RECENT DEVELOPMENTS IN STOCHASTIC MODELING AND UPSCALING OF HYDROLOGIC PROPERTIES IN TUFO

Christopher A. Rautman
Geoscience Assessment and Validation Dept.
Sandia National Laboratories
Albuquerque, NM 87185
(505) 844-4584

ABSTRACT
A set of detailed geostatistical simulations of porosity has been produced for a layered stratigraphic sequence of welded and nonwelded volcanic tuffs at Yucca Mountain, Nevada. These simulations are produced using a composite model of spatial continuity and they are highly conditioned to abundant drill hole (core) information. A set of derivative simulations of saturated hydraulic conductivity has been produced, in the absence of conditioning data, using a cross-variable relationship developed from similar data elsewhere. The detailed simulations reproduce both the major stratigraphic units and finer scale layering indicated by the drill hole data. These simulations have been scaled up several orders of magnitude to represent block-scale effective hydrologic properties suitable for use in numerical modeling of groundwater flow and transport. The upscaling process involves the reformulation of a previously reported method that iteratively adapts an initial arbitrary grid to "homogenize" the detailed hydraulic properties contained within the adjusted cell limits and to minimize the size of cells in highly heterogeneous regions. Although the computation of the block-effective property involves simple numerical averaging, the blocks over which these averages are computed are relatively inhomogeneous, which reduces the numerical difficulties involved in averaging non-additive properties, such as permeability. The entire process of simulation and upscaling is rapid and computationally efficient compared with alternative techniques. It is thus suitable for the Monte Carlo evaluation of the uncertainty in site characterization as it affects the results of groundwater flow and transport calculations.

INTRODUCTION
Assessing the performance of a potential high-level nuclear waste repository, such as that proposed for construction at Yucca Mountain, Nevada, requires calculating ground water travel times and rates of radionuclide releases, among other measures of repository performance. These hydrologic calculations require a description of the geology and material properties of the site itself. Classical geologic depictions of a site, such as verbal lithologic descriptions and graphical portrayals of geometry, are inadequate in themselves. Numerical process models necessitate numerical descriptions of the hydrologic properties of a site. Additionally, because the total quantity of material actually observed and sampled inevitably will be a very minute fraction of the three-dimensional block of rock that contains an engineered facility such as a repository, the results of those calculations and models should reflect geologic uncertainty. Licensing requirements mandate that this uncertainty be addressed in a quantitative and objective manner.

In this paper, we present the results of recent modeling activities focused on a small portion of the Yucca Mountain site to demonstrate the development of capabilities to model detailed geology in a stochastic fashion, and to upscale that detail to represent effective properties of blocks suitable for flow (process) modeling. The methodology is well suited to assess uncertainty that results from incomplete site characterization.

GEOSTATISTICAL SIMULATION
Geostatistical simulation comprises a diverse set of techniques for producing numerical models of geologic materials and rock properties. Simulation is distinct from estimation -- often better known by its geostatistical name kriging -- which is simply a means of interpolating between measured values. In contrast with kriging and other interpolation techniques that merely smooth the transition from one measured value to another, simulation fills in between measurements with random values sampled from some type of probability density function. Simulated models are designed to reproduce measured condition values at their spatial location, tend to reproduce the model of spatial continuity provided as input, and appear to vary more realistically on a small scale than an equivalent kriged model. Journel and Alabert, among others, have demonstrated the "excessive" smoothness of kriged models in contrast both to simulations and to an exhaustively known set of data. Such excessive smoothness may produce an unwarranted degree of spatial connectedness. If used in a physical process model, such spatial continuity may suggest more (or less) rapid movement of ground water and contaminants than is justified in reality.

