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Ranking stochastic realizations for improved aquifer response uncertainty assessment

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Abstract

Incomplete sampling leads to uncertainty in the detailed 3-D distribution of conductivity in every subsurface formation. Stochastic/geostatistical techniques are being increasingly used to generate alternative fine scale 3-D realizations of subsurface parameters that are consistent with the available data. Ideally, an assessment of aquifer response uncertainty is provided by processing a large number of fine scale realizations through a groundwater modeling program. To avoid excessive CPU times the fine scale realizations are often averaged to a coarse resolution for fast flow and transport simulation. The problem with this approach is that the aquifer response is often sensitive to fine scale heterogeneities and such coarse flow models may lead to erroneous results. An alternative approach is proposed in this paper. The coarse scale responses are used to rank the realizations, i.e. identify low and high response realizations. A limited number of fine scale realizations are then processed through the flow and transport simulator. Thus, aquifer response uncertainty can be analyzed at the fine scale with less computational effort. The proposed method is applied to a hypothetical aquifer, which is characterized by variogram statistics derived for the Columbus aquifer, Mississippi. The value of ranking is shown by comparing the approximate uncertainty with the reference fine scale aquifer response.

Keywords: Aquifer response uncertainty; Stochastic realizations; Ranking

1. Introduction

Natural aquifers show heterogeneous characteristics since a variety of geological processes were involved in their genesis. The geological processes may be understood in general; however, the initial and boundary conditions can never be known in sufficient detail to provide a unique deterministic image of the aquifer.

A number of researchers have pointed out the importance of considering spatial varying parameters in solving groundwater problems. Peck et al. (1988) compiled a broad review about the consequences of spatial variability on groundwater modeling. Tyler et al. (1995) discuss how fluvial heterogeneities influence production profiles. Silliman and Wright (1988) have shown that the knowledge of pathways and their distribution in the subsurface is important to predict the spread of pollutants.

Typically, only a few spatial distributed measurements are available (e.g. flowmeter measurements, lab analysis of cores) to describe the distribution of

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aquifer parameters (e.g. conductivity). Hence, apart from the problem of integrating measurements from different measurement devices, uncertainty due to incomplete sampling exists in describing the distribution of conductivity.

A deterministic distribution of conductivity could only be obtained by having a measurement of conductivity at every location of the aquifer. Since this is not possible, conductivity has been treated within a stochastic framework where it is modeled using space random functions (Delhomme, 1979; Gomez-Hernandez and Wen, 1994; Poeter and McKenna, 1994). Probabilistic distribution models characterize the uncertainty in the spatial distribution of conductivity. If the stochastic representation of conductivity is used, the governing equations describing groundwater flow and transport turn into stochastic partial differential equations. Resulting aquifer response distributions, e.g. hydraulic head or flow velocity, become random functions.

In this paper we want to quantify by a numerical simulation approach, how the uncertainty due to incomplete sampling of conductivity affects the aquifer response. Our approach starts by generating a number of equiprobable distributions of conductivity, all of which honor the available data and their spatial structure, by using geostatistical methods (Isaaks and Srivastava, 1989; Journel, 1989; Deutsch and Journel, 1997). All conductivity realizations are processed through a groundwater flow and transport simulator. Analyzing the distribution of simulation results will give a measure of the uncertainty due to incomplete sampling of conductivities. This procedure is known as the "Monte Carlo approach". Most often, incomplete sampling of conductivity is considered to be the only source of uncertainty. In practical cases, additional sources of uncertainty might exist, e.g. unknown boundary conditions or distribution of recharge. For any decision making in the context of aquifer management it is of utmost importance to quantify all sources of uncertainty (Ballin et al., 1992).

Analytical approaches are very valuable to predict aquifer responses in cases where underlying assumptions are met by the actual aquifer. Recent developments in analytical approaches to describe concentration uncertainty e.g. Kabala and Sposito (1994) and Dagan et al. (1996) show that their applicability has been extended to conditions including transient boundary conditions or rate limited sorption. Analytical approaches generally gain their computational efficiency at the cost of various simplifying assumptions, in particular with respect to the variability of input variables. The significance of their results may also be limited by the use of a multi-Gaussian random function model for conditional probabilities. In this paper the numerical approach is selected because of its larger flexibility.

Setting up a numerical groundwater model requires a spatial discretization of the model domain. Because it is infeasible to process multimillion node grids through a groundwater flow and transport simulator, fine scale conductivity values have to be scaled up to a coarser grid of blocks. Before scale-up the scale of the measurement support and the scale that captures the behavior of interest must be identified. Consideration of the dimensions of the model domain and CPU resources leads to the selection of the modeling scale. We implicitly assume that relevant variations of conductivity can be captured with a fine scale resolution grid and that the flow and transport processes of interest may be modeled with this detailed grid.

