

# Assessment of Hydraulic Conductivity Upscaling Techniques and Associated Uncertainty

FARAG BOTROS<sup>1,2,4</sup>, AHMED HASSAN<sup>3,4</sup>, AND GREG POHLL<sup>2</sup>

<sup>1</sup>*Division of Hydrologic Sciences, University of Nevada, Reno*

<sup>2</sup>*Desert Research Institute, 2215 Raggio Parkway, Reno, NV, 89512*

<sup>3</sup>*Desert Research Institute, 755 E. Flamingo Rd., Las Vegas, NV, 89119*

<sup>4</sup>*Also at: Irrigation and Hydraulics Department, Faculty of Engineering, Cairo University, Orman, Giza 12613 - Egypt.*

## ABSTRACT

Upscaling is the process of transforming the detailed description of hydraulic parameters in a grid constructed at measurement scale (fine grid) to a coarser grid with less detailed description (coarse grid) for the purpose of numerical subsurface modeling. One technique of upscaling (the power averaging technique) is investigated and evaluated using numerical simulations. The optimum exponent and the associated uncertainty are obtained for different log-conductivity variances, different covariance structures and upscaled block sizes. The optimum exponent shows slight variation from one realization to another with the same conductivity distribution. However, when a different distribution is used, the optimum exponent changes significantly. The results of this technique are compared to the numerical averaging technique and they are found to give better results in terms of preserving the average flow. This technique can be used to stochastically populate and solve thousands of coarse grid simulations with considerably less effort.

## 1. INTRODUCTION

The use of numerical models for studying subsurface flow and transport has become common practice in hydrology over the last three decades. Data are usually collected at scales much smaller than that used in numerical models. Hydraulic parameters cannot be measured at all points in the area of interest but using geostatistical techniques, available measurements can be used to stochastically populate the entire domain of the studied area. Models built based on these geostatistical techniques should be on the same scale as the supporting measurements. This leads to a very large number of cells ranging from  $10^{11}$  to  $10^{18}$  cells depending on the size of modeled area (*Warren and Price, 1961*). Although computational power is continuously increasing, the maximum domain size that can be simulated at present is limited to few million cells. This indicates the importance of the upscaling process in subsurface modeling.

Upscaling of hydraulic conductivity drew the attention of many investigators. Their goal was to upscale or “to average” the hydraulic conductivity of a group of cells in the detailed description grid (at measurement scale) to only one representative value of hydraulic

conductivity in the coarser grid (at numerical model scale). The grid at the measurement scale is called hereinafter the fine grid, while the one at the modeling scale is called the coarse grid.

The first objective of this paper is to examine and evaluate the power averaging technique (one of the techniques used to upscale hydraulic conductivity) in such a way that groundwater flow characteristics are preserved when moving from the fine-grid model to the coarse-grid upscaled model. The second objective of this paper is to construct curves (similar to type curves) that can be used to get the upscaling parameters (optimum exponent in this case) with associated uncertainty without solving the fine grid.

## 2. BACKGROUND

*Durlofsky* (1991) defined two terms of the upscaled hydraulic conductivity; effective conductivity and equivalent conductivity. If the scale over which the averaged conductivity in the coarse grid is defined is large enough to encounter all types of heterogeneities in the fine grid, then this averaged conductivity is referred to as effective conductivity. If this large scale does not encompass all scales of variations, this averaged conductivity is referred to as equivalent conductivity. The effective conductivity can be viewed as a constant property of the medium as it does not depend on flow conditions to which the medium is subjected, while equivalent conductivity is not a constant property of the medium and shows some variation under different flow conditions.

Averaging of perfect stratified medium conductivities into the arithmetic mean in the direction of strata and the harmonic mean in the perpendicular direction of the strata provides good examples of effective conductivity. *Matheron* (1967) showed that for an infinite domain in which conductivities follow lognormal distribution and have an isotropic spatial correlation, geometric mean is a precise estimate for effective conductivity. Many stochastic approaches dealt with determination of the effective conductivity in a probabilistic sense where the spatial variations of the natural logarithm of hydraulic conductivity ( $\ln K$ ) are modeled as a random field (*Dagan*, 1989; *Gelhar*, 1993). Effective conductivity approach is appropriate and can provide a reasonable description of flow through regions which are large relative to the correlation length of heterogeneous conductivity field.

However, for the purpose of numerical modeling the domain is usually discretized into blocks of size not large enough to encompass all types of heterogeneity, and therefore, equivalent conductivity has to be calculated for this block rather than effective conductivity. The equivalent conductivity is sometimes referred to as block conductivity.