The probabilistic mechanism underlying geostatistical simulation gives rise to the interpretation of simulations as equally likely alternative realizations. Because each realization is consistent with a given state of knowledge (conditioning data and variogram), there is no obvious objective means for deciding which one of a set of simulations "best" represents the true, but unknown, reality. The uncertainty that results from less than
exhaustive characterization of a site can thus be assessed in a probabilistic, Monte Carlo fashion. The technique of Monte-Carlo style uncertainty assessment in hydrology is well known. Geostatistical simulation merely provides a more sophisticated numerical model of the underlying site geology than is usually implemented.7,8

MODELING OF YUCCA MOUNTAIN

The application of geostatistical simulation to flow modeling of the Yucca Mountain site is not necessarily straightforward. Many applications of simulation involve a single geologic unit (a porous sandstone aquifer, for instance). In contrast, the Yucca Mountain region consists of an apparently simple, but geostatistically complex, layered sequence of welded and nonwelded tuffs. The rocks are characterized by pronounced changes in mappable features and corresponding changes and gradations in hydrologic properties.9 Additionally, the potential repository at Yucca Mountain is located within the unsaturated zone above the water table and process modeling of unsaturated flow and transport is a difficult issue at best.10 Nonlinearity of permeability as a function of (partial) saturation state increases the complexity of the modeling effort. Although the geometric problem is potentially solvable simply by breaking the complex stratigraphy at Yucca Mountain into its various components and modeling them separately, it is apparent that the computational effort involved in generating a large number of geostatistical simulations for Monte Carlo-style evaluation of flow and transport quickly expands beyond reason as the number of separate "layers" or distinct zones to be modeled increases.11

Strategic Approach

We are developing tools and approaches suitable for practical geostatistical simulation at Yucca Mountain. In this exercise, we attempt to simulate a diverse lithologic interval consisting of both welded and nonwelded tuff in one computational pass. This modeling is a small-scale example of what Rautman and Flint termed a "highly conditioned simulation approach" using "major stratigraphic units." Under this approach, the modeled region contains an abundance of actual site data that act to constrain the resulting simulation of unsampled locations. In the presence of abundant field data, the simulation algorithm is less sensitive to errors or purposeful distortions in the model of spatial continuity used to control the generation of in-fill values; the simulation is constantly "brought back" to reality by the conditioning information. A generalized model of spatial continuity developed for a composite stratigraphy, such as in the current example, may necessarily be a compromise among more accurate models that could be developed for a more finely divided layered sequence (compare, for example, Figures 7 and 8 of Rautman and Flint).12

We have chosen to create our preliminary models using a fast, sequential Gaussian simulation algorithm, SGSIM.5 The hydrologic property of primary focus is relative-humidity-oven-dry porosity because the set of drill hole data used to condition the simulations does not yet contain permeability values. Because these simulations are intended to support modeling of groundwater flow and transport, models of permeability are essential. An independent data set containing values of both porosity and saturated hydraulic conductivity was used to develop a quantitative cross-variable regression (described below). Following simulation of a detailed porosity model conditioned to data from drill holes, a similar detailed model of hydraulic conductivity was produced using the porosity-conductivity relationship.

Sequential Gaussian Simulation

The simulation process used in this study entails defining a block-style grid covering the modeled region and determining a random path to each and every grid node within that grid. Measured data to condition the simulation either may be mapped onto the nearest grid node or may be left in their proper spatial position with respect to the grid. Simulation of a new node is initiated by searching for conditioning data within a specified search pattern and by estimating the complete probability density function at that grid node, given surrounding nearby information. In Gaussian-based algorithms, that probability distribution is assumed to be bivariate normal. A hydrologic property value is then sampled from that probability distribution and assigned to that grid location, and the simulation process moves to the next node along the random path. A node completely isolated from conditioning data may either be left unsimulated (flagged as "missing") or be simulated based on the marginal probability distribution, or overall probability of occurrence. In the sequential method, once simulated, a grid node counts as part of the data upon which the remainder of the simulation is conditioned.