Wen and Gomez-Hernandez (1996) provide an extensive overview and discussion of various scale-up techniques. They distinguish among the local techniques (e.g. geometric mean), the nonlocal techniques that solve the groundwater flow equation at the measurement scale, the block geometry methods, where the grid for flow simulation is deformed to account for subsurface structure and the direct block conductivity generation. Recent applications of scale-up in the context of groundwater modeling include the work of Rautman and Robey (1992) at the Yucca Mountain site, Nevada and of Follin and Thunvik (1994) on the crystalline rock in Sweden. In general, aquifer responses obtained from a scaled-up conductivity distribution are approximative since, with the exception of elastic grid-based algorithms, high and low conductivities are averaged out, which leads to a poor representation of formerly connected extreme values.

In this paper, we claim that uncertainty in aquifer response cannot be directly determined from the results of coarse scale flow modeling. Nevertheless, the coarse scale response may rank the results at the fine scale. For example, a realization that leads to a

fast coarse scale response may also lead to a fast fine scale response. A limited number of fine scale conductivity fields can then be selected according to their coarse scale aquifer response. An alternative to this procedure is to process a small number, *n*, of fine scale realizations. The proposal amounts to using the available coarse scale information to select a better set of *n* realizations. Of course, there will be no benefit if the coarse scale realizations do not "rank" the detailed realizations.

Deutsch and Srinivasan (1996) investigate different ranking techniques to choose low-side, expected and high-side realizations for oil recovery and reservoir management. They quantify the value of ranking realizations in terms of expected loss. Gomez-Hernandez and Carrera (1994) show the application of the ranking principle with respect to uncertainty analysis of the groundwater- modeling response. They use the first-order approximation of piezometric heads as a function of element-averaged log transmissivities to derive the probability of extreme (large) response values. Due to the first-order approximation, this method is restricted to only moderately varying transmissivity fields. In contrast, the method presented in this paper is applied to a highly varying conductivity distribution that is typical of many aquifers.

2. Methodology

Given uncertainty in the spatial distribution of subsurface hydraulic properties, we characterize the aquifer response variable *r* as a random variable (RV) *R*, the probability distribution of which characterizes the uncertainty about r_{true}, the unknown true value. The conditional cumulative distribution function (ccdf) is denoted:

$$F(r) = \text{Prob}\{R \leq r | (\text{all data})\} \tag{1}$$

Consider a domain of interest A. The distribution of hydraulic properties $z(\mathbf{u})$, $\mathbf{u} \in \text{A}$, where $z(\mathbf{u})$ is the hydraulic property at location $\mathbf{u}$, can be modeled with stochastic simulation. We construct alternative, equally probable, realizations denoted by the superscript l: $\{z^{(l)}(\mathbf{u}), \mathbf{u} \in \text{A}\}$, $l = 1, \ldots, L$. Some large number of realizations ($L = 100$) could then be processed through a flow simulator to yield possibly different flow responses, $r^{(l)}$, $l = 1, \ldots, L$. These responses can be used to model the distribution $F(r)$.

An approximation to the distribution of the fine scale aquifer response can be constructed with the much faster coarse scale flow simulation:

$$F_{\text{cs}}(r) = \text{Prob}\{R_{\text{cs}} \leq r | (\text{all data})\} \tag{2}$$

The random variable R_{CS} is not the same as the fine scale flow response *R*. In general, the coarse scale distribution $F_{\text{CS}}(r)$ will not be the same as *F(r)* obtained from the fine scale flow simulation. The difference will be pronounced when the flow response *r* depends on the fine scale details of the heterogeneous hydraulic property distribution.

We propose a measure of mismatch between the reference distribution *F(r)* and our estimate $F^*(r)$ (obtained from running a limited number of fine scale realizations) so that the benefit of either running more simulations or ranking the realizations can be quantified:

$$\Delta = \int_{r_{\min}}^{r_{\max}} \left| \frac{1 - \dfrac{F^*(r)}{F(r)}}{1 - F(r)} \right| \text{d}r \tag{3}$$

$r_{\max}$ and $r_{\min}$ refer to the maximum and minimum flow response, respectively, of each of the distributions (i.e. reference or approximate) considered. By weighting the discrepancy between the approximate and the "true" cdf by $1/[F(r)(1 - F(r))]$, more emphasis is put on the mismatch at the tails of the distribution to better account for the relative importance of extreme results. Eq. (3) will be used to assess the value of ranking.

In detail, the procedure consists of the following steps:

1. Generate a large number (L) of fine scale conductivity distributions.
2. Upscale all fine scale realizations to a coarse resolution using an appropriate averaging method. While the geometric mean modified by a term accounting for the variance of conductivity is used here (following Gelhar, 1993), the choice of the appropriate averaging method may impact the success of using coarse scale realizations to mimic fine scale behavior.
3. Process all coarse conductivity distributions