The techniques that are used to calculate the block conductivity can in general be divided into two main categories; local averaging techniques and numerical averaging techniques. Local techniques estimate values of block conductivities by taking the average of cell conductivities inside the block regardless of the boundary conditions the block is subjected to. In numerical techniques, the fine grid is divided into blocks and each of these blocks is isolated and subjected to a certain type of boundary conditions where the groundwater flow equation is solved at measurement scale for this block. Block conductivity is then estimated as the value that preserves the flow at the block boundaries under the same boundary conditions. For a good

review of such upscaling techniques and the limitation of each technique, one could refer to (Wen and Gomez-Hernandez, 1996; Renard and de Marsily, 1997). In the following we evaluate the power averaging technique which is categorized as a local averaging technique and assess the uncertainty in upscaling parameters used with this technique.

### 3. METHODOLOGY

Two-dimensional fine grid realizations with  $512 \times 1024$  cells are generated using different conductivity spatial correlation structures with varying values of the log-conductivity variance,  $\sigma_{\ln K}^2$ , and length,  $\lambda$ . The boundary conditions imposed on the flow domain for these fine grid realizations are specified hydraulic head at the right and left faces and no-flow conditions at the top and bottom faces. Porosity is considered constant and equals to 0.3. The variability of hydraulic conductivity in fine grids is described in a geostatistical framework through a spatial structure that may follow exponential, Gaussian, or hole-type covariance functions. The isotropic covariance models of these structures are given as

$$C_Y(r) = \sigma_{\ln K}^2 e^{-r/\lambda} \quad (1-a)$$

$$C_Y(r) = \sigma_{\ln K}^2 e^{-(r/\lambda)^2} \quad (1-b)$$

$$C_Y(r) = \sigma_{\ln K}^2 \left(1 - \frac{r^2}{2}\right) e^{-(r/2\lambda)^2} \quad (1-c)$$

for the cases of exponential, Gaussian, and hole-type covariance structures, respectively, where  $r$  is the lag distance and  $C_Y(r)$  is the log-conductivity covariance at spatial lag  $r$ .

Different combinations of  $\sigma_{\ln K}^2$  and  $\lambda$  are used to generate conductivity realizations having these covariance structures. These fine-grid realizations are then upscaled using power averaging technique and assuming different sizes of the coarse grid block,  $L$ .

**3.1 Power averaging technique** *Journel et al.* (1986) proposed to use a power average to compute block conductivities which can be given as

$$K_b = \left( \frac{1}{N} \sum_{i=1}^N K_i^P \right)^{1/P} \quad (2)$$

where  $K_b$  is upscaled block conductivity,  $N$  is the number of fine grid cells within this block,  $K_i$  is the hydraulic conductivity of the  $i$ -numbered cell in the fine grid, and  $P$  is an exponent. When  $P = 1.0$ , the block conductivity is equal to the arithmetic mean of cell conductivities; when  $P = -1.0$ , block conductivity is equal to the harmonic mean. As  $P$  approaches zero, the block conductivity approaches the geometric mean and when  $P$  approaches  $\infty$ , the block conductivity approaches the largest value of cell conductivities inside the block and as  $P$  approaches  $-\infty$ , the block conductivity approaches the smallest value of cell conductivities inside the block. In his three-dimensional model, *Desbarats* (1992) suggested to use the exponent  $P = 1/3$  and showed that it gives good estimation for different types of heterogeneities. *Noetinger* (1994) suggested calculating the exponent  $P$  from the formula:

$$P = 1 - \frac{2}{E} \quad (3)$$

where  $E$  is the Euclidean dimension of the space modeled, which means to use harmonic mean in 1-D flow; geometric mean in 2-D flow, and  $P = 1/3$  for 3-D flow.

*Scheibe and Yabusaki* (1998) used power average technique for a three-dimensional synthetic hydraulic conductivity distribution. They generated the distribution based on geological considerations consistent with relevant depositional processes and field observations of stratification geometries (*Scheibe and Freyberg*, 1995). They found that the best estimate for the exponent  $P$  in terms of preserving the bulk flow characteristics at the upscaled grid scale is approximately 0.7 which is close to the arithmetic mean for perfectly stratified medium. This is because stratification was taken into consideration when generating the conductivity distribution.

