulic properties of the soil, their spatial variability and the sampling schemes. Although some of the processes explored here are already known from past experimental work, this is the first time (to our best knowledge) that a sound and rigorous mathematical framework is developed and presented. We believe that models like the one explored here, although approximated and with limitations, can provide interesting insights and help in formulating and testing suitable conceptualizations of the physical systems.

The main conclusions of the work can be listed as follows.

1. The correlation scale I of the hydraulic properties plays a fundamental role in the physical and averaging processes that take place in the soil; the interplay between I and the "scale triplet" rules the behavior of the standard deviation of water saturation SD_S.
2. The shape of SD_S under ergodic conditions (very large L/I) resembles previous results, although the importance of a fully three-dimensional analysis is underlined. In particular, the dimensionless factor $\Gamma'=\Gamma I$, i.e., the product of the macroscopic capillary length scale and the horizontal scale of the soil structure, manifests the resistance of vertical flow to laterally deflect the streamlines.
3. A scale effect manifests for small to intermediate L/I, for which SD_S increase with the extent L. This nonergodic effect depends on the structural and hydraulic parameters as well as the scales of the problem, and it is consistent with a similar effect found in experiments.
4. The influence of the support ℓ is to decrease the saturation variability and increase its spatial correlation. This circumstance generally leads to a departure from the ergodic conditions, i.e., a larger relative extent L/I is needed to stabilize SD_S around its ergodic, limit value.
5. The procedure indicates that a relatively small number of measurements N is typically required for getting a quite accurate estimate of the ensemble average of SD_S, of the order of $N \gtrsim 16$ or even less for small domains; the required N may increase with the spatial variability of log conductivity σ_f^2.

We remark that the solutions proposed here model the ensemble average of the saturation standard deviation over the domain extent, while the variability of saturation within a particular realization may differ from its expected value, typically when $I/L=O(1)$ or less; one of the consequences could be that the value for N discussed above is larger than indicated by the present analysis. Also, we remind that the method focuses on the medium heterogeneity as the main driver for the spatial variability of soil moisture, neglecting other important components (vegetation, topography, rainfall heterogeneity, and others) that may have a deep impact on the spatial variability of saturation. Nevertheless, the method can provide a useful tool to assess the impact of scales on the saturation variability.

While the nature of the present contribution is mainly theoretical, the proposed methodology may represent a first step toward the development of a modeling framework for quantitative prediction of the spatially distributed water content in soils. There are several potential hydrological applications that may benefit from such modeling framework, like, e.g., the setup of measurement networks, the upscaling of soil parameters, the local calibration and validation of remote sensing products and the development of suitable downscaling tools to mention a few. Such goal could be achieved by a thorough validation against detailed data at the different scales, which in turn calls for a more systematic monitoring and experimental effort, and the relaxation of some assumptions, like, e.g., considering spatially variable precipitation and nonstationary soil properties. At any rate, the present model could be used as a screening tool for preliminary assessment of the spatial variability of water content under scenarios involving different soil parameters or saturation conditions. The approach could also be employed for a preliminary inference of relevant soil properties like Γ, $\sigma_f^2, \sigma_a^2, I$ if enough measurements are available, and it may provide a framework for data interpolation when in presence of sparse data.

Appendix A: Derivation of SD_S and $SD_{S,\Delta}$

First, we consider the case of continuous sampling, i.e., when the measurement spacing is very small ($\Delta = 0$), such that the domain W is fully sampled. Thus, the spatial mean and variance of S over the domain W are given by

$$\bar{S}=\frac{1}{W}\int_W S(\mathbf{x})d\mathbf{x} \tag{A1}$$

$$\overline{\sigma_S^2}=\frac{1}{W}\int_W (S(\mathbf{x})-\bar{S})^2 d\mathbf{x} \tag{A2}$$

We emphasize that both $\bar{S}$ and $\overline{\sigma_S}$ are stationary random variables, and their expected values are achieved through suitable ensemble averaging over the local saturation $s(\mathbf{x})$. The expected values are given by

$$\langle \bar{S} \rangle = \langle S \rangle = \langle s \rangle \tag{A3}$$

$$SD_S^2 = \langle \overline{\sigma_S^2} \rangle = \left\langle \frac{1}{W} \int_W (S(\mathbf{x}) - \bar{S})^2 d\mathbf{x} \right\rangle \tag{A4}$$