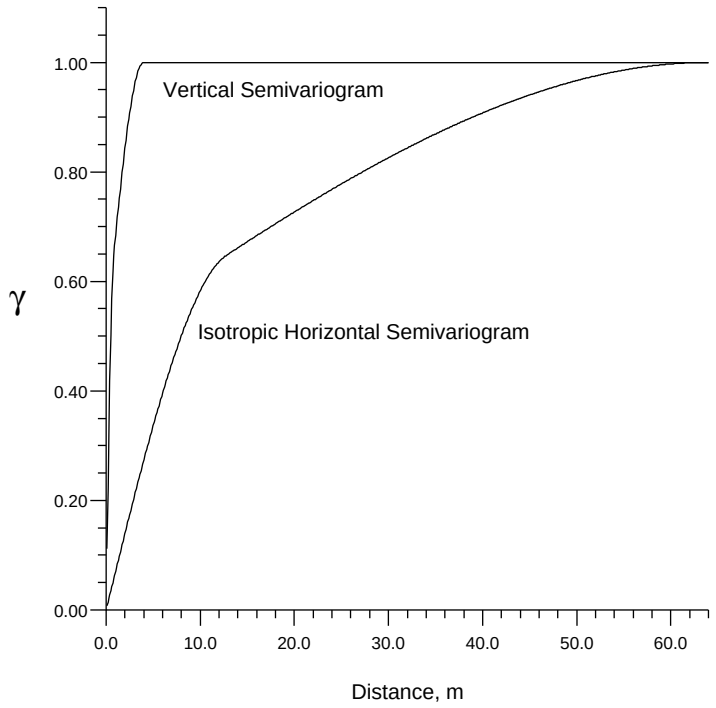


Fig. 1. Normal scores semivariogram used to generate the 100 conductivity realizations.

through a flow and transport simulator; for illustration purposes, we also process the fine scale realizations.

4. Rank the coarse scale aquifer responses (and their associated realizations).
5. Divide the range of coarse scale results into a number of classes.
6. Randomly sample within each class to obtain a realization number.
7. Calculate the fine scale aquifer responses of the selected realizations.
8. Construct an approximate cdf based on the fine scale flow results and on the mean probabilities of the respective classes.
9. Compute the mismatch between the approximate and the true fine scale cdf.

To test the method, we additionally perform the following:

10. Steps 6–9 are repeated 100 times to ensure representative sampling within every stratum; the mean of the mismatches is kept.
11. Repeat steps 5–9 for varying number of strata (between 3 and 100).

3. Example

The hypothetical aquifer extends 192 m × 192 m in the horizontal domain and 8 m in the vertical. It is discretized by cubic elements with side lengths of 1 m yielding a total of 294,912 elements and 335,241 nodes. The statistics to characterize the conductivity field are adopted to a large extent from the results of the aquifer field study conducted at the Columbus Air Force Base, Mississippi (Gelhar et al., 1992; Rehfeldt et al., 1992). In this way, we ensure working with a heterogeneous conductivity distribution. A mean hydraulic conductivity of $k = 250$ m d^{-1} and a coefficient of variation of three are used. A horizontal correlation length λ_h of 1/3 of the model domain and a ratio between horizontal and vertical correlation length of 16:1 (Gelhar, 1993) are chosen.

