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MODELLING AND UPSCALING UNSATURATED FLOW THROUGH RANDOMLY HETEROGENEOUS SOILS

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1 INTRODUCTION

While applying physically-based mathematical models of flow and transport (Darcy's law and conservation equations) to an actual field situation, the spatial variability of soil hydraulic properties have to be considered in order to provide realistic predictions of unsaturated flow and transport at field scale. This heterogeneity can be included in the modelling by various approaches, depending on the problem of interest. In this study, samples of heterogeneous soils are generated using sets of spatially correlated random field parameters that are either geometrically isotropic, or else anisotropic with perfect or imperfect stratification. Numerical simulations of unsaturated flow are then performed on each sample, with the mean flow either perpendicular or parallel to stratification, using a gravitational boundary condition at the bottom of the sample. The resulting effective unsaturated conductivity is then analyzed at the scale of the sample as a function of mean pressure or suction, and compared to stochastic and probabilistic theories (spectral perturbations, and nonlinear probabilistic power average).

2 STOCHASTIC THEORY AND NUMERICAL METHODOLOGY

The soil hydraulic parameters, which are random space functions, are represented in each case by a single realization. One realization for each of the soil parameter is used as input for the simulation model, to obtain a single realization of the unsaturated flow field. The method has been used previously for saturated 3D flow simulations[1], and for 2D unsaturated flow and transport simulations[2], among others. The realizations of 1D and 2D parameter fields are generated using the XIMUL 123D code (Ababou), which is based on the 3D turning bands random field generator[3]. More details on parameters and numerics can be found in reference [12].

2.1 Unsaturated Constitutive Relationships

The relationship between hydraulic conductivity $K(x)$ and suction head $\psi(x)$, for each grid point x within the discretized domain, is represented by the Gardner [1958] model as:

$$K(x) = K_S(x)\exp(-\beta(x)\psi(x)) \quad (1)$$

where $K_s(x)$ is the saturated hydraulic conductivity, and $\beta(x)$ is the pore size distribution parameter, a pressure scaling parameter, generally known as Gardner's "constant". In this study both parameters are considered as regionalized variables. The van Genuchten [1980] moisture retention function is used (assumed to be independent of space):

$$\Theta(x) = \frac{\theta(x) - \theta_r}{\theta_s - \theta_r} = \left\{ \frac{1}{1 + \alpha|\psi(x)|^{n_v}} \right\}^{m_v} \quad (2)$$

where, θ_r is residual moisture, θ_s is saturated moisture, $\theta(x)$ is the suction-dependent moisture content, Θ is the "effective" degree of saturation, and finally, "α" , "n" and m=(1-1/n) are the van-Genuchten parameters (used here only for the moisture curve).

Upscaled constitutive relationships for a given heterogeneous domain are obtained by repeated numerical flow experiments, for a series of given infiltration rates.

2.2 Analytical $K_{EFF}(\psi)$ through Spectral Perturbation Theory

In this approach, the effective unsaturated conductivity curve $K_{EFF}(x)$ is expressed analytically from the stochastic spectral solutions of unsaturated flow obtained by [4,5,6] based on linearization and perturbation approximations of unsaturated Darcy equations (steady state case). The effective conductivity components in the two principal directions (orthogonal and parallel to strata) are given by:

$$K_V = \exp\left[F - \frac{\sigma_f^2}{2(1+B\lambda_z)} - \left(B - \frac{(2\lambda_z + |H|)}{2(1+B\lambda_z)}\sigma_\beta^2 \right)|H| \right] \quad (3)$$

$$K_H = \exp\left[F + \frac{\sigma_f^2}{2(1+B\lambda_z)} - \left(B - \frac{(2\lambda_z - |H|)}{2(1+B\lambda_z)}\sigma_\beta^2 \right)|H| \right] \quad (4)$$

where F is the mean and σ_f^2 is the variance of $Ln(K_S)$, B is the mean β, σ_β^2 is the variance of β, and H is the mean suction. A major drawback is that this method is valid only for small variability (σ_f <1 and σ_β << 1), and applicable only for moderate suctions (not very dry soils).

