NUMERICAL VALIDATION OF VARIOUS MIXING RULES USED FOR UP-SCALED GEO-PHYSICAL PROPERTIES

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ABSTRACT

Mixing rules are widely used to express effective properties of coefficients appearing in heterogeneous diffusion like processes. Since most of the mixing rules were derived to compute the effective dielectric constant, ε_{eff}, in this work, we confine our interest to the electrostatic behaviour of mixtures. This paper focuses on the validation of mixing rules by comparing them with the effective properties computed from the numerical solution of div(εgradΦ) =0 including boundary conditions. One of the issues concerns the very large number of grid blocks required to obtain convergence. We choose the checkerboard configuration as the input for the heterogeneous ε field as a realistic example that is amenable to analysis. We compare the convergence rates of a Finite Element Model (FEM) and a Finite Difference Model (FDM). Different choices of internodal dielectric coefficients are used in the FDM. For the 2-dimensional case it can be shown that the result for both the FEM and FDM converge to the geometric average. The FEM uses a 9 (27) points scheme, whereas the FDM uses a 5 (7) points in 2- (3)-dimensional computations. It is found that the convergence rate for the FE model is faster for both the 2- and 3-dimensional models. Indeed, using a geometric average for the internodal dielectric constant leads to the fastest convergence rate when the different FD models are compared. From the 3-dimensional computations it is possible to estimate ε_{eff} for different ratios of ε for a two component system. From comparison with existing mixing formulas we conclude that the cubic power-law or the Looyenga-Landau-Lifshitz and the Bruggeman mixing rule give the best estimate. For the given volume ratio of constituents, the Hashin-Shtrikman bounds show the range of values that can be obtained for different spatial distributions. We conclude that for a given volume ratio fine gridded numerical computations can be used to analyze the measured effective dielectric constant.

1. INTRODUCTION

In heterogeneous diffusion like processes, mixing rules are used to obtain averaged values of the coefficients, e.g., the diffusion coefficient D, the thermal conductivity λ, the Darcy permeability k, the magnetic susceptibility μ, the electric conductivity σ and the dielectric constant ε. In the literature references cited in this paper we mainly concentrate on effective dielectric constant for electrostatics and the equivalent Darcy permeability for flow through porous media. Without loss of generality we express all results in terms of the dielectric constant The average dielectric constant for up-scaled heterogeneous media is denoted by the effective dielectric constant ε_{eff}.

The classical mixing rules are the Maxwell-Garnett mixing rule (MGM) [*Maxwell-Garnett*, 1904] and the Bruggeman formula (BRM) [*Bruggeman*, 1935]. Summaries and applications of various mixing rules are given by [*Renard and de Marsily*, 1997; *Sihvola*, 2000; *Kärkkäinen et al.*, 2000; *Seleznev*, 2005]. The mixing rules seek the single optimal effective value for ε_{eff}, which replaces the heterogeneous ε field. An important class of mixing rules is derived from the effective medium approximation. The concept of the effective medium theory implies that the mixture responds to electromagnetic excitation as if it were homogeneous [*Sihvola*, 2000]. All of these theories use the effective field due to an average dielectric constant and subsequently average local contributions with a specific volume fraction. At low concentrations of the guest component (inclusions), all mixing rules show more or less the same results due to linear approximations in the component fraction. Hence at higher concentrations of the guest component in the host component (background), the results can strongly vary [*Kärkkäinen et al.*, 2001]. Moreover, in order to validate the computed ε_{eff}, the Wiener bounds [*Wiener*, 1912] and the Hashin–Shtrikman bounds [*Hashin and Shtrikman*, 1962] are often used. The Hashin–Shtrikman bounds are equivalent to the Maxwell-Garnett estimate of the relative dielectric constant for a two component mixture. Both types of bounds are based on spherical inclusions embedded in the background medium [*Choy*, 1999]. These sets of bounds are represented by a lower and an upper bound and are applicable for the averaged dielectric coefficient in a macroscopically isotropic (Hashin-Shtrikman bounds) or anisotropic (Wiener bounds) homogeneous medium. The bounds are independent of the spatial distribution of the constituents.