For poorly conditioned simulations, including grids within which the conditioning data are particularly unevenly distributed spatially, early simulation of nodes far removed from conditioning data and based solely upon the marginal probability distribution can lead to propagation of these randomly selected values in accordance with the input model of spatial continuity. This process can lead to the production of models that may appear unrealistic in that bodies of one type of material may randomly appear in an "improper" geologic context. These geologic oddities do not indicate a failure of the simulation methodology; rather the results are simply reflecting uncertainty in the factual information. A "surprised" human observer most likely has additional soft information that has not been incorporated into the simulated model. The challenge in these cases is to quantify that soft information in some manner and use it to reduce uncertainty. The issue of soft data in geostatistical modeling is beyond the scope of this discussion.

Location and Geology of the Modeled Region

The model region selected to develop and evaluate geostatistical capabilities is located in the southeastern portion of the region proposed for the potential repository at Yucca Mountain in the vicinity of two recently drilled holes (Figure 1). In this portion of Yucca Mountain, welded and nonwelded tuffs of the Miocene Paintbrush Tuff have been gently tilted toward the east by Basin-and-Range-style block faulting. Surface exposures of the Paintbrush Tuff consist of welded ash flows belonging to the Tiva Canyon Member. The Tiva Canyon becomes gradationally nonwelded at its base, and overlies a sequence of nonwelded ash flows and air fall tuffs typically lumped together as the "Paintbrush nonwelded interval." These porous and permeable rocks are underlain by a very thick sequence of densely to moderately welded ash flows assigned to the Topopah Spring Member.
Figure 1

To be inserted
The modeled region consists of a cross section (Figure 1) that extends 62 m in a roughly north-south direction, essentially parallel to strike, between two shallow drill holes, USW UZN-54 on the south (74 m deep) and USW UZN-55 on the north (78 m deep). The south end of the section is located in the bottom of a small drainage, and the northern end extends onto the adjacent side slope. Because the depth of drilling is relatively shallow, the modeled section encompasses only a small portion of the overall Paintbrush Tuff stratigraphic unit. However, the section contains rocks belonging to three of the four major lithologic units present in the unsaturated zone in the vicinity of the potential repository at Yucca Mountain (the fourth is zeolitic nonwelded tuff), and thus represents an excellent data set for developing strategies to model complex layered stratigraphy.

**Available Drill-hole and Other Data**

A number of hydrologic properties have been measured on core samples (nominally 6.3 cm diameter) collected on average every 0.7-0.8 m in each drill hole. These properties include bulk density, porosity, particle density, volumetric water content and relative saturation. The porosity data from drill holes N-54 and N-55 were used to develop a model of vertical spatial variability for porosity in the immediate vicinity of the cross section. The drill hole data suggest a vertical range of correlation of approximately 37 m. This compares with the vertical range of 30 m previously reported for outcrop studies of the entire Paintbrush Tuff interval. Data are not available in the vicinity of the NS4-N55 cross section to compute location-specific variograms in the horizontal direction. Therefore, we have combined previously published estimates of horizontal correlation for welded and nonwelded vitric (but not zeolitic) tuffs at Yucca Mountain with the drill hole variograms to obtain an approximate model of spatial continuity for this exercise. This estimated composite model has a horizontal major axis of anisotropy with a range of 150 m, and a vertical-to-horizontal anisotropy ratio of 0.24.

The drill hole data for the modeled cross section do not include permeability-type measurements. Additional data that include values of matrix saturated hydraulic conductivity relevant to the tuffs at Yucca Mountain are available from surface transects and a number of other sources. These data were used to develop a cross-variable correlation between porosity and conductivity, which is illustrated in Figure 2. Data from a number of independent sources were used to cover the expected magnitude of variability in both parameters at Yucca Mountain and to help eliminate any sampling biases inherent in a single study. Samples considered to contain zeolite minerals were omitted from the analysis, because the modeled cross-section does not include the zeolitic unit. The data are described by the linear regression