2.3 Analytical $K_{eff}(\psi)$ through the Power Averaging theory

The Power Averaging theory ("RA model") was developed in reference [7] and in earlier reports, and was also presented briefly in ref. [8]. In the Power Averaging model, it is assumed that the local conductivity curves of the randomly heterogeneous medium are of the form:

$$K(\psi, x) = K_s(x)\exp(-\beta(x)\psi) \Leftrightarrow LnK(\psi, x) = LnK_S(x) - (\beta(x)\psi) ,$$

where $K_S(x)$ and $\beta(x)$ are random positive coefficients, and ψ is suction head (*meters*). The coefficients may have lognormal or any other positive distributions. In the analytical developments below, it will be assumed that $f(x) = LnK_s(x)$ and $a(x) = Ln(\beta(x))$ are spatially correlated Gaussian random fields, generally cross-correlated (ρ). The effective conductivity curve resulting from the "RA model" (Gardner version) can be expressed as follows in the case of unimodal (e.g. lognormal) statistical parameters Ks(x) and β(x) :

$$K_i(\Psi) = K_G \exp\left\{\frac{1}{2}(A_i\Psi^2 + B_i\Psi + C_i)\right\} \qquad (5)$$

where $A_i = p_i\sigma_a^2$; $B_i = -2(1 + p_i\rho\sigma_a\sigma_f)$; $C_i = p_i\sigma_f^2$; ψ = -h is suction head, and $\Psi = \beta_G\psi$ is the dimensionless suction head.

The curve $K_i(\Psi)$ is the principal effective conductivity component along direction X_i. The parameter p_i is the power averaging used for obtaining conductivity along direction X_i: it may be treated for the moment as a semi-empirical adjustable parameter. In addition, statistical parameters are defined as follows: β_G is the geometric mean of $\beta(x)$, where :

$$\beta = \frac{\partial LnK(h,x)}{\partial h}$$ is the log-conductivity slope;

σ_a is the standard deviation of log-coefficient $a(x)$; σ_f is the standard deviation of log-coefficient $f(x)$; ρ is the cross-correlation between the random log-parameters ($a(x)$, $f(x)$).

The averaging powers p_i can be chosen tentatively as follows (a more complete conjecture is available, but in this work, we will calculate the p_i's from the numerical experiments): p_i = 0 in each direction Xi if the medium is perfectly isotropic; p_i = -1 (harmonic) in the direction orthogonal to layers (e.g. vertically); p_i =+1 (arithmetic) in the direction parallel to layers (e.g. horizontally). Eqn. (5) can also be expressed as a function of p_i as follows:

$$K_i(\Psi) = K_G \exp\left\{\frac{1}{2}\left[(p_i\sigma_a^2)\Psi^2 - 2(1 + p_i\rho\sigma_a\sigma_f)\Psi + p_i\sigma_f^2)\right]\right\} \qquad (6)$$

Remarkably, the "RA" Power Averaging model in Eqn (5) yields an effective conductivity curve Ki(Ψ) of the same form as the spectral perturbation theory, which can also be cast in terms of (Ai,Bi,Ci), but with different expressions for these coefficients. In 3D, the parameters of the "RA" model are the 3 averaging powers "p_i" (i=1,2,3) which can be taken different horizontally and vertically. For a horizontally stratified medium, assuming p_i = +1 horizontally and p_i = -1 vertically yields arithmetic mean and harmonic mean of the nonlinear K(h,x) curve. With this choice, the RA model becomes similar but not identical to the model proposed in reference [9], which was further investigated by [10, 11]. However, [9] did not include the cross-correlation parameter, which plays an important role according to our simulation results and analytical results as well (both spectral perturbations and power averaging).