The effective value of a mixture depends on the method of measurement and the scale at which the heterogeneities occur. For a large class of measurements the processes in the isotropic case are described by the stationary diffusion equation with a given set of boundary conditions. Validation of the mixing rules partly consists of comparing the results with experimental data [*Noetinger and Jacquin*, 1991]. It is, however, also possible to validate the mixing rules by comparison with numerical computations using the stationary diffusion equation [*Pekonen et al.*, 1999; *Kärkkäinen et al.*, 2000, 2001; *Renard et al.,* 2000a, 2000b]. In these investigations, an analysis of the two- and three-dimensional dielectric mixture has been done using the Finite Difference Method (FDM). *Renard et al.* [2000b] investigated the difference in convergence rate of the numerical solution obtained from FDM and the Finite Element Method (FEM). They concluded that for coarse gridded models the FEM overestimated ε_{eff} and FDM underestimated it when the harmonic average is applied on the grid cell boundaries.

The two component checkerboard configuration as the input for the locally heterogeneous ε field has been investigated extensively. Analytical functions for the two–dimensional checkerboard configuration with periodic boundary conditions have been discussed by *Keller* [1964], *Dykhne* [1971] and *Ke-da* [1990]. It is generally concluded that the analytic ε_{eff} for this configuration equals the geometric average. Moreover, this field is sufficiently realistic to be representative of practical heterogeneity distributions, amenable to analysis (periodicity, simplicity, uniformity of internodal permittivities) and the role of the host, ε_{host}, and guest component, ε_{guest}, is indistinguishable.

FDM is a widely accepted numerical method to compute the effective dielectric constant and to investigate the role of the component distribution. To evaluate the effective dielectric constant obtained from FDM computations, numerical properties must be investigated. The convergence of the numerical solution toward the theoretical solution can only be obtained for a large number of grid blocks [*Romeu and Noetinger*, 1995; *Renard et al.*, 2000b]. Moreover, in FDM computations an effective dielectric constant, denoted by ε_{ij}, must be ascribed to the grid cell boundaries. The way ε_{ij} is defined, influences the validity and thus the convergence of the solution [*Romeu and Noetinger*, 1995; *Renard et al.*, 2000b; *Roth et al.*, 1996].

In this paper, we investigate the role of two numerical methods, FEM and FDM, for the computation of the effective dielectric constant. The convergence for four different finite difference approximations and the finite element model is evaluated. For each FD model we apply the arithmetic average, the harmonic average, the geometric average or the third-order power law (or cubic law) as input for ε_{ij} [e.g., *Noetinger and Jacquin*, 1991; *Wen and Gómez-Hernández*, 1996]. The results obtained for the 3-dimensional checkerboard configuration for different ratios between ε_{host} and ε_{guest} are compared to existing mixing rules.

The objective of this study is to give the methodology for validation of mixing formulas by comparing them to accurate numerical computations. The long term objective is to use accurate numerical computations to obtain a mixing rule that includes a parameter that describes the spatial distribution of the constituents, i.e., a parameter that specifies the effective dielectric constant from combined dielectric and capillary pressure measurements.

2. NUMERICAL METHODS

To obtain ε_{eff} of a two component mixture two types of numerical models have been developed based on the finite difference method and finite element method. The sample is composed by the background material, ε_{host}, and the inclusions, ε_{guest}. Both the models solve the equation for a static electromagnetic problem in a square or cubic domain. For the model description we restrict to the 2-dimensional case where the diffusion equation reads

$$\nabla_{x,y} \cdot \left(\varepsilon(x,y) \nabla_{x,y} \Phi \right) = 0 \text{ on } \Omega\text{: } \{0 \le x < L, 0 \le y < L\}, \tag{1}$$

where ε is the dielectric constant and Φ is the electric potential. In the y-direction the potential has an ordinary periodic boundary condition [e.g., *Kärkkäinen et al.*, 2001]. A constant potential difference, $\Delta\Phi$, is applied in the x-direction. These periodic boundary conditions are given as

$$\Phi(x = L, y) = \Phi(x = 0, y) - \Delta\Phi \text{ and } \Phi(x, y = 0) = \Phi(x, y = L). \tag{2}$$

After solving for the potential field, the effective dielectric constant can be computed with

$$\varepsilon_{eff} = \frac{Q}{\Delta\Phi} \frac{L}{A}, \tag{3}$$

where A is the total surface perpendicular to the flow and $Q=\int_A \varepsilon \frac{d\Phi}{dn} dS$, is the total charge.