\[
\ln(K_p) = -26.676 + 25.961\phi
\]

where \(\phi\) is porosity as a fraction continuity and \(K_p\) is saturated hydraulic conductivity in m/s. The correlation coefficient \(r\) for this regression line is 0.86. Residuals from the regression have a mean of zero and appear to be normally distributed with a standard deviation of 2.63. To avoid a one-to-one, singular relationship between porosity and hydraulic conductivity, \(\ln(K_p)\) values for the model were predicted from the simulated values of porosity by adding a Gaussian random noise component with the appropriate standard deviation to the value computed through equation 1. A direct (co)simulation of spatially correlated conductivity values would have been preferable. However, values of \(K_p\) are not available from the drill holes in the cross section, and thus spatial continuity within the error component is not considered.

**Simulation Results**

Two different simulations of porosity are shown in Figures 3(a) and 4(a). The transformed derivative simulations of saturated conductivity are shown in the corresponding (b) portions of the same figures. The simulations appear quite similar in that the relatively thick upper portion of the cross sections represents the low-porosity, low-conductivity welded tuffs of the Tiva Canyon Member. The Tiva Canyon portion of the section is underlain generally by the much higher porosity-conductivity Paintbrush nonwelded interval, which is, in turn, underlain by the densely welded, low-porosity-permeability, uppermost portions of the...
Topopah Spring Member. Differences in detail between the two simulations represent uncertainty, because there are no samples in the undrilled middle portion of the section to prove or disprove any of the modeled values.

Note that the transformed conductivity simulations (Figures 3b and 4b) have a more erratic "pepper-and-salt" appearance than the primary porosity simulations from which they are derived. This effect is attributed to the addition of a random, regression-error component to the primary regression prediction (Equation 1) that describes the correlation between these two variables. The gross lithologic layering of the stratified tuff sequence is well preserved, however. Had the conductivity data been available to create a direct simulation, the final result might have been somewhat similar, in that permeability-type properties might be expected to be more variable spatially than porosity.

UPSCALING

The models of hydrologic properties presented in the preceding section are too detailed for general use in hydrologic flow and transport calculations. However, it is not sufficient to generate models that simply consist of larger grid blocks. The type of samples and measurements used to construct the models must be considered.

Figure 3. Simulated model of (a) porosity and (b) ln saturated hydraulic conductivity for random number seed 1711.

Figure 4. Simulated model of (a) porosity and (b) ln saturated hydraulic conductivity for random number seed 1723.

Data Support

Support is the typical geostatistical term used to denote the "size" of the measurements under consideration. The support for the geostatistical models presented in the previous section is the centimeter-sized core pieces on which porosity and the other hydrologic properties were measured. The geostatistical models just presented (Figures 3 and 4) consist of blocks of approximately 0.38 m$^2$. This change of support is not particularly extreme.

Hydrologic modeling of this small portion of Yucca Mountain using the fractional-meter grid cells of the geostatistical simulations would be feasible; however, modeling such processes on a repository scale using this amount of detail almost certainly is impossible. We must therefore change the support of the hydrologic process model many orders of magnitude from the support of the actual data. The hydrologic literature is replete
with examples of the difficulty of performing this change of support in a realistic and reasonable manner.23

Practitioners of geostatistics have invested a significant effort in identifying the effects of changes in support, and a number of approaches and algorithms have been proposed. However, this effort has focused on “additive” properties, principally ore grades in mining applications, other compositional measurements, and (by extension) porosity. The critical flaw in the conventional geostatistical approach is that the various correction algorithms leave the mean of the distribution unchanged.24 The approach simply is not applicable in general to flow properties such as hydraulic conductivity. Although it is a relatively simple matter to scale up the porosity simulations of Figures 3a and 4a to whatever flow-simulation grid scale is desired, the equivalent computation for the conductivity simulations is a completely different issue. This issue assumes major proportions in modeling unsaturated flow systems, because there currently is no large-scale unsaturated permeability measurement similar to the classical aquifer well test that can be used to calibrate upscaling of the model from what are essentially point measurements.