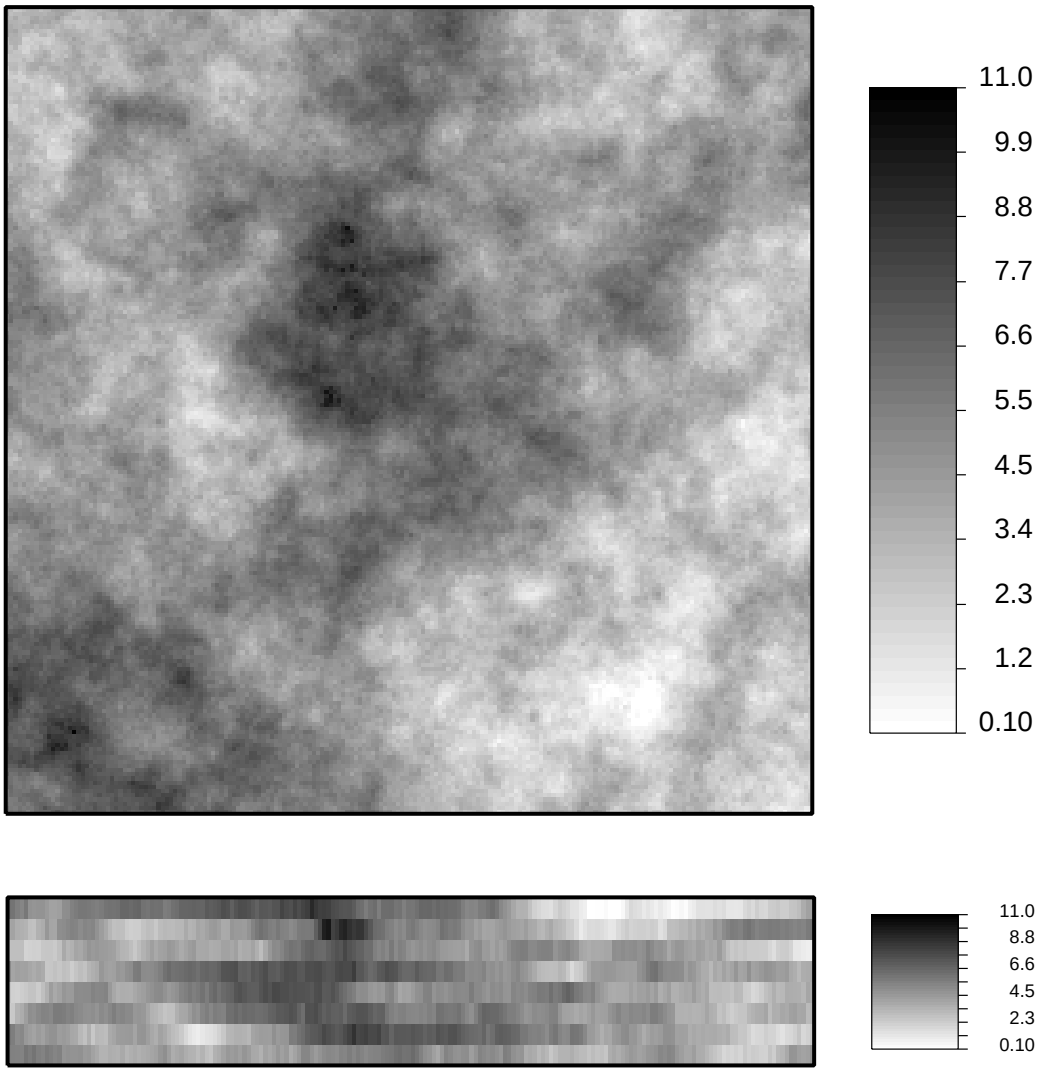


Fig. 2. Example layer (top) and example cross section (bottom) for one realization of the conductivity distribution. For more detailed display, a logarithmic scale has been used for conductivity. Horizontal dimensions are 192 × 192 m, vertical extension is 8 m. The cross section is displayed using a five-fold vertical exaggeration.

The normal scores semivariogram model $\gamma(h)$ adopted to generate the conductivity fields is shown in Fig. 1. The semivariogram has two nested spherical variogram structures:

$$\gamma(h) = 0.5\mathrm{Sph}\sqrt{\frac{h_\mathrm{v}^2}{0.8^2} + \frac{h_\mathrm{h}^2}{12.8^2}} + 0.5\mathrm{Sph}\sqrt{\frac{h_\mathrm{v}^2}{4.0^2} + \frac{h_\mathrm{h}^2}{64.0^2}} \quad (4)$$

h_v is the lag separation distance in the vertical direction and h_h is the lag separation distance in the horizontal direction. Sph(d) is the unit range spherical variogram model (e.g. Deutsch and Journel, 1992).

A total of 100 conductivity fields are generated with the sequential Gaussian simulation technique (Deutsch and Journel, 1992). The conductivity distributions of a layer and a vertical cross-section of one of the realizations are shown in Fig. 2. For every fine scale conductivity field, a medium case with 96 ×