For the specific equations in the FD method we refer to *Patankar et al.* [1980]. The model area is subdivided in square grid blocks and the internodal dielectric constant, ε_{ij}, used in the FDM description is represented by

$$\varepsilon_{ij} = \left(\frac{\varepsilon_i^{\alpha} + \varepsilon_j^{\alpha}}{2} \right)^{1/\alpha}. \tag{4}$$

Hence, the arithmetic average, the harmonic average and the third-order power law average corresponds respectively to α=1, α=-1, α=1/3. The fourth internodal average applied, is the geometric average described by $\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}$.

The FEM is also based on an equidistant grid and bilinear test functions are applied in the two-dimensional configuration and trilinear test functions in three-dimensional configuration [*Zienkiewicz et al.*, 2005]. The test function used for two dimensions is represented by

$$v_\beta(x,y) = 1 + ax + by + cxy\,, \tag{5}$$

in the domain spanned by the grid points *β=P, N, NE, N* with coordinates (0,0), (0,Δ*y*), (Δ*x*,Δ*y*) and (Δ*x*,0) respectively. At the points *N, NE, E* the function $v_\beta = v_P = 0$. Hence we obtain

$$v_P(x,y) = \left(1 - \frac{|x - x_P|}{\Delta x}\right)\left(1 - \frac{|y - y_P|}{\Delta y}\right). \tag{6}$$

3. NUMERICAL RESULTS

Simulations with the FEM and FDM, with different estimations for the internodal dielectric coefficients, are performed for the checkerboard configuration. In other words the volume fraction for each of the components is 0.5 in all simulations. Grid refinement is applied in combination with the multi-grid method to find ε_{eff}. The results for a two component mixture with ε_{host}=3 and ε_{guest}=10 for the 2-dimensional and 3-dimensional configuration are presented in FIGURE 1 and FIGURE 2 respectively.

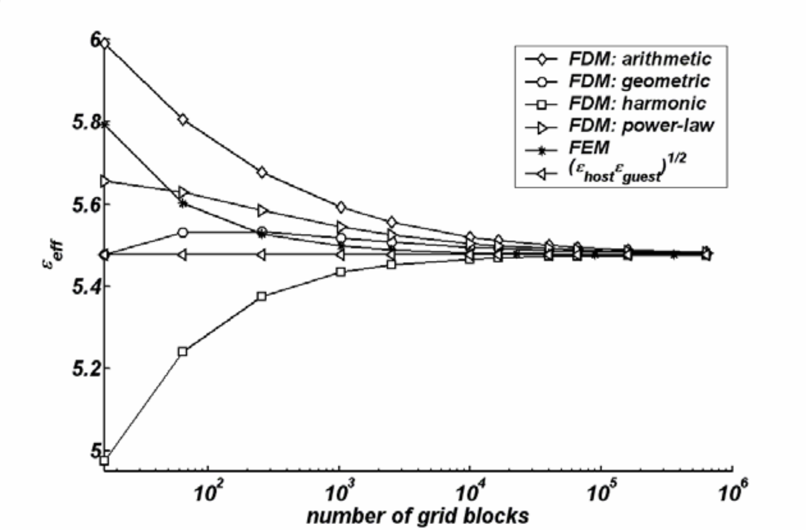

FIGURE 1. Comparison between FDM and FEM for a 2 dimensional checkerboard configuration with ε_{host}=3 and ε_{guest}=10

For the 2-dimensional case, for all ε_{ij}, both the FEM solutions and FDM solutions , converge to the geometric average. In the case where the geometric average is applied as estimator for ε_{ij}, the computed ε_{eff} is approximated well for the coarse grid (see FIGURE 1). Moreover, the under- and overestimation for the harmonic and arithmetic average applications satisfy the Wiener bounds. For these bounds a layered system is assumed, hence the upper and lower bound are represented by the harmonic and arithmetic average respectively. The solutions obtained for all refinements satisfy the lower and upper Hashin-Shtrikman bounds, respectively given by 4.68 and 7.36.