2.4 Numerical Experiments Approach

Steady state gravity drainage flow simulations are performed using the 2D numerical model presented in references [12, 13]. The transient mixed form of the unsaturated Richards equation is solved by Finite Differences, using Modified Picard iterations for handling the inherent nonlinearity. The resulting set of equations is solved by the 2D Strongly Implicit Procedure. A uniform infiltration rate q is specified over the top boundary of the domain, and a unit hydraulic gradient is imposed at the bottom boundary, lateral boundaries are impervious. The initial condition is uniform pressure head. Transient simulations are performed till the steady state is reached by time marching. The numerical simulations are performed for a series of infiltration cases, i.e., for different values of "q". Note that the transient flow results were also analyzed, and solute transport simulations were conducted on the steady flow fields (see references [12,13]).

3 UPSCALING UNSATURATED FLOW

The effective conductivity is calculated numerically by interpreting the numerical simulation results in terms of global quantities: mean flux and mean gradient. The resulting K is plotted versus mean suction ψ, and it is then compared with the two available analytical results: the spectral perturbation solution, and the power averaging result (RA Model). In the latter case, the upscaled numerical conductivity curves were fitted to the power averaging formula in eqn.(6) to obtain the unknown coefficient p_i by a nonlinear least squares optimization method. The numerical $K(\psi)$ curve is also compared to the Arithmetic, Harmonic and Geometric mean $K(\psi)$ curves (computed with RA model).

The β parameter plays an important role in the resulting value of the averaging powers p_i. Note that β is a pore size distribution parameter, whose inverse represents a capillary length scale ($1/\beta = \lambda_{CAP}$). This scale is compared to layer thickness or correlation length (λ_Z). The cases $\beta\lambda_Z \sim 1$, $\beta\lambda_Z < 1$, $\beta\lambda_Z > 1$ are explored.

It was found that perfectly stratified unsaturated soils can behave like saturated media, with arithmetically averaged $K(\psi)$ in parallel flow and harmonically averaged $K(\psi)$ in perpendicular flow - *however* in some cases, depending on flow regime and layer thickness, this classical behavior does not hold.

3.1 Statistical representation of flow parameters of soil.

The mean and standard deviation values (Table 1) are taken from [14] for the generation of single realizations of Ln(Ks(x)) and β(x), corresponding to a coarse-textured sand from the upper Hanford formation at the Hanford site, Washington. Although the two parameters are generated independently, the correlation lengths of both the parameters are the same, which relates each parameter unto itself spatially.

In this study mainly three types of generated random fields are used:

- In the first case, a perfectly layered "1D" random field is generated, with $\lambda_X >> \lambda_Z$, or equivalently, $\lambda_X \to \infty$ and λ_Z finite. in a domain discretized into 1001 nodes.

- In the second case, a 2D anisotropic field with imperfect random stratification is generated ($\lambda_X > \lambda_Z$) in a domain discretized into 501x501 grid points.
- In the third case, a 2D random isotropic field is generated ($\lambda_X = \lambda_Z$) in a domain of size 10mx10m discretized into 1000x1000 grid points.

Table 1 Statistical Parameters of Gardner's exponential conductivity curve

Parameters	Mean	Standard deviation	Correl. length horizontal (m)λx	Correl. length vertical (m) λz	Δx (m)	Δz (m)
1. Perfectly stratified"1D" random field ; $\lambda_X >> \lambda_Z$; βλ=0.8133						
Ln Ks *(*)*	0.253	0.771	∞	0.10	2.0	0.20
β*(1/m)*	8.133	1.493	∞	0.10	2.0	0.20
2. Imperfectly stratified "2D"random field; $\lambda_X > \lambda_Z$;βλ=1.6266						
Ln Ks *(*)*	0.253	0.771	2.0	0.20	0.10	0.05
β*(1/m)*	8.133	1.493	2.0	0.20	0.10	0.05
3. Isotropic "2D" random field Field; $\lambda_X >> \lambda_Z$; βλ=8.133						
Ln Ks*(*)*	0.253	0.771	1.0 m	1.0 m	0.01	0.01
β*(1/m)*	8.133	1.493	1.0 m	1.0 m	0.01	0.01

*Ks in m/d

Table 2. Moisture retention Properties of vGM curve, assumed to be constant in space

$\theta_s\left(m^3/m^3\right)$	$\theta_r\left(m^3/m^3\right)$	$\alpha_v\left(m^{-1}\right)$	n_v
0.397	0.027	4.306	1.82212