Introducing in the latter the residuals $s' = s - \langle s \rangle$, $S' = S - \langle S \rangle$, $\bar{S}' = \bar{S} - \langle S \rangle$ we obtain

$$\begin{aligned} SD_S^2 &= \left\langle \frac{1}{W} \int_W (S'(\mathbf{x}) - \bar{S}')^2 d\mathbf{x} \right\rangle = \\ &= \frac{1}{W} \int_W \langle S'^2(\mathbf{x}) \rangle d\mathbf{x} - \frac{1}{W^2} \int_W \int_W \langle S'(\mathbf{x}') S'(\mathbf{x}'') \rangle d\mathbf{x}' d\mathbf{x}'' \end{aligned} \tag{A5}$$

The above formula can be written as

$$SD_S^2 = \sigma_S^2 - R_S \tag{A6}$$

where

$$\sigma_S^2 = \frac{1}{v^2} \int_v \int_v \langle s'(\mathbf{x}) s'(\mathbf{x}') \rangle d\mathbf{x} d\mathbf{x}' = \frac{1}{v^2} \int_v \int_v C_{ss}(\mathbf{x}' - \mathbf{x}'') d\mathbf{x} d\mathbf{x}' \tag{A7}$$

is the ensemble (*ergodic*) variance of the spatially averaged saturation, i.e., when $L \to \infty$, and R_S is the variance of the spatial mean $\bar{S}$, being

$$R_S = \frac{1}{v^2 W^2} \int_v \int_v \int_W \int_W C_{ss}(\mathbf{x}' + \mathbf{y}' - \mathbf{x}'' - \mathbf{y}'') d\mathbf{x}' d\mathbf{x}'' d\mathbf{y}' d\mathbf{y}'' \tag{A8}$$

Equation (A6), together with (A7) and (A8), provides the standard deviation of saturation S as function of the scales L and ℓ, respectively, the extent and the support scales, from which W and v depend. The statistical structure of the heterogeneous hydraulic properties is embedded in the covariance local saturation C_{ss}, which shall be addressed later.

Expression (A6) is theoretically valid when the spacing scale Δ is very small, while in practice the measurements are separated by a finite distance $\Delta > 0$. Thus, we consider in the following also the case of incomplete sampling of S over the volume W, i.e., when $(\Delta \neq 0)$. With N the number of measurements, and $\mathbf{x}_i$ the generic measurement location $(i = 1, N)$, the sample variance, denoted as $SD_{S,\Delta}^2$, is equal to

$$SD_{S,\Delta}^2 = \left\langle \frac{1}{N} \sum_{i=1}^{N} \left[S_i - \frac{1}{N} \sum_{j=1}^{N} S_j \right]^2 \right\rangle \tag{A9}$$

where $S_i = S(\mathbf{x}_i)$. Further elaboration gives

$$SD_{S,\Delta}^2 = \frac{1}{N} \sum_{i=1}^{N} \langle S_i'^2 \rangle - \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \langle S_i' S_j' \rangle \tag{A10}$$

Taking expectation, the final result is

$$SD_{S,\Delta}^2 = \sigma_S^2 - \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} C_{SS}(\mathbf{x}_j - \mathbf{x}_i) \tag{A11}$$

It is easy to see that if $N \to \infty$ then $SD_{S,\Delta}^2 \to SD_S^2$, the latter given by (A6), while if $N = 1$ it is $SD_{S,\Delta}^2 = 0$ and the number of measurements is clearly inadequate to capture the spatial variability of water saturation.

The relation between C_{SS} and C_{ss} is

$$C_{SS}(\mathbf{r}) = \frac{1}{v^2} \int_v \int_v C_{ss}(\mathbf{r} + \mathbf{x}' - \mathbf{x}'') d\mathbf{x} d\mathbf{x}' \tag{A12}$$

with $\mathbf{r}$ the separation distance vector.

Appendix B: First-Order Analysis

In this section, we briefly recast the first-order analysis of the unsaturated flow field. The main scope is to obtain an expression for the covariance C_{ss} of the point saturation s which is the key component of the present framework; further details of the first-order procedure can be found in Russo (1998, 1995) and Yeh et al. (1985a).