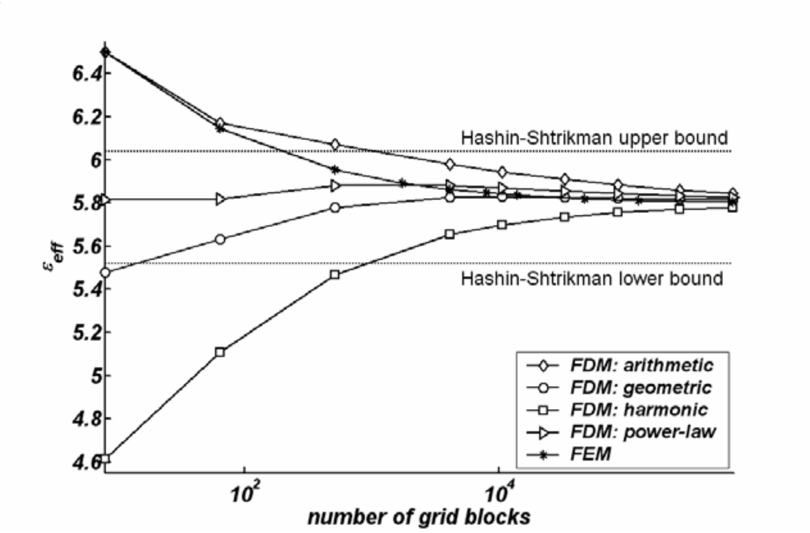

FIGURE 2. FDM and FEM computations for a 3–dimensional checkerboard with ε_{host}=3 and ε_{guest}=10

From FIGURE 2 it can be seen that the solutions obtained for the power law FDM approximation for the 3-dimensional checkerboard satisfy the Hashin-Shtrikman bounds, even for very coarse grids. The harmonic and the arithmetic FD models have the smallest convergence rate and are valid for $\Delta x/L < 0.087$. Not much difference in convergence rate can be observed between FEM and the FDM based on both the geometric average and power law average. The overestimation ε_{eff} for the FE model and the underestimation of the FD model, except from the "arithmetic" based FDM, is in agreement with the results of *Renard et al.* [2000b]. The result obtained from the power law based FDM for a very coarse grid already gives a reasonable and valid estimate for ε_{eff}.

To investigate which mixing rule (MR), provides the best estimate for ε_{eff}, we compute the ε_{eff} of the 3-dimensional checkerboard for different ε-ratios on a very fine grid, consisting of 681472 grid blocks. We normalize ε_{eff} with the mixing rule considered and plot the results as a function of the contrast on a logarithmic scale (see FIGURE 3). The BRM and the Looyenga-Landau-Lifshitz mixing rule (LLMF) both give the best estimates for ε_{eff} with increasing deviations for increasing contrasts. For the region of $\varepsilon_{host}/\varepsilon_{guest}$ between 0.7 and 2, the BRM (FIGURE 3a) and LLMF (equation (2) with α=1/3, FIGURE 3b) give a very good approximation of ε_{eff}. In spite of the fine gridded solutions for the FEM and FDM, the deviation in ε_{eff} between the different numerical models still exists for bigger contrasts. Especially for the geometric, arithmetic and harmonic FDM approximations a finer grid is required. The FD model based on the power law average and the finite element model show both the best convergence and overlap each other (see also FIGURE 2), which might indicate that these solutions have converged. The worst approximation is provided by the power law mixing formula (PF) (FIGURE 3f), with α=0.65. This suggests that α<0.5 should be used and that α =1/3 is almost optimal.