4 NUMERICAL EXPERIMENTS AND UPSCALING

A series of gravity drainage experiments are performed using the above-described method (Section 2.4) on one and two-dimensional random fields. The mass balance is also observed simultaneously, which is the right method to check the steady state attainment. The simulated flow field will be under the unit gradient condition, thus the flux is equal to the effective unsaturated K for which the mean pressure is obtained by corresponding pressure fields. The simulations are carried out for different flux rates to get the curve of effective unsaturated K. Two principal flow directions considered are, flow perpendicular to bedding and flow parallel to bedding. Flow parallel to bedding is considered on the same sample rotated by 90 degrees (*vertical instead of horizontal strata*). The flow direction remains the same, still parallel to gravity (*gravitational flow*). The resulting set of unsaturated flow fields is used to upscale numerically the hydraulic conductivity against mean suction.

4.1 Flow though Perfectly Stratified "1D" fields($\lambda z=\infty$, $\lambda z=0.1m$); $\beta\lambda=0.8133$

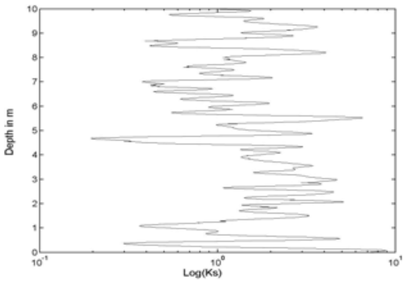

Figure 1. Generated random field of Ln(Ks) profile for the perfectly stratified case.

A set of horizontally stratified 1D random fields Log(Ks) and β are generated, with the statistical parameters from Table 1, on a 1001 node grid. The generated field of Ln(Ks(x)) is as shown in **Fig.1**.

Flow Perpendicular to Stratification

A series of simulations are performed and the upscaled conductivity curve is plotted and compared with the spectral perturbation results of [4,5,6] in **Fig. 2** which match quite well. Fig.2 also shows the best fitted curve to the power average p = -0.0484 for the Ln(K/Kg) fit; p = -0.0634 for the K/Kg fit. It is seen from this figure that the numerical K(ψ) curve matches with the harmonic mean at low suctions (wet range), as could be anticipated, but the curve moves away from the harmonic mean (closer to geometric mean) at higher suctions (dry range).

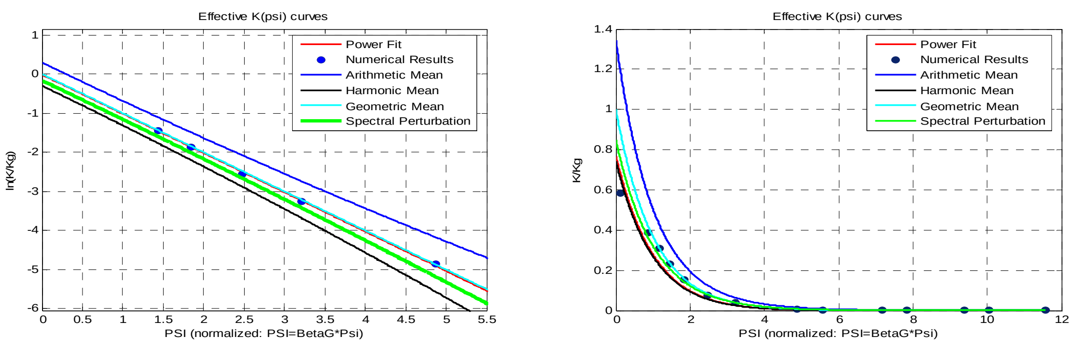

Figure 2 Numerical results compared with Spectral perturbation theory and best fit to poweravaraging equation (RA model) for flow perpendicular to perfect stratification Left Ln(K/KG) fit; p_i= -0.0484. right (K/KG) fit; p_i= -0.0634.

Flow parallel to Stratification.