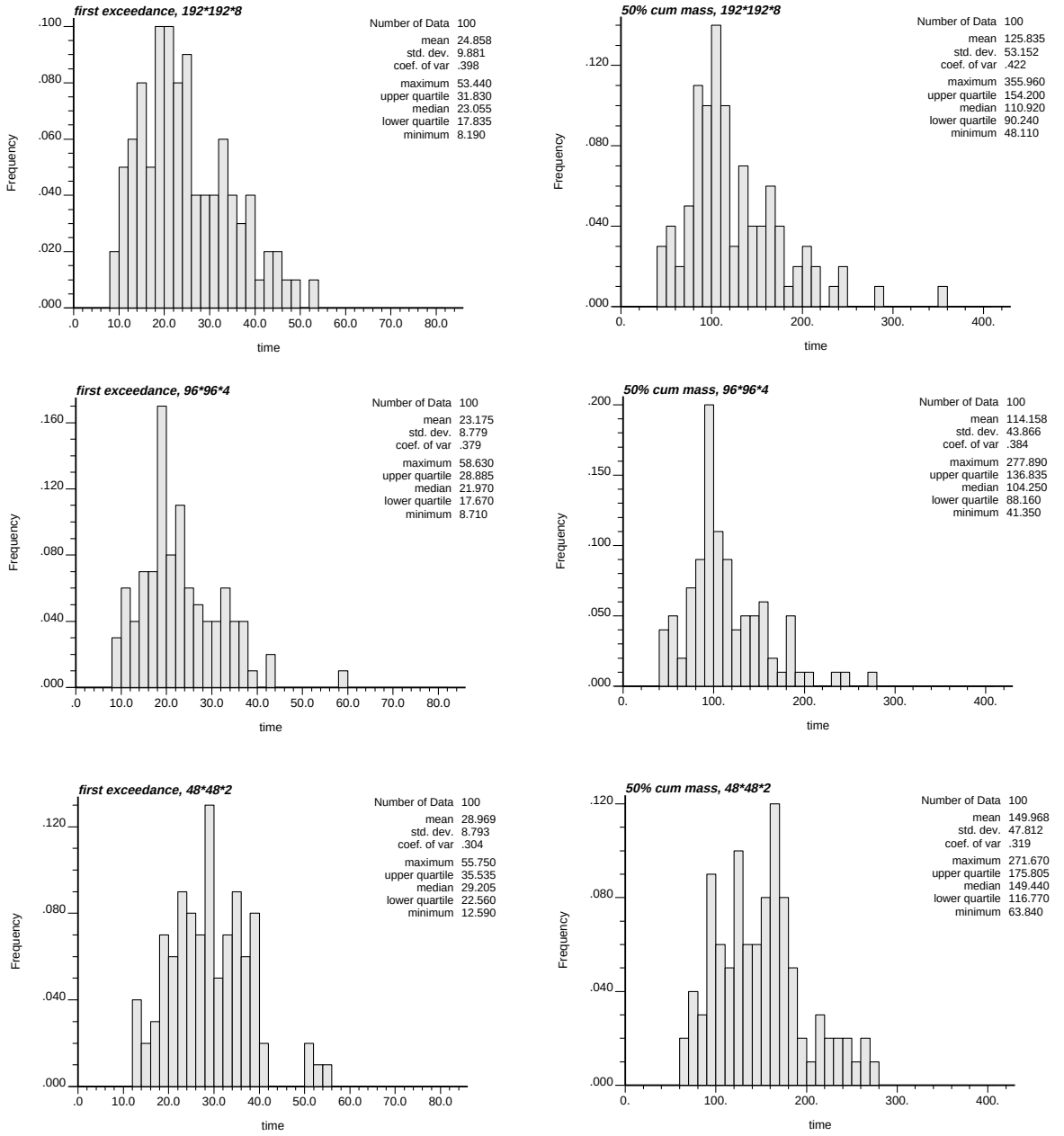


Fig. 3. Histograms of the time of exceeding the threshold of 10^{-10} kg m^{-3} for the first time (left side) and the time at which 50% of the input mass has passed the outflow plane (right side) for fine (top), medium (middle) and coarse resolution (bottom).

96×4 elements and a coarse case with $48 \times 48 \times 2$ elements is computed using the modified geometric mean to up-scale the conductivities.

Groundwater flow and transport modeling is performed using the FRAC3D code (Therrien and Sudicky, 1996) for every realization and each level of discretization. In FRAC3D the 3-D equations for variably saturated groundwater flow and advective–dispersive solute transport in porous or discretely fractured media can be optionally