With these different recommendations for the exponent,  $P$ , it is important to evaluate this technique and estimate the value of  $P$  for a large number of simulations. It is also important to assess the uncertainty in the parameter  $P$  that may stem from different realizations of the same spatial covariance model or from different spatial models.

In our numerical simulations, the groundwater flow equation is first solved at the scale of the fine grid and the groundwater fluxes at the coarse grid block boundaries are then obtained. Coarse grid conductivities are then calculated using Eq. (2) with different exponent  $P$  values. Our objective is to get the optimum exponent which minimizes the root mean square error (RMSE) function which is defined as follows:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N_C} (q_f - q_c)_i^2}{N_C}} \quad (4)$$

where  $q_f$  is the specific discharge at coarse block boundaries obtained from the solution of the groundwater flow equation at the scale of the fine grid,  $q_c$  is the specific discharge at coarse block boundaries obtained from the solution of the groundwater flow equation at the scale of coarse grid, and  $N_C$  is the number of coarse grid blocks.

*Cardwell and Parsons* (1945) showed that effective conductivity must have a value between arithmetic and harmonic means of cell conductivities. Although this rule might not hold true here because we are dealing with small blocks and using different objective function, we use the bounds for exponent  $P$  as suggested by *Cardwell and Parsons* (1945) (i.e.,  $P$  ranges from -1.0 to 1.0) with increments of 0.01. In some cases, we found that the optimum exponent lies outside this range, so we used a wider range of the exponent for these individual cases.

## 4. RESULTS

The results of these simulations are shown in Figure 1 where the log-conductivity is assumed to have exponential (Figure 1a), Gaussian (Figure 1b), or hole-type (Figure 1c) covariance. In this analysis, 30 realizations are examined with  $\sigma_{lnK}^2 = 0.1$ ,  $\lambda$  is equivalent to four fine-grid cells and the coarse grid block taken as  $8 \times 8$  fine grid cells (i.e.,  $L = 8$ ). Each line in the figure

represents a different realization. For any combination of  $\sigma_{\ln K}^2$ ,  $\lambda$ , and  $L$ , the optimum exponent lies in a narrow range for all 30 realizations, however, this range changes for different covariance structures.