A series of simulations are performed to obtain the upscaled K(ψ) relation point by point. The numerical K(ψ) points are compared with the spectral perturbation theory of [4,5,6], to the best fitted power averaging model (RA Model), and to the arithmetic, harmonic and geometric mean curves (also computed with the aid of the RA model). The best fitted parameter is p_i = -0.1749 for the Ln(K/Kg) fit, and p_i = +0.9640 the K/Kg fit. Indeed, it can be seen that the numerical points K(ψ) coincide with the arithmetic mean curves for low suctions (wet range) but deviate somewhat from it (in favour of the geometric mean) for higher suctions (dry range).

The different values obtained for the fitted power "p_i" depend on the direction "i" (as expected) but also on the type of fit. The latter can be explained as follows. The LnK fit attributes more weight to the dry range than the K-fit. In fact, the K-fit almost completely neglects high suctions (low conductivities) compared to the LnK-fit, and that was one reason to try the LnK-fit as an alternative fit.

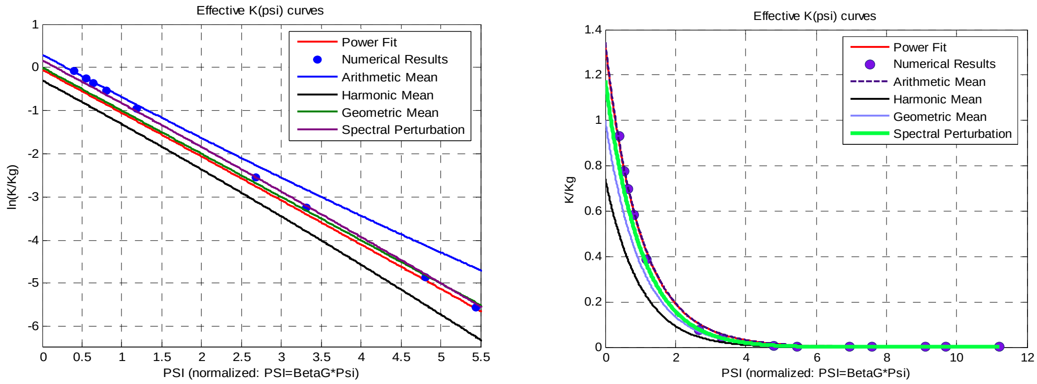

Figure 3. Numerical results compared with Spectral perturbation theory and best fit to poweravaraging equation (RA model) for flow parallel to perfect stratification Left: Ln(K/Kg) fit; p_i= -0.1749. Right: (K/Kg) fit; p_i= -+0.

4.2 Flow through Imperfectly Stratified Field (λx>>λz);); βλ=1.6266

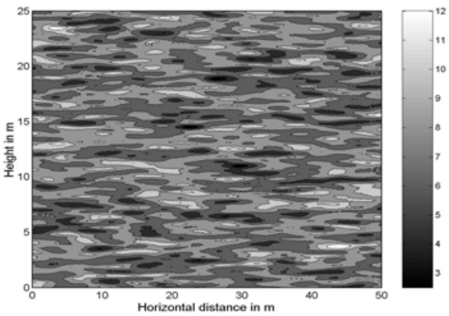

Figure 4. Generated 2D anisotropic Random Field of Ln(Ks)

In this case flow in imperfectly stratified medium is explored. The hydraulic properties of the soil remain the same as in Table 1 and 2, with the horizontal correlation length chosen much greater than the vertical one (λx >> λz). This yields horizontally elongated strips of soil (elongated imperfect layers). The generated field of the saturated lnKs is shown in **Fig 4**.

Flow Perpendicular to Imperfect Stratification. Fig. 5 shows the comparison of numerical results with the Yeh's spectral perturbation results, which match very well, and the same figure also plots the the upscaled conductivity curve with best fitted power averaging parameter "p": p = -0.0484 for the Ln(K/Kg) fit, and p = -0.0634 for the K/Kg fit. As anticipated, the numerical results in this case do not really match with the harmonic mean values, and some more tests need to be performed near saturation to explore the behavior of the imperfect stratification.

Flow Parallel to Imperfect Stratification. Fig. 6 shows the comparison of numerical results with the Yeh's spectral perturbation results, which match quite well, and also plots the best fit of the upscaled power average conductivity curve, which is p =+0.0636 for the Ln(K/Kg) fit and pi = -0.0777 for the K/Kg fit. The numerical results in this case do not really match with the arithmetic mean values. More points should be tested in the wet range of suctions.