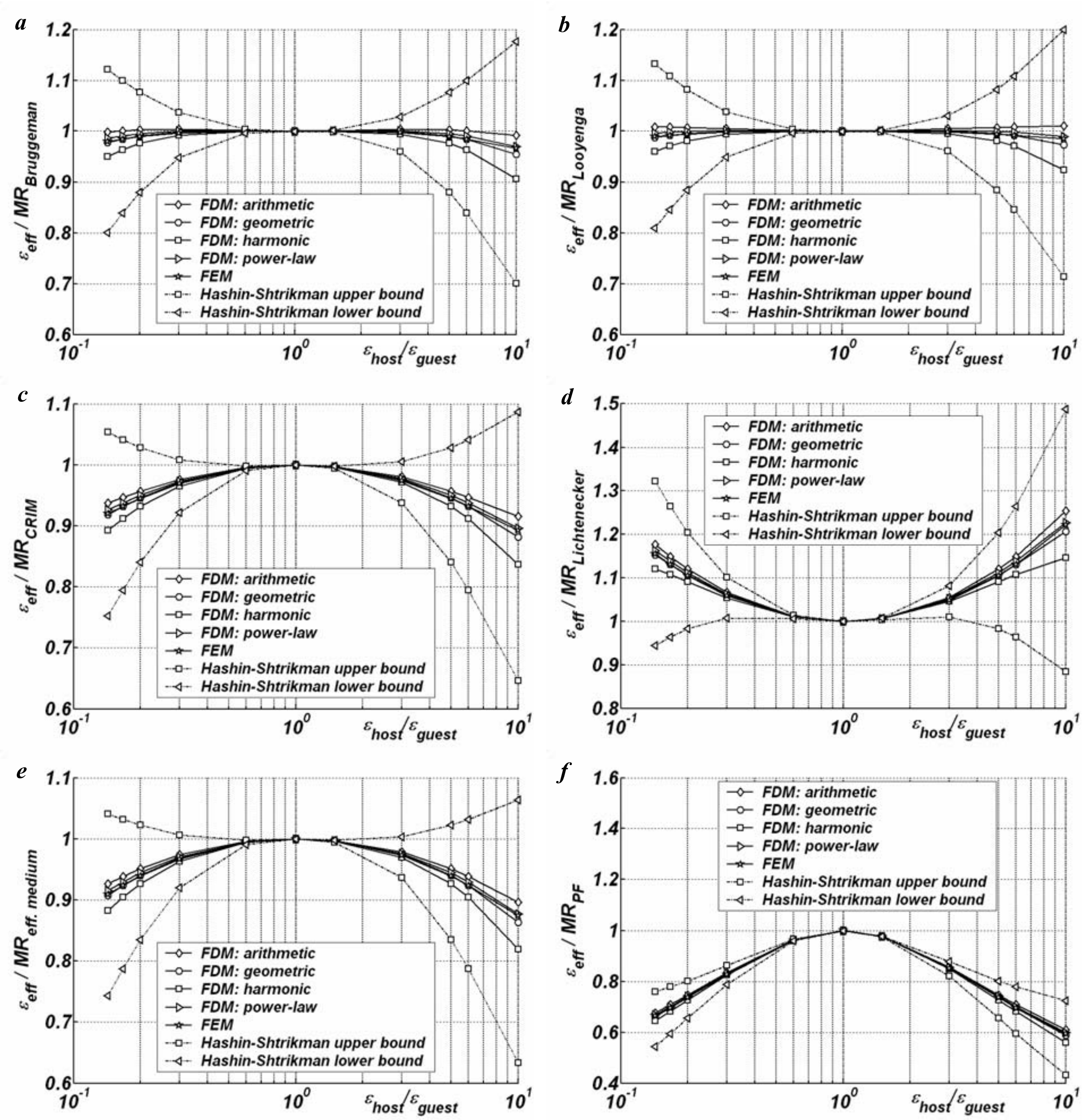

FIGURE 3. Normalization of ε_{eff} for different contrasts with various mixing rules: *a)* Bruggeman Mixing formula, BMF *b)* Looyenga-Landau-Lifshitz Mixing formula (LLMF, *Seleznev*, 2005) *c)* Complex Refractive Index Mixing formula, CRIM [*Seleznev*, 2005] *d)* Lichtenecker Mixing formula, LMF [*Seleznev*, 2005] *e)* Effective Medium Approximation, EMA [*Sahimi*, 1994] for a percolation threshold, p_c=0.2495 [*Stauffer and Zabolitzky*, 1986] *f)* Power law formula, PF with α=0.65 [*Ghose and Slob*, 2006]. The Hashin-Shrtrikman bounds equal the Maxwell-Garnett Mixing formula, GMF, for a two component mixture.

We investigate the applicability of the geometric average used for ε_{eff}, as obtained for the 2-dimensional checkerboard. All computations are done with the FE model. We computed ε_{eff} for 100 uniformly distributed random field realizations. All these realizations consists of a two component mixture with ε_{host}=3 and ε_{guest}=10 and an expected volume fraction of 0.5, with a 2-dimensional percolation threshold p_c= 0.5. To test the isotropy of the fields, we compute ε_{eff} both in x- and y-direction. The mean value for ε_{eff} for both directions is μ_x=5.4804 and μ_y=5.5824 and the corresponding standard deviations are σ_x= 0.0512 and σ_y=0.0541. In FIGURE 4 the convergence rate is presented for the average value of μ_x and μ_y. It is clear that the both solutions converge towards the geometric average. Comparison of the results from the checkerboard field (FIGURE 1) and the results from the uniformly distributed random field (FIGURE 4) shows that the convergence rate for the random field is slower than for the checkerboard configuration and both configurations converge towards the geometric average. This is also described by the effective medium approximation, from which we obtain indeed the geometric average, using p_c=0.5 for bond percolation in 2 dimensions.