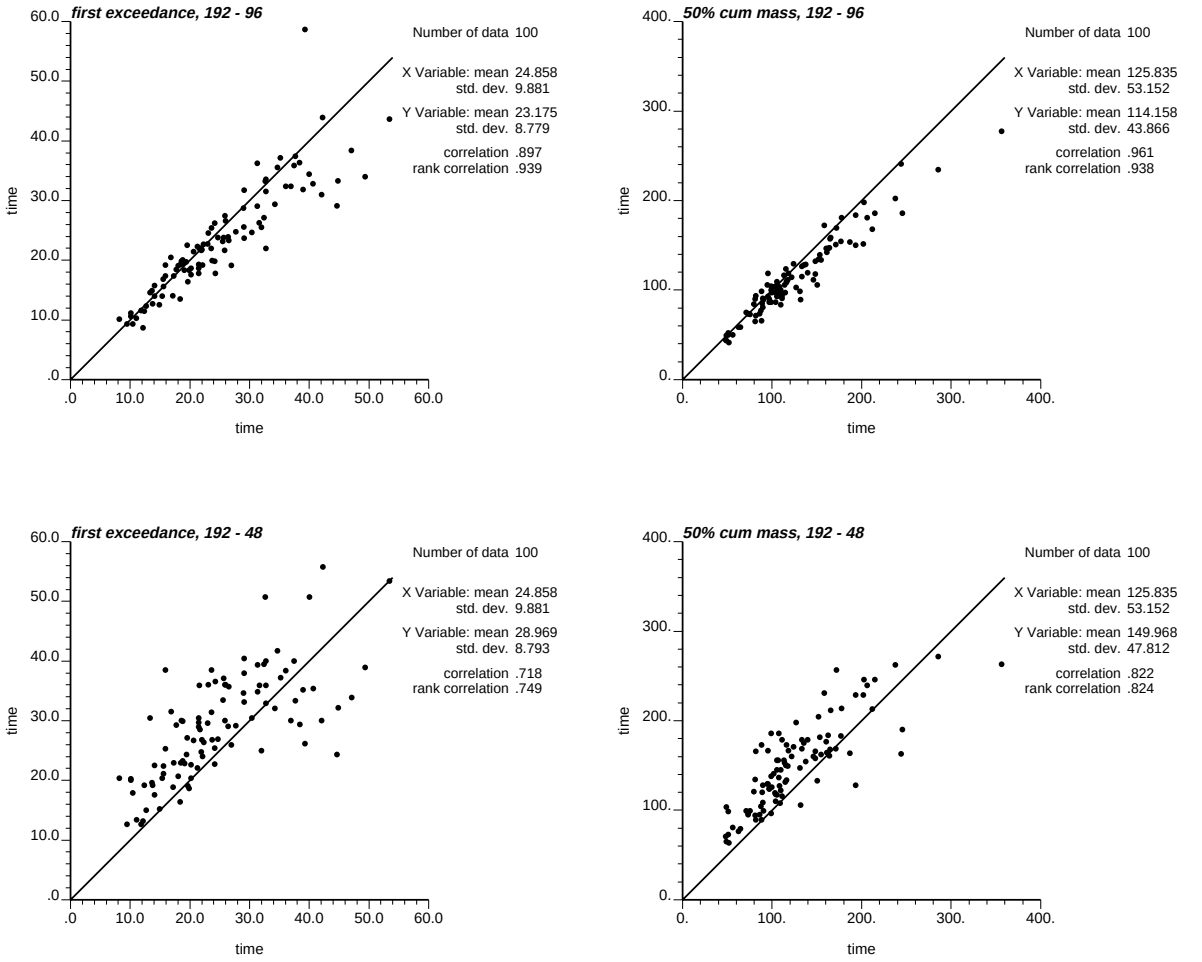


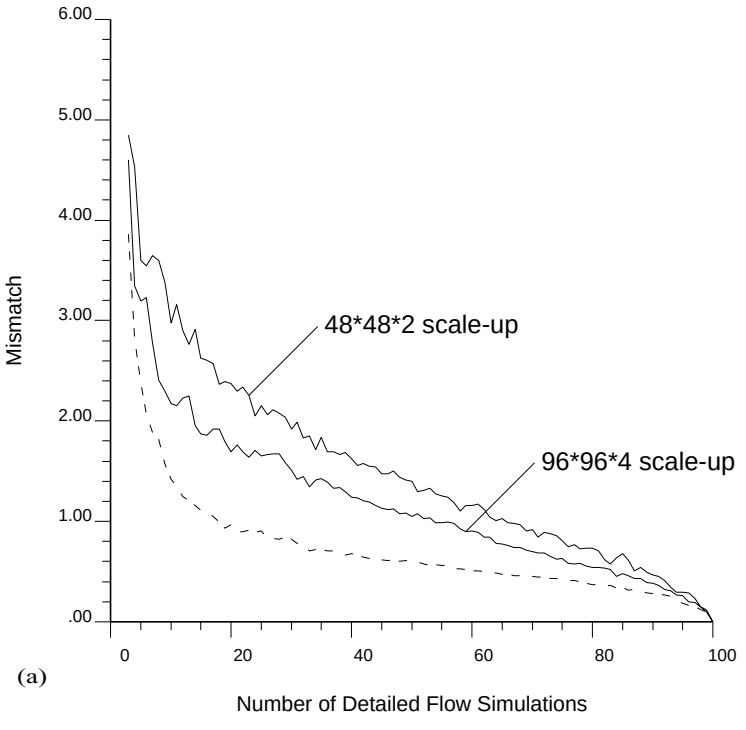
Fig. 4. Scatter plots of the time of exceeding the threshold of 10^{-10} kg m^{-3} for the first time (left side) and the time at which 50% of the input mass has passed the outflow plane (right side) between the fine scale case (reference values) and the medium (top) and the coarse resolution (bottom). Fine scale results are displayed on the *x*-axis and coarse scale results on the *y*-axis.

solved with the finite element or the finite difference method.

Boundary conditions for the flow field consist of prescribed heads at the inflow and outflow plane with a piezometric head difference of 0.3 m. All other boundaries of the hypothetical aquifer are set to no-flow boundaries. With reference to the Columbus aquifer (Gelhar et al., 1992), a spatially uniform porosity of 0.35 is used. Transport of a mass conservative pollutant is simulated assuming an instantaneous release of 625,000 kg of mass at location $x = 10$ m, $y = 96$ m and $z = 6$ m.

The transport problem is dominated by advection, which in turn is mainly determined by the distribution

Fig. 5. Mismatch between the reference cdf obtained from all fine scale flow simulation results and their approximation using only a limited number of detailed flow simulations selected according to coarse scale modeling results: (a) mismatch for the time at which any of the nodes in the outflow plane exceeds the threshold of 10^{-10} kg m^{-3} for the first time; (b) mismatch for the time at which 50% of the input mass has passed the outflow plane (dashed line represents the approximate cdf using a limited number of "true" fine scale simulation results).