4.3 Flow Through Isotropic Field (λx = λz); βλ=1.6266

In this case the numerical simulations are performed on a two-dimensional (2D) isotropic random field of 10m×10m size, with a mesh grid of 1000×1000 nodes. The statistical parameters given in Table 1 are used to generate isotropic field for hydraulic conductivity and for Gardner's scaling parameter (exponent) in the 2D domain. Ln(Ks) field is shown in **Fig. 7**. A correlation length of 0.1 m is used. The statistical resolution is therefore 10 nodes per correlation length. A set of gravity drainage numerical experiments are carried out for various flux rates (q).

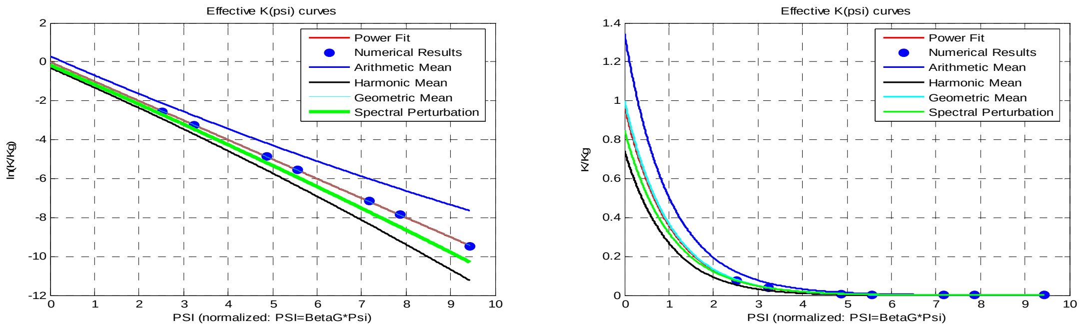

Figure 5. Numerical results compared with Spectral Perturbation and Best fit to power averaging equation (RA Model) for flow perpendicular to imperfect stratification. Left: Ln(K/Kg) pi= -0.0484. Right: (K/Kg) fit : pi = -0.0634.

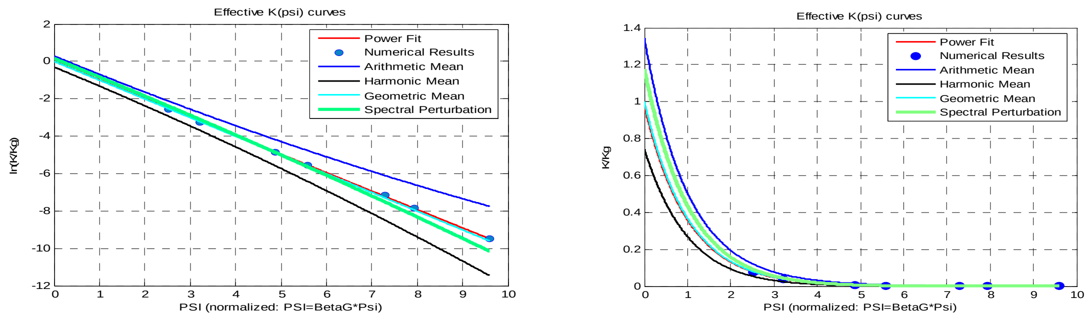

Figure 6. Numerical results compared with Spectral Perturbation results and Best fit to power averaging equation (RA Model) for flow parallel to imperfect stratification . Left: Ln(K/Kg) fit, pi=+0.0636. Right: (K/Kg) fit, pi= -0.0777.

Fig.8 shows the comparison of numerical results with the Yeh's spectral perturbation results, which match quite well, and it also shows the best fitted curve of the upscaled conductivity from power averaging theory (RA model), with a fitted power "p" equal to -0.0484 for the Ln(K/Kg) fit, and -0.0634 for the K/Kg fit.