Proposed Solutions to the Scaling of Permeability

A number of approaches to the upscaling of permeability-type data have been proposed, and these have been implemented with varying degrees of success in certain applications.

A simple, but geologically common, binary lithologic system consisting of sand and shale is of significant interest in the petroleum industry. In certain sedimentary environments and for purposes of predicting the effective permeability of large reservoir blocks, it has been demonstrated that an empirical power-law average based on the sand-shale ratio can produce reasonable estimates of block-scale effective permeability over the economically important range of values.25,26,27 The technique relies on the fact that in a given geologic context, “sand” tends to have a relatively constant permeability, particularly by comparison (in hydrocarbon production) to “shales” of near-zero permeability. Block-scale effective permeability is essentially an “average” of the relative proportions of sand and shale. The value of the power-law exponent for a given field can be developed in an empirical manner.

Another major approach to the upscaling of permeability data has focused on the “direct” simulation of block effective permeabilities in a manner similar to the generation of the stochastic images in Figure 3 and 4. The generation of the images is not difficult; rather the problem here focuses on determining the probability distribution and spatial correlation structure of those block-scale values. Current solutions to this problem28,29,30 have focused on numerical computation of the effective permeability of a “limited” number of block-scale cells positioned within a large microscale simulation, similar to Figure 3, conditioned to existing well data. The assumption, appropriate for most enhanced-recovery applications in the petroleum industry, is that flow will be in a particular known direction (i.e., stratigraphically horizontal from injector well to producer well). The effective permeabilities of a number of such block-scale cells are computed, and the variograms and cross variograms for the (exhaustive) point values and (sparser) block values can be computed. Once the point-to-block correlation structure has been approximated, it is a relatively simple matter to directly simulate a large field of block values conditioned to data measured on the smaller scale.

Both of these potential solutions to the issue of upscaling flow properties possess serious difficulties when applied to Yucca Mountain. Although to some extent the welded-nonwelded distinction relevant to ash-flow tuffs constitutes a binary lithologic system, the two lithotypes are not interspersed in the classical manner of a deltaic or fluvial sand-shale depositional system. Thus, it appears unlikely that the effective permeability of tuff is related to the proportion of welded and nonwelded material.

The direct simulation of block-scale effective permeabilities offered by the second methodology could be used at Yucca Mountain in certain limited instances. The requisite microscale realizations of, for example, hydraulic conductivity can be generated (i.e., Figure 3b). It is also possible to perform the numerical upscaling of block-sized volumes located within a microscale realization. Finally, the methodology and techniques for inferring the necessary covariances and cross-covariances exist. The difficulty is a practical one, in that the Yucca Mountain problem is 1.5-dimensional (implies more complex numerical upscaling computations) and multi-layered (each layer presumably would need to be scaled-up separately).27 In addition, a major focus within the Yucca Mountain project is on assessing uncertainty, which implies that numerous realizations must be produced, scaled-up, and evaluated. Even if the generation of “production” Monte Carlo stochastic images for final flow calculations is restricted to the direct simulation of blocks based on a single inference of the point-to-block relationship, the methodology would appear to be computationally intensive. What is needed is a fast, approximate method that is applicable to the unsaturated-zone setting of Yucca Mountain, the large number of discrete layers, and a reasonable site-characterization program. The adaptive grid methodology, described below, offers a potential solution to this need.