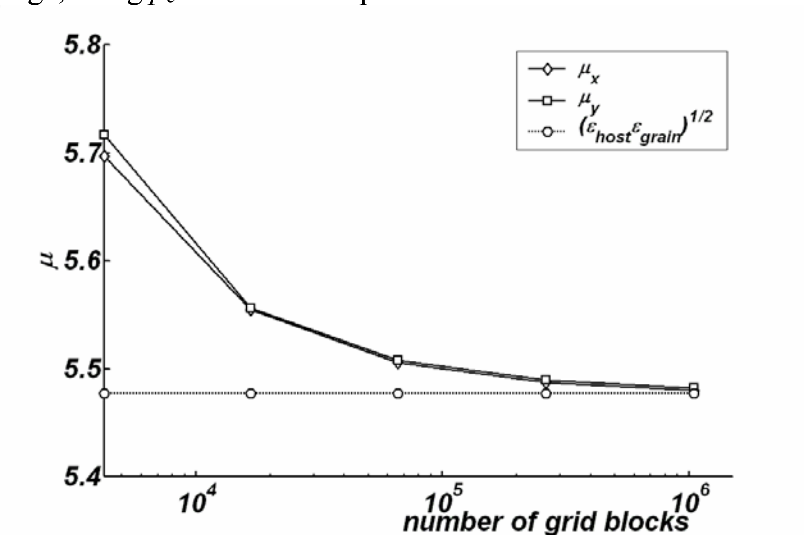

FIGURE 4. Estimated means in x- and y-direction, μ_x and μ_y, obtained for 100 uniformly distributed random field realizations

4. DISCUSSION AND CONCLUSIONS

Based on the numerical computations we conclude that for fine gridded models the different proposed FD models and the FE model converge to the analytical ε_{eff}. However, in the 3-dimensional case the applicability of the FE model and the harmonic and arithmetic FD approximations are not valid for a coarse grid because the solution does not satisfy the Hashin-Shtrikman bounds. Application of the finite difference method for effective parameter computation is restricted by the choice of internodal averaging. For the 2-dimensional case the geometric average FDM approximation has the best convergence rate and it provides a good estimate for ε_{eff} for coarse gridded models. Based on the same criteria, the power law FDM approximation (with α=1/3) is the most powerful model for 3-dimensional computations.

Moreover, for increasing contrasts between ε_{host} and ε_{guest} the convergence rate decreases for both FDM and FEM, hence more grid refinement is required. The same can be concluded from the computations obtained for uniformly distributed random fields in comparison to the checkerboard configuration. However, the numerical solution for both the 2-dimensional random fields and the 2-dimensional checkerboard field indeed converge to the geometric average according to the effective medium approximation. As opposed to this, the 3-dimensional solution for the checkerboard field is not approximated well by the effective medium theory, when the percolation threshold is set to 0.2495 (see FIGURE 3e). We conclude that the cubic power-law or the Looyenga-Landau-Lifshitz mixing rule and the Bruggeman formula give the best estimate for the 3-dimensional case.

REFERENCES

Bruggeman, D. A. G. (1935), Berechnung verschiedener physikalischer konstanten von heterogenen substanzen, i. dielektrizitätskonstanten und leitfähigkeiten der mischkörper aus isotropen substanzen, *Ann. Phys*, 24(5), 636–664.

Dykhne, A. M. (1971), Conductivity of a two dimensional two-phase system, *Sov. Phys. JETP*, 32(1), 63 – 65.

Choy, T. C. (1999), *Effective Medium Theory: Principles and Applications*, Clarendon Press, Oxford.

Ghose, R., and E. C. Slob (2006), Quantitative integration of seismic and GPR reflections to derive unique estimates for water saturation and porosity in subsoil, *Geoph. Res. Let.*, 33, L05404.