As anticipated the numerical results in this case are quite close to the geometric mean curve ($p_i = 0$). The *dimensionless* capillary length scale is $\beta\lambda = 8.133 >> 1$.

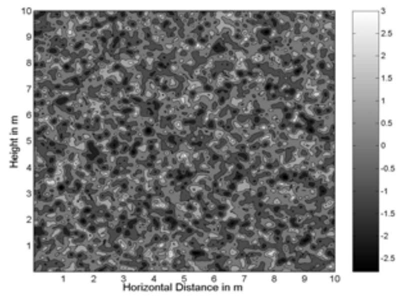

Figure 7. Generated random field Ln(Ks) with 2D isotropic auto-correlation structure.

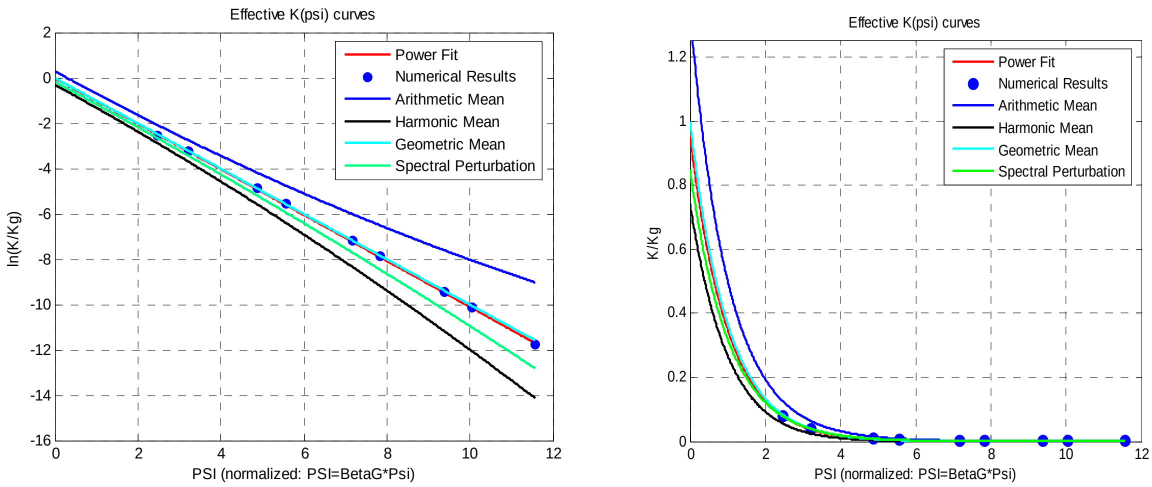

Figure 8. Numerical results compared with Spectral Perturbation theory for flow through isotropic field. Left: Ln(K/KG) fit, pi= -0.0484. Right: (K/KG) fit, pi= -0.1517

5 CONCLUSIONS

Unsaturated steady flow through randomly heterogeneous soils was simulated numerically, analyzed and upscaled. The β parameter described in Gardner's exponential conductivity curve is a pore size distribution parameter, whose inverse represents a capillary length scale ($1/\beta = \lambda_{CAP}$). This capillary scale is compared to layer thickness or correlation length (λ_Z) to produce a dimensionless capillary scale βλ. Cases $\beta\lambda_Z \sim 1$, $\beta\lambda_Z < 1$, $\beta\lambda_Z > 1$ are explored.

It is found that perfectly stratified unsaturated soils can behave like saturated media, with arithmetically averaged K(h) in parallel flow, and harmonically averaged K(h) in perpendicular flow. However in some cases, depending on flow regime and layer thickness, this 'classical' behaviour does not hold.

Overall, it was shown that the behavior of effective unsaturated conductivity can be captured parametrically via a probabilistic nonlinear '*power average model*', where the product $\beta\lambda_Z$ plays a direct role (*Ababou et al.*). The latter model was compared to linearized spectral perturbation theory: the two models are in a way "complementary"; they are not exclusive of each other, and they can be made to coïncide totally in some cases.

Given these encouraging results, further work is currently being conducted to investigate more completely the upscaled unsaturated conductivity versus suction and the behavior of the power averaging exponent.

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