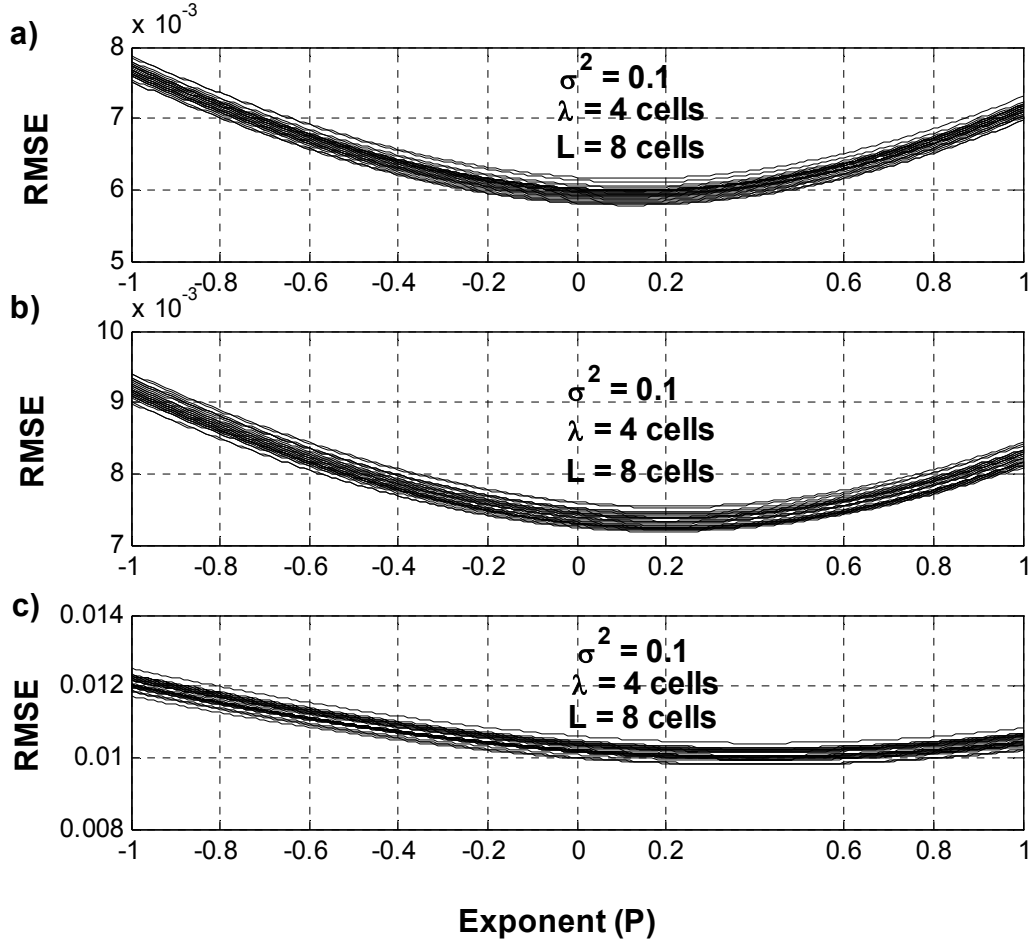


FIGURE 1. RMSE of the flux values between the fine and coarse grids for 30 realizations using a) exponential covariance, b) Gaussian covariance, and c) hole-type covariance.

Figure (2) shows the optimum exponent for different  $L/\lambda$  ratios and different covariance structures where the lines represent the median values and the symbols represent the 90% confidence interval of the optimum exponent  $P$ . The range of the optimum exponent changes slightly with  $\sigma_{\ln K}^2$ , however, it changes significantly with  $L/\lambda$  and the covariance structure. For small variances and for highly correlated values, the difference between the arithmetic and harmonic means is so subtle, and that is why the confidence interval for optimum  $P$  for small  $\sigma_{\ln K}^2$  is wider than that for larger  $\sigma_{\ln K}^2$ . This also explains why the confidence interval at small  $L/\lambda$  ratios (i.e., highly correlated values) is wider than that for larger  $L/\lambda$  ratios. That is clear in

case of Gaussian and hole-type covariance structures because for these spatial correlation structures, the correlation is higher than the exponential covariance for small  $L/\lambda$  as can be calculated from Eq. (1).