Given the steady state 3-D Richards equation with unit mean vertical gradient, and adopting the Gardner-Russo constitutive relations (3), the procedure consists in a formal perturbation of the Richards equation over the relevant variables $\psi, f=\ln K_s, a=\ln \alpha, s$ around their mean and taking expectation of the moment of interest, in our case the saturation mean $\langle s \rangle$ and the covariance C_{ss}. The result is encapsulated in formula (13a) of Russo (1998) which is reproduced here for the sake of convenience

$$C_{ss}(\boldsymbol{\xi})=B^2\left[C_{hh}(\boldsymbol{\xi})+H^2C_{aa}(\boldsymbol{\xi})+HC^*_{ha}(\boldsymbol{\xi})\right] \tag{B1}$$

where $C^*_{ha}(\boldsymbol{\xi})=C_{ha}(\boldsymbol{\xi})+C_{ha}(-\boldsymbol{\xi})$ and

$$B=\frac{\Gamma^2 H}{4}\exp\left[-\frac{\Gamma H}{2}\right] \tag{B2}$$

In the above expressions H, h are the mean capillary head and its fluctuation, respectively; C_{yz} is the covariance between generic variables y, z, and $\boldsymbol{\xi}$ is the separation vector. The latter covariances, are given in the Fourier space by formula (10) of Russo (1998). The evaluation of (B1) as function of $\langle S \rangle$ requires a functional relationship between the capillary head H and the saturation statistics, the latter can be achieved by the perturbation expansion of the second of 3, the result being

$$\langle s \rangle=\exp\left(-\frac{1}{2}\Gamma H\right)\left(\frac{\Gamma H}{2}+1\right) \tag{B3}$$

The covariances are manipulated by assuming a vertical unit gradient $\mathbf{J}=(1,0,0)$ free drainage i.e., and by adopting axisymmetric exponential covariances (e.g., equation (11) of Russo, 1998) for both f and a; after few algebraic passages the various terms appearing in (B1) can be written with the dimensionless variables $x_i=\xi_i/I, \Gamma'=\Gamma I, h'=h/I$, with x_1 aligned with the vertical, as follows

$$\frac{C_{hh}(x_1,r)}{I^2}=\frac{4e\left(\Gamma' H'\left(\Gamma' H'\sigma_a^2-2\sigma_a\sigma_f\rho_{af}\right)+\sigma_f^2\right)}{\pi}\cdot \int_0^\infty\int_0^1\frac{\kappa^2u^2J_0\left(\kappa r\sqrt{1-u^2}\right)\cos(\kappa u x_1)}{\left[e^2\kappa^2u^2+\kappa^2(1-u^2)+1\right]^2\left(\kappa^2+\Gamma'^2u^2\right)}du\,d\kappa \tag{B4}$$

$$\frac{C_{ha}(x_1,r)}{I}=\frac{4e\left(\sigma_a\sigma_f\rho_{af}-\Gamma' H'\sigma_a^2\right)}{\pi}\cdot \int_0^\infty\int_0^1\frac{\kappa^2uJ_0\left(r\kappa\sqrt{1-u^2}\right)\left[\Gamma' u\cos(\kappa u x_1)-\kappa\sin(\kappa u x_1)\right]}{\left[\kappa^2\left((e^2-1)u^2+1\right)+1\right]^2\left(\kappa^2+\Gamma'^2u^2\right)}du\,d\kappa \tag{B5}$$

$$C_{aa}(x_1,r)=\sigma_a^2\exp\left(-\sqrt{x_1^2/e^2+r^2}\right) \tag{B6}$$

where $e=I_v/I$ is the formation anisotropy, ratio between the vertical and horizontal integral scales of the hydraulic properties, $r=\sqrt{x_2^2+x_3^2}$ is the horizontal separation distance and $J_n(z)$ is the Bessel function of the first kind.

The above formulas differ from those reported in Russo (1998) in that they are somewhat simpler to integrate and manipulate; their solution still requires numerical quadratures. Formula (B1), together with expressions (B5), (B4), and (B6), provide the necessary input for the calculation of the standard deviation of water saturation as function of the mean saturation, as described in section 3.

A particular case for which an analytical solution can be found is the statistically isotropic formation $e=1$, for which the saturation variance can be written as

$$\sigma_s^2=C_{ss}(0)=\frac{\Gamma'^4H'^2}{16}e^{-\Gamma' H'}\left\{H'^2\sigma_a^2+\frac{\left(\sigma_f^2-H'^2\sigma_a^2\Gamma'^2\right)\left[\Gamma'(\Gamma'+2)-2(\Gamma'+1)\ln(\Gamma'+1)\right]}{(\Gamma'+1)\Gamma'^3}\right\} \tag{B7}$$

Acknowledgments
The data for the SPG99 experiment reproduced in Figure 7 were taken from Famiglietti et al. (2008a); all of the other numerical information is provided in the figures produced by solving the equations in the paper.

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