Adaptive Grid

An adaptive grid algorithm has been developed based on concepts originally described by Garcia and others.31 The concept is to construct a mesh covering the area (or volume) of interest, for which the sides of each cell are conceptually and mathematically represented as springs with an appropriate coefficient of elasticity (Figure 5). By setting each coefficient of elasticity proportional to some measure of heterogeneity of the detailed geostatistical simulation composing the adjoining cells, it is possible to have the “springy” sides of the cells expand or contract to minimize some aspect of that heterogeneity.32 Alternatively, the area (volume) of particularly heterogeneous cells can be minimized. Presumably the impact of a “bad” estimate of effective permeability for a small grid cell on the entire simulation is relatively small. The effect of this algorithm is that the final grid adapts to follow geological features reflected in the underlying geostatistical simulation of a material property, and that the individual cells are as “homogeneous” as possible. Because the detailed hydrologic properties within a given cell tend to resemble each other more than would be the case for an arbitrary grid, the numerical difficulties encountered in computing an average, “effective” property for the cell are reduced.
The grid adaptation process is divided into three parts. The first part is the actual adjustment or movement of the cell-bounding nodes, which proceeds in several individual steps. In the second part, the heterogeneities of the adjusted cells are computed and these are translated into coefficients of elasticity for each cell boundary. A set of norms, or measures of the effectiveness of the grid-adjustment process in reducing overall heterogeneity of the grid is also computed during this portion of the process. The third part is to accept or reject the new mesh. If the new grid is accepted as an improvement over the previous version, the process begins again to see if additional improvement can be obtained. If the grid is rejected, a new “relaxation factor” may be computed or the grid may be considered “frozen” and the program exits.

For a given problem, the number of nodes in the x and y, and, for three dimensions, the z directions are fixed, as are the corner nodes that define the region under consideration. The external sides are not fixed, but are adjusted to user-specified boundary functions. Adjustments in the x and y directions are performed separately. Thus the steps in the adjustment process are:

1. adjust the x coordinates of the nodes using the current elasticities;
2. adjust the y coordinates of the top and bottom of the mesh to the specified boundary functions;
3. adjust the y coordinates of the nodes using the current elasticities;
4. adjust the x coordinates of the left and right sides of the mesh to the specified boundary functions.

At the end of the adjustment process, all nodes on the exterior of the mesh lie on the specified boundary.

The second part of the adaptation process requires finding in which element each data point of the underlying geostatistical simulation lies. Then, the numerical average, standard deviation and number of data points for each grid element is computed. The area, $a_i$, of each element is also determined, as are the minimum element area and maximum cell standard deviation ($max(a_i)$). Four norms describing the overall heterogeneity of the new grid are computed. These are:

\[ \| \sigma_i \|_\infty = max(\sigma_i) \]  
(EQ 2)

\[ \| \sigma_i \|_2 = \left( \sum_{i=1}^{n} \sigma_i^2 \right)^{0.5} \]  
(EQ 3)

\[ \| \sigma_i^a \|_\infty = max(\sigma_i^a) \]  
(EQ 4)

\[ \| \sigma_i^a \|_2 = \left[ \sum_{i=1}^{n} (\sigma_i^a)^2 \right]^{-0.5} \]  
(EQ 5)

The last norm (equation 5) is recommended, but the others may be advantageous for particular meshes. For each element, a measure of heterogeneity, $\beta_i$, is calculated:

\[ \beta_i = \frac{\sigma_i a_{min}}{\sigma_{max} a_i} \]  
(EQ 6)

The elasticities, $k$, for each side or link are computed as

\[ k_{side} = 1 + \left( \frac{r}{n_{adj}} \right) \sum_{i=adj}^{n_{adj}} \beta_i \]  
(EQ 7)

for those $n_{adj}$ elements adjacent to $k_{side}$. The relaxation factor, $r$, and the elasticities, $k$, initially are set equal to 1.

In the third and final step, acceptance of the computed grid depends on the value of the selected norm. The new norm computed after adjustment of the grid is compared to the smallest norm previously encountered. If the new norm is smaller, indicating that the adjusted grid blocks are more homogeneous internally or that the heterogeneity is confined to smaller grid cells, the new grid is accepted and the relaxation factor is set equal to 1. If the grid is not accepted, the relaxation factor is reduced by half, and the evaluation process repeated. If the relaxation factor becomes less than 0.001, the adjustment process terminates, retaining the grid with the lowest norm encountered. A minimum number of 10 detailed data points are required within each element to prevent the formation of excessively small grid blocks.