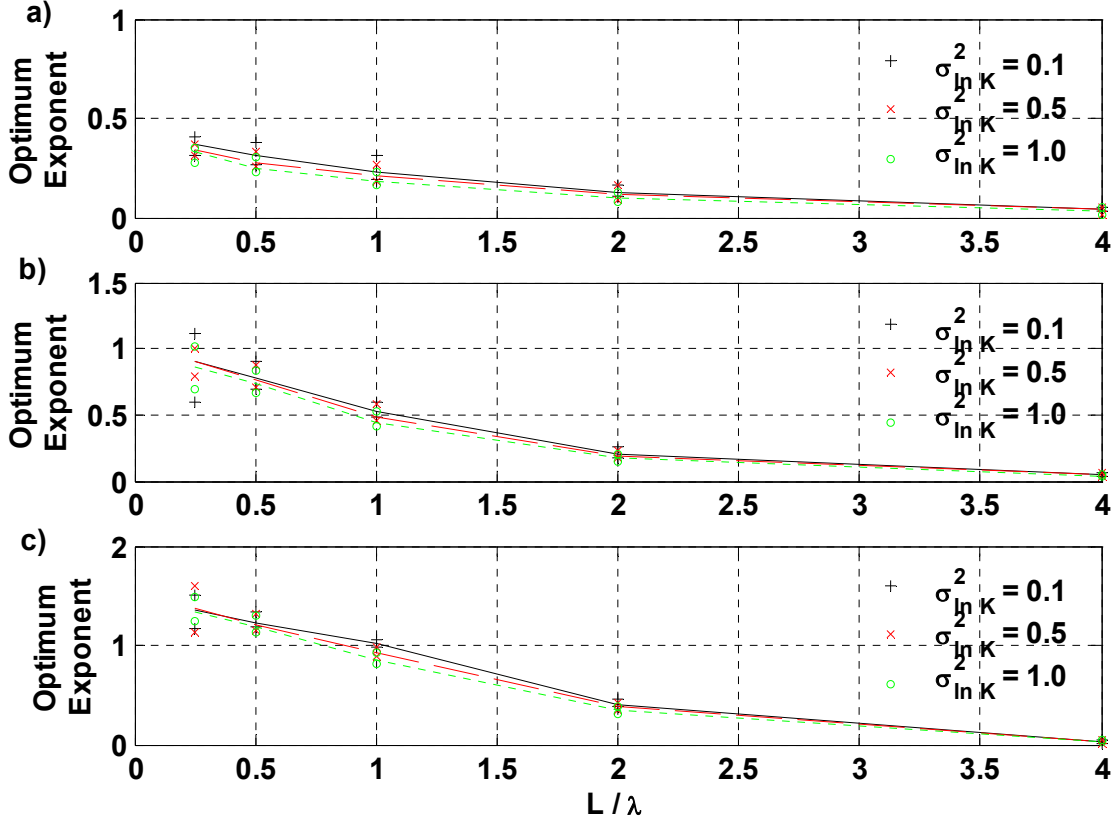


FIGURE 2. Optimum exponent as a function of  $(L/\lambda)$  and  $\sigma_{\ln K}^2$  using a) exponential covariance, b) Gaussian covariance, and c) hole-type covariance. Solid line for  $\sigma_{\ln K}^2 = 0.1$ , dashed line for  $\sigma_{\ln K}^2 = 0.5$ , and dotted line for  $\sigma_{\ln K}^2 = 1.0$ . Symbols represent 90 % confidence interval.

## 5. COMPARISON TO NUMERICAL AVERAGING TECHNIQUE

Rubin and Gomez-Hernandez (1990) used the average flow rate as a criterion for the equivalence between the coarse grid and the fine grid. They defined the block conductivity as:

$$\frac{1}{S} \int_S q(x) dx = K_b \frac{1}{S} \int_S \nabla h(x) dx \quad (5)$$

where  $S$  represents the block surface in 2-D and the block volume in 3-D,  $q(x)$  is the specific

discharge at a point  $x$  inside the block, and  $\nabla h(x)$  is the head gradient at the same point, and  $K_b$  is the block conductivity.

Using the same fine grid realizations used with power averaging technique, the grids are divided into blocks and each block is isolated and imposed to certain boundary conditions where the groundwater flow equation is solved for each block at the fine grid scale to get the flux at block sides. One value of block conductivity is then obtained in a way that preserves the flux at block sides under the same boundary conditions. The boundary conditions around each block that are used in the current study are permeameter boundary conditions where specified head are defined for two parallel sides of the block and no flow boundary along the other two sides.

After obtaining the hydraulic conductivity for each block, the coarse grid is solved using these conductivities and the fluxes around coarse-grid blocks are compared to those obtained from fine grid solution. Figure (3) shows a comparison between RMSE obtained by power average technique and numerical averaging technique for  $\sigma_{lnK}^2$  equals to 1.0.