Hashin, Z., and S. Shtrikman (1962), A variational approach to the theory of the effective magnetic permeability of multiphase materials, *J. Appl. Phys.*, 33(10), 3125 – 3131.

Kärkkäinen, K. K., A. H. Shivola, and K. I. Nikoskinen (2000), Effective permittivity of mixtures: numerical validation by the FDTD method, *IEEE Trans. Geosci. Remote Sensing*, 38(3), 1303 – 1308.

Kärkkäinen, K. K., A. H. Shivola, and K. I. Nikoskinen (2001), Analysis of a three-dimensional dielectric mixture with finite difference method, *IEEE Trans. Geosci. Remote Sensing*, 39(5), 1013 – 1018.

Ke-da, B. (1990), Electrical conduction in checkerboard geometries, *Phys. Rev. B.*, 41(7), 4330 – 4333.

Keller, J. B. (1964), A theorem on the conductivity of a composite medium, *J. Math. Phys.*, 5(4), 548 – 549.

Maxwell-Garnett, J. C. (1904), Colours in metal glasses and in metallic films, *Phil. Trans. R. Soc. A*, 203, 385 – 420.

Noetinger, B., and C. Jacquin (1991), Experimental tests of a simple permeability composition formula, paper presented at the 66th Annual Technical Conference and Exhibition of the society of the SPE, Dellas, TX, 6 – 9 October.

Noetinger, B. (1994), The effective permeability of a heterogeneous porous medium, *Transp. Porous Media*, 15, 99 – 127.

Patankar, S.V., W. J. Minkowycz, and E. M. Sparrow (1980), *Numerical Heat Transfer and Fluid Flow,*: Hemisphere, Washington.

Pekonen, O., K. Kärkkäinen, A. Sihvola, and K. Nikoskinen (1999), Numerical testing of dielectric mixing rules by FDTD method, *J. Electromagn. Waves Applicat.*, 13, 67 – 87.

Renard, P., and G. de Marsily (1997), Calculating equivalent permeability: a review, *Adv. Water Resour.*, 20(5-6), 253 – 278.

Renard, P., G. Le Loc'h, E. Ledoux, G. de Marsily, and R. Mackay (2000a), A fast algorithm for the estimation of the equivalent hydraulic conductivity of heterogeneous media, *Water Resour. Res.*, 36(12), 3567 – 3580.

Renard, P., E. Ledoux, and P. Ackerer (2000b), Scale up of hydraulic conductivities: comparison of laboratory experiments and numerical analysis, Proceedings of the 13th Conference on Computational Method in Water Resources, Calgary, Alberta, 25 – 29 June.

Romeu, K. R., and B. Noetinger (1995), Calculation of internodal transmissivities in finite difference models of flow in heterogeneous porous media, *Water Resour. Res.*, 41(4), 943-959.

Roth, C., J. Chilès, J., and C. de Fouquet (1996), Adapting transmissivity simulations to finite difference flow simulators, *Water Resour. Res.*, 32(10), 3237 – 3242.

Sahimi, M. (1994), *Applications of Percolation Theory*, Taylor and Francis, London.

Seleznev, N. V. (2005), *Theoretical and Laboratory Investigation of Dielectric Properties of Partially Saturated Carbonate Rocks*, Delft University Press, Delft.

Sihvola, A. (2000), Mixing rules with complex dielectric coefficients, *Subsurface Sens. Technologies and Appl.*, 1(4), 393-415.

Stauffer, D., and J. G. Zabolitzky (1986), Re-examination of 3D percolation threshold estimates, *J. Phys. A: Math. Gen.*, 19, 3705-3706.

Wen, X-H., and J. J. Gómez-Hernández (1996), Upscaling hydraulic conductivities in heterogeneous media: an overview, *J. of Hydr.*, 183, 9 – 32.

Wiener, O. (1912), Die Theorie des Mischkorpers fur das Feld des stationaren Stromung,.Abh. Math., *Physischen Klasse Konigl. Sacsh. Gesel. Wissen*, 32, 509 – 604.

Zienkiewicz, O. C., R. L. Taylor, and J. Z. Zhu (2005), *The Finite Element Method : its Basis and Fundamentals*, 6th ed., Elsevier Butterworth-Heinemann, Oxford.