### Hydrologic Properties and Upscaling

Adapting the grid to the geostatistical simulation minimizes the heterogeneity of hydrologic properties contained within each element. In regions of relatively high heterogeneity, the adaptive grid algorithm using the norms given by Equations 4 or 5 will tend to reduce the size of elements within that region. Although the grid adaptation creates grid blocks that are by no
means completely homogeneous, the elements thus created do
tend to be either (a) more homogeneous than a general, arbitrary
grid and/or (b) relatively smaller in size and presumably of lesser
importance to the overall flow calculation.

At this time, upscaling of hydrologic properties within
the final, adjusted grid blocks is accomplished through simple
numerical averaging of the comprised geostatistically generated
values (note: the arithmetic mean is computed for porosity; the
geometric mean is computed for conductivity). The effect of nu-
merical problems related to the averaging of widely varying val-
ues (such as permeability data) are inherently less pronounced
because values within each adjusted cell are less variable than for
an arbitrary grid, or the size of the cell(s) containing the widely
disparate values is small. Although they have not been imple-
mented at present, we are investigating other computational
methods for averaging/upscaling that are less sensitive to a few
extreme values within the detailed simulated values.44

Because the scaled-up hydrologic property within each
grid block is computed as a simple numerical average, the implic-
it assumption is that intra-block spatial correlation of pore sizes
and other factors that affect the hydrologic pathways do not exist.
Correlations that exist within the underlying detailed geostatis-
tical simulation at less than the block scale are discarded.

If the scale of the flow phenomena of interest is smaller
than the block scale, it cannot be captured; this is a fundamental
computational limitation. Significant spatial structure is retained
if the range of correlation extant in nature and reproduced in the
detailed simulation is large by comparison with the average scale
of the final grid blocks. Such long-range spatial correlation pat-
terns will be preserved in the admittedly simplified block-scale
models. However, as the actual range of correlation converges to-
ward the dimension of the individual blocks, more and more of
the spatial structure will be intentionally (and unfortunately) dis-
carded.

**Upscaled Models of Porosity and Conductivity**

The adaptive grid algorithm and simple numerical aver-
ing process has been applied to the simulated detailed models
of porosity and permeability produced for the N-54/N-55 cross
section. An example of these upscaled models corresponding to
Figure 3 is shown in Figure 6. The adjusted grid boundaries at-
tempt to follow the macroscopic layering created by the welded-
nonwelded lithologic subdivisions that are the major feature of the
modeled region. The Tiva Canyon Member, Paintbrush non-
welded unit, and Topopah Spring Member are all evident in the
upscaled version of the geostatistical simulation. Grid-cell
boundaries also attempt to conform to the internal stratigraphic
layering, which reflects smaller scale changes in hydrologic
properties as indicated by the conditioning measurements in the
bounding drill holes. Finally, the areas of the block-scale grid el-
ements vary as the grid-adjustment algorithm has attempted to
homogenize the included, microscale hydrologic properties and
limit the influence of more extreme heterogeneity. Even though
intra-block spatial correlation has been eliminated by the simplis-
tic numerical averaging technique applied to the contained mi-
acro-scale values, the large scale features of the real rocks have
been preserved.

![Figure 6. Upscaled models of (a) porosity and (b) in saturated hydraulic conductivity corresponding to the detailed, microscale models of Figure 3.](image)

Although it is difficult to determine by simple visual ob-
servation of the grey-scale images, the improvements obtained
through the adaptive grid algorithm are real. For the simulation
shown in Figures 3 and 6 (random number seed 1711), the norm
of Equation 5 decreased from 209.56 to 155.37, an improvement
over the initial uniform grid of 26 percent. The simpler measure
of grid-cell heterogeneity, the maximum standard deviation
(Equation 2) decreased 27 percent. Much less improvement oc-
curred for the adaptive gridding of the simulation shown in Fig-
ure 4 (seed 1723). The primary norm in this case decreased from
192.31 to 188.14, a mere 2 percent reduction. The maximum cell
standard deviation decreased 6 percent.