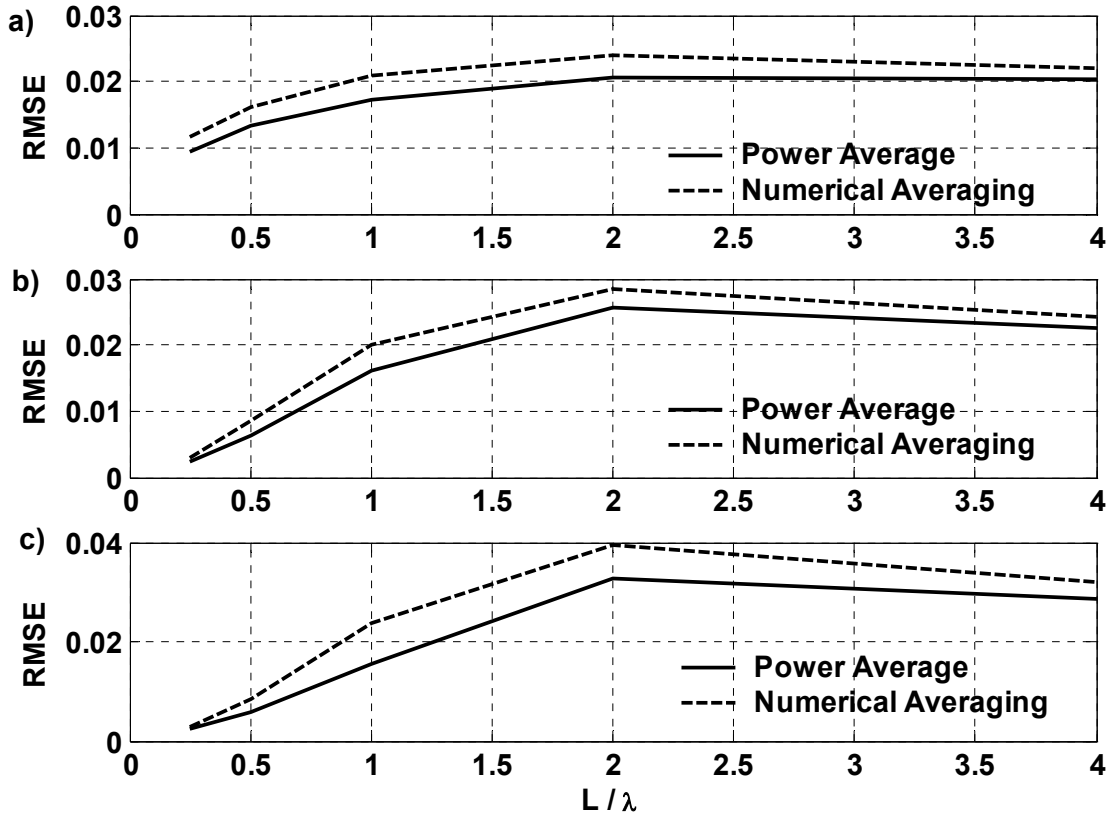


FIGURE 3. Comparison between power averaging technique and numerical averaging technique for a) exponential covariance, b) Gaussian covariance, and c) hole-type covariance.

Although, in the numerical averaging technique, we upscale each block individually to preserve the flow for this block (i.e., we use different exponent for each block) which provides

more degrees of freedom, the power averaging technique gives better results in terms of preserving the flow (Figure 3). That is because we use permeameter boundary conditions around each block without any justification. These boundary conditions should be as close as possible to those existing around the block sides in the fine grid model. This requires the solution of flow equation for the whole fine grid domain, defeating the purpose of upscaling.

## 6. DISCUSSION AND CONCLUSIONS

The analysis performed here indicates that the optimum exponent  $P$  used in the power averaging technique depends on the spatial structure in the fine grid, the variance of log hydraulic conductivity in the fine grid,  $\sigma_{\ln K}^2$ , and  $L/\lambda$  ratios. For a certain combination of these parameters, the optimum exponent  $P$  does not significantly change from one realization to another. This means that one can populate many fine grid realizations and upscale these realizations with the optimum exponent obtained from Figure 2 and then solve the coarse grid realizations which will considerably save time and effort. This study also shows that the power averaging technique may give better results than numerical averaging techniques as the latter use some boundary conditions around each block without any justification.

## REFERENCES

- Cardwell, W. T., and R. L. Parsons (1945), Average permeabilities of heterogeneous oil sands, *Trans. Am. Inst. Min. Metall. Pet. Eng.*, 160 34-42
- Dagan, G. (1989), *Flow and transport in porous formations*, Springer-Verlag, New York
- Desbarats, A. J. (1992), Spatial averaging of hydraulic conductivity in three-dimensional heterogeneous porous media, *Math. Geology*, 24 (3), 249-267
- Durlofsky, L. J. (1991), Numerical calculation of equivalent grid block permeability tensors for heterogeneous porous media, *Water Resources Research*, 27 (5), 699-708
- Gelhar, L. W. (1993), *Stochastic subsurface hydrology*, Prentice Hall, New Jersey
- Journel, A. G., C. V. Deutsch, and A. J. Desbarats (1986), Power averaging for block effective permeability, *Soc. of Petrol. Eng.*, (Paper No. 15128 - 56th California SPE meeting, Oakland),
- Matheron, G. (1967), *elements pour une theorie des milieux poreux*, Mason, Paris
- Noetinger, B. (1994), The effective permeability of a heterogeneous porous medium, *Trans. Porous Media*, 15 99-27
- Renard, P., and G. de Marsily (1997), Calculating equivalent permeability: A review, *Adv. Water Res.*, 20 (5-6), 253-278
- Rubin, Y., and J. J. Gomez-Hernandez (1990), A stochastic approach to the problem of upscaling of conductivity in disordered media: Theory and unconditional numerical simulations, *Water Resources Research*, 26 (4), 691-701
- Scheibe, T., and S. Yabusaki (1998), Scaling of flow and transport behavior in heterogeneous groundwater systems, *Adv. in Water Resour.*, 22 (3), 223-238
- Scheibe, T. D., and D. L. Freyberg (1995), Use of sedimentological information for geometric simulation of natural porous media structure, *Water Resources Research*, 31 (12), 3259-3270
- Warren, J. E., and H. S. Price (1961), Flow in heterogeneous porous media, *Soc. of Petrol. Eng. Jour.*, 1 153-169
- Wen, X. H., and J. J. Gomez-Hernandez (1996), Upscaling hydraulic conductivities in heterogeneous media: An overview, *J. Hydrol.*, 183 (1-2), ix-xxxii