6.00
5.00
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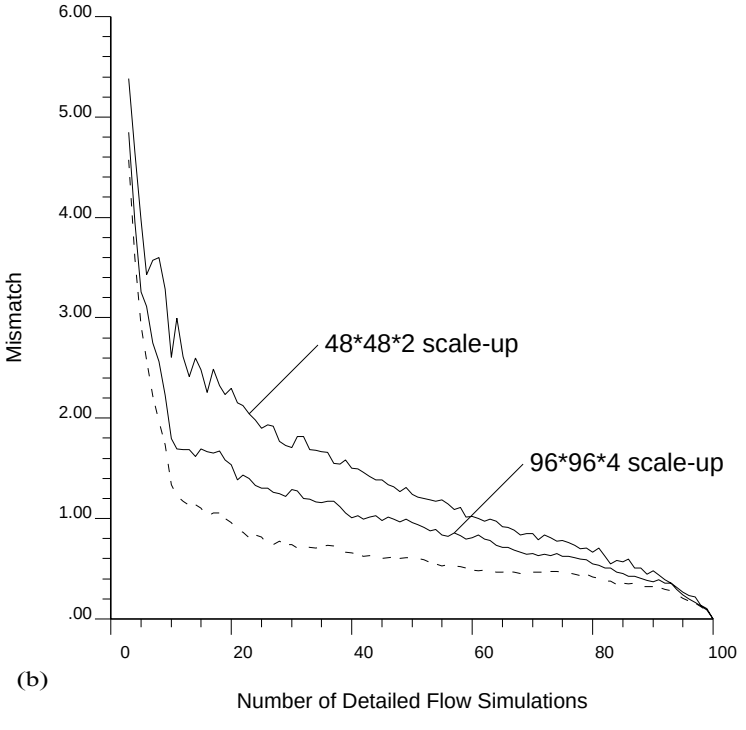
3.00
2.00
1.00
.00
Mismatch
48*48*2 scale-up
96*96*4 scale-up
0
20
40
60
80
100
Number of Detailed Flow Simulations

(a)


6.00
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Mismatch
48*48*2 scale-up
96*96*4 scale-up
0
20
40
60
80
100
Number of Detailed Flow Simulations

(b)

and possible connectivity of extreme conductivity values. Two different responses are statistically analyzed at the outflow plane of the hypothetical aquifer:

- the first time any of the nodes exceeds a small threshold concentration of 10^{-10} kg m^{-3};
- the time at which 50% of the input mass has passed the outflow plane.

It is anticipated that the time of first exceedance gives insight to the connectivity of high conductivities (single best flowpath leading to early mass arrival) whereas the measure of 50% of initial mass going through gives a more "average" description of the plume movement.

4. Results

Fig. 3 shows histograms of the time at which the concentration at the outflow plane exceeds the threshold value of 10^{-10} kg m^{-3} for the first time and of the time at which 50% of the initial input mass has passed the outflow plane for the three different resolutions of the conductivity distribution. The fine scale case ($192 \times 192 \times 8$) represents the reference against which the results of the coarser resolutions are compared.

The mean time for both measures slightly decreases at the medium scale ($96 \times 96 \times 4$) but then significantly increases at the coarse scale ($48 \times 48 \times 2$). In general, the results at the coarse scale seem to be notably skewed to longer response times whereas the results at the medium scale reproduce the distribution characteristics of the fine scale quite well. For the 50% cumulative mass measure the maximum value consistently decreases with coarsening of the resolution (from 355.96 to 271.67 days). The variability of both measures also decreases (coefficient of variability decreases from 0.4 to 0.3 and from 0.42 to 0.32) with coarsening of the discretization. This is due to averaging out high conductivity values in the scale-up leading to longer response times with less spread. Low conductivities, of course, also become averaged out, but do not significantly affect the distribution of the results in this case.

In terms of scatter-plots, Fig. 4 shows the correlation between the fine scale and the coarse scale results. The larger mean response times of the coarse resolution are expressed by the majority of data points falling above the 45° line. For the medium resolution, a strong correlation between the actual results (0.90 and 0.96) and the rank-order (both 0.94) can be seen for both mass arrival measures; there is a high probability that a realization which leads to a fast response at the medium scale will also show a fast response at the fine scale.

The rank correlations for the coarse resolution are considerably smaller (0.75 and 0.82), mainly due to some data points showing significantly different values. For example, the same realization yields a first exceedance time of about 16 days at the fine resolution whereas the coarse resolution gives 38 days. Although the overall trend is overestimation (longer times) the reverse can also be found. For example, a fine scale response of 45 days corresponds to only 24 days for the coarse resolution. In general, the 50% cumulative mass measure shows less deviation from the reference results at coarser scales compared to the time of first exceedance. For each combination of scale and arrival time measure it can be seen that the spread between fine and coarse scale results increases with increasing response times. This behavior is less pronounced at the $96 \times 96 \times 4$ grid where little variation is encountered, even for the tails of the cdfs. Yet, the examples of the coarse resolution illustrate the need to run simulations at the fine scale to verify consistency with coarse scale results and, perhaps, obtain more reliable time estimates.

Fig. 5 shows the mismatch between the approximate cdf constructed from a limited number of fine scale realizations and the reference cdf using all 100 fine scale results. Fig. 5a displays the mismatch for the time at which the threshold concentration of 10^{-10} kg m^{-3} is exceeded for the first time at the outflow plane and Fig. 5b displays the mismatch for the time at which 50% of the input mass has passed the outflow plane. In each figure, three curves are given: the top curve represents the coarse case and the center curve represents the medium case. For reasons of comparisons, limited numbers of fine scale realizations were also sampled from the "true" cdf (dashed lines) and the mismatch between the approximate and the complete reference scale was computed. These results are shown in the bottom curve.