**DISCUSSION**

The large-scale stratigraphic features reflected in Figure
6 almost certainly are a first-order control on groundwater move-
ment and contaminant transport at Yucca Mountain. Their conti-
nuity or lack thereof, and the uncertainty in their general location
and approximate material properties are important considerations
in assessing the hydrologic performance of the site. Uncertainty resulting from the inevitably "incomplete" site description will be an important consideration in assessing the performance of any potential repository at Yucca Mountain.

The models developed in this exercise are admittedly imperfect representations of the real Yucca Mountain; however, they possess a number of significant advantages over models created by many other techniques. First, creation of the underlying detailed models is fast. The sequential Gaussian algorithm required only one model of spatial variability and one computational pass to represent a composite of three separate lithologic units. Second, creation of the conductivity models in this instance was accomplished by a simple algebraic transform based on an inexpensive, easy-to-measure, and spatially abundant material property: porosity. Third, the block-scale grid, which ultimately will be used for hydrologic calculations, is quickly adapted to the unique spatial characteristics of each individual realization. The adaptation of the grid is based directly upon the simulated hydrologic properties, thus minimizing the errors introduced by the fast, simple numerical averaging technique applied to the values contained in each cell, which is a fourth important characteristic of this methodology.

Finally, the methodology described in this paper is amenable to incremental improvement at several points in the process. Actual hydraulic conductivity measurements could be used to create and condition the microscale simulations of that property. More sophisticated nonparametric techniques can be substituted for all or part of the process of creating the underlying, detailed hydrologic-property models. Techniques such as indicator simulation may be particularly suitable for representing the properties of relatively disparate lithologies within a single computational (simulation) environment. They may also be relevant in evaluating the performance impacts of various scenario-related distortions of the expected spatial continuity patterns. Additionally, the various norms (Equations 2 through 5) associated with the adaptive grid algorithm could be adapted to distinguish grid blocks for which simple numerical averaging is a "reasonable" approximation from those that might need to be represented by a more sophisticated form of numerical upscaling, perhaps involving numerical flow computations.

CONCLUSIONS

We have demonstrated that Monte-Carlo-style simulations of important hydrologic rock properties can be generated in a labor- and computationally efficient manner, even for a lithologically diverse geologic setting. The key to using simplifying assumptions and simulation techniques in a composite stratigraphic interval is the presence of adequate conditioning data. We have also scaled-up these detailed, microscale simulations, for which the data support and the model values are approximately equivalent, to represent block-effective properties suitable for flow calculations in a tractable, computationally efficient, if approximate manner.

Major stratigraphic and hydrologic features of the Yucca Mountain region are preserved in these fast, approximate stochastic images of block-scale effective properties. The limitations imposed by the composite stratigraphy, Gaussian-related simulation algorithm, and simple numerical averaging technique for upscaling non-additive properties such as hydraulic conductivity are not trivial. However, the difficulty and additional effort inherent in more accurate and theoretically elegant approaches to the same problem may preclude them from use on a routine basis. If adequate conditioning data are available from site characterization, the limits to our approximate approach may be sufficiently small to justify their use in initial performance calculations. More sophisticated simulation algorithms and techniques for estimating block-scale effective permeability-type properties exist, and these can then be applied to resolve finer-scale performance issues and sensitivities.

ACKNOWLEDGMENT

This work was supported by the U. S. Department of Energy, Yucca Mountain Site Characterization Project Office, under contract DE-AC04-76D00789.

REFERENCES


DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.