To explain how the mismatch values are obtained, let us consider the case, where the approximate cdf is constructed from five realizations selected from all the first exceedance results at medium resolution. The times are sorted from the fastest response at 8.71 days to the slowest response at 58.63 days and divided into five classes each containing 20 values. Within every class a realization which has been sorted into this class is selected at random (the respective realization numbers are 41, 73, 45, 15, 100). Now, the approximate cdf is constructed from the fine scale results of these realizations (11.96, 18.42, 21.61, 31.26, 37.52). The fine scale results are considered to represent the mean cdf-value of the corresponding classes (0.1, 0.3, 0.5, 0.7, 0.9). Finally the mismatch between the approximate and the reference cdf is computed using Eq. (3). The described procedure is repeated 100 times for each number of strata and the arithmetic mean is retained. The number of strata is varied between 3 and 100.

Fig. 5 shows that the mismatch decreases on increasing the number of realizations. The mismatch for both aquifer responses is similar. Obviously, the mismatch becomes zero if all detailed flow simulations are used. If the approximate cdf is constructed from the "true" cdf (dashed lines) there is only little improvement when more than 35 fine scale flow simulations are used. For the medium and the coarse resolution, the approximate and the reference cdf still become closer as more realizations are used. The steep decrease in mismatch within 10–15 detailed realizations is slightly more pronounced for the 50% mass measure (Fig. 5b) than for the first exceedance measure, which corresponds to the higher correlation values given in Fig. 4. These numbers indicate that the approximate cdf of the first arrival measure is more affected by the scale-up of the detailed conductivities than the 50% mass measure.

5. Discussion

The coarse scale groundwater models yield interpretable estimates with good rank-order correlation to the fine scale model results. Yet, occasionally, different response times for the same realization compared to the reference values can be seen. The correlation between fine and coarse scale modeling results appears to depend on both, the degree of averaging and the type of aquifer response analyzed. Typically, we cannot expect coarse models, regardless of the scale-up technique, to reproduce the results of fine scale simulation. Groundwater modeling with coarse grids may be biased, and in general, show too small variability.

Processing fine scale realizations, selected according to their coarse scale aquifer response, results in reduced CPU time. The CPU requirements for the three levels of discretization are about 10 min, 1 h and 8 h (workstation with a RISC R5000 processor) for the coarse, medium and fine cases, respectively. Ranked coarse scale aquifer responses indicate which fine scale realizations should be processed in order to describe the uncertainty due to incomplete sampling. In practice, we can process a large number of coarse scale results and then process a limited number through the detailed flow simulation; however, the correlation between the coarse scale and the detailed response will remain unknown. One simple approach to tell if the ranking has been successful is to see whether the results appear rank preserving. For example, if the detailed response for the 20% coarse scale quantile is greater than the detailed response for the 80% quantile, then the ranking has not been successful. Ranking will help if the detailed response values are rank preserving.

Even future increases in computing resources will not make it feasible to process all fine scale realizations. Rather, it will lead to more fine scale representations of even larger model domains; the merit of ranking techniques will remain valid.

In our case study, a particular technique of scale-up in combination with two different types of aquifer response was used to determine the merit of ranking coarse scale realizations. One might argue that there is a best scale-up technique for the conductivity distribution of a given aquifer and the simulated aquifer response. The scale-up of fine scale conductivities to block values presumably has only little impact on groundwater heads whereas the influence is likely larger in dispersion dominated aquifers or in the case where a cleanup time has to be predicted. Sanchez-Villa et al. (1995) compare the three different "practical" scale-up methods: a Darcian type approach, power averaging and defining block conductivities as the ratio of average flux to average

gradient. They conclude that all the methods yield similar results. Gomez-Hernandez and Wen (1994) suggest that the simple geometric average performs as good as the more sophisticated scale-up techniques, if the conductivity distribution is not dominated by streaks of high or low values. Warren and Price (1961) and Bouwer (1969) conclude that the geometric average yields a reasonable estimate of block conductivities for 3-D flow.

6. Summary and conclusions

There is a unique heterogeneous distribution of rock properties in each aquifer; however, there is unavoidable uncertainty due to data paucity. Geostatistical techniques are being increasingly used to create fine scale stochastic numerical models that mimic the heterogeneous features of real aquifers. The uncertainty in aquifer response due to incomplete sampling is quantified by processing a large number of realizations through flow and transport simulators.

Computer resources restrict the number of fine scale realizations that can be processed. Thus, we propose coarse scale groundwater flow and transport simulation with all realizations followed by a fine scale simulation on a number of realizations selected according to their ranks. The value of ranking is assessed by computing the mismatch between the "true" cdf and the cdf approximated by the fine scale aquifer responses of the selected realizations. Constructing a high resolution hypothetical aquifer based on variogram statistics that were derived for the Columbus aquifer, Mississippi, two aquifer responses are analyzed at the outflow plane: the first time at which a small threshold concentration is exceeded and the time at which 50% of the initial mass has passed. For scale-up ratios of 8 and 64, rank correlation coefficients between the coarse and the fine resolution results, range from 0.75 to 0.94 for the two different aquifer responses. In general, the 50% mass measure leads to a better representation of the "true" cdf than the first arrival measure. Because the results of coarse scale simulations are only approximate, it will, however, still be necessary to run a number of fine scale simulations to confirm consistency with coarse scale results.

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