Hydrogeologic Flow Unit Characterization Using Transition Probability Geostatistics

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Abstract

This paper describes a technique for applying the transition probability geostatistics method for stochastic simulation to a MODFLOW model. Transition probability geostatistics has several advantages over traditional indicator kriging methods including a simpler and more intuitive framework for interpreting geologic relationships and the ability to simulate juxtapositional tendencies such as fining upwards sequences. The indicator arrays generated by the transition probability simulation are converted to layer elevation and thickness arrays for use with the new Hydrogeologic Unit Flow (HUF) package in MODFLOW 2000. This makes it possible to preserve complex heterogeneity while using reasonably sized grids. An application of the technique involving probabilistic capture zone delineation for the Aberjona Aquifer in Woburn, Ma. is included.

Keywords: MODFLOW, T-PROGS, transition probability geostatistics, stochastic simulations, indicator kriging

Introduction

The essential feature of a Monte Carlo simulation is that multiple equally probable hydrogeologic model realizations are generated and solved. Typically, the realizations are generated by combining random instances of parameter values from user-defined probability distribution functions or by generating a spatial distribution of parameters using techniques such as sequential Gaussian simulation (Deutsch and Journel, 1992). Another approach is to randomize the spatial distribution of the parameter zones using a technique such as indicator kriging (Journel and Alabert, 1989). The resulting indicator distributions are generally conditioned to borehole data, and each distribution represents an equally probable interpolation of the observed zonation at the boreholes (McKenna and Poeter, 1995).

While both approaches are useful, the parameter randomization approach requires the modeler to delineate parameter zones, often resulting in gross simplification of the complex heterogeneity inherent at most sites. The indicator simulation approach treats the uncertainty associated with such heterogeneity as an integral part of the stochastic simulation process. One potential drawback of the indicator simulation approach is that it requires the modeler to assign a single value of hydraulic conductivity within each material - an obviously difficult task. However, if sufficient observation data are available, the model can be run in a "stochastic inverse" mode, where the properties associated with the indicators are parameterized and each model instance can be calibrated to head and flow observations.

In this paper we describe a method for performing indicator simulation-based stochastic flow modeling with the MODFLOW model. We also describe a method for combining the transition probability-based indicator simulation approach (Carle, 1996; Carle and Fogg, 1996; Carle 1997a) with the new Hydrogeologic Unit Flow (HUF) Package in MODFLOW 2000 (Anderman and Hill, 2000). The combination of the HUF package and transition probability geostatistics makes it possible to consider detailed heterogeneity while maintaining relatively simple grids with reasonable computational requirements. It also allows the use of variable cell thicknesses for the MODFLOW grid, something that is typically not possible with indicator simulations.

Transition Probability Geostatistics

The stochastic simulation approach described in this paper is based on the T-PROGS software (Carle, 1997a). The T-PROGS software utilizes a transition probability-based geostatistical approach to model spatial variability by 3-D Markov Chains (Carle and Fogg, 1997) and formulate indicator cokriging equations (Carle and Fogg, 1996) and the objective function for simulated annealing (Carle, 1997b).

The transition probability approach has several advantages over traditional indicator kriging methods. First, the transition probability approach considers asymmetric juxtapositional tendencies, such as fining-upwards sequences. Second, the transition probability approach has a conceptual framework for incorporating geologic interpretations

into the development of cross-correlated spatial variability. The transition probability

approach does not exclusively rely on empirical curve fitting to develop the indicator (cross-)

variogram model. This is advantageous because geologic data are typically only adequate to

develop a model of spatial variability in the vertical direction.

The transition probability approach provides a conceptual framework to integrate

geologic insight into a simple and compact mathematical model, the Markov chain. This is

accomplished by linking fundamental observable attributes – mean lengths, material

proportions, anisotropy, and juxtapositioal tendencies – with Markov chain model

parameters.

The first step in performing a transition probability analysis using the T-PROGS

software is to review the available borehole logs at a site and merge or simplify hydrofacies

categories (if necessary) to a reasonably small number; typically five or less. The borehole

data are then passed to a utility within T-PROGS called GAMEAS that computes a set of

transition probability curves as a function of lag distance for each category for a given

sampling interval. A sample matrix of measured vertical direction transition probability

curves are shown by the dashed lines in Figure 1. Each curve represents the transition

probability from material j to material k. The transition probability t_{jk}(h) is defined by:

$$t_{jk}(h)= \Pr(j \text{ occurs at } x + h \mid k \text{ occurs at } h) \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (1)$$

where x is a spatial location, h is the lag (separation vector), and *j,k* denote categories. Note that the curves on the diagonal represent auto-transition probabilities, and the curves on the off-diagonal represent cross-transition probabilities.

The next step in the analysis is to develop a Markov Chain model for the vertical direction that is consistent with the observed vertical transition probability data. The Markov Chain curves are shown as solid lines in Figure 1. Mathematically, a Markov chain model applied to one-dimensional categorical data in a direction ϕ assumes a matrix exponential form:

$$T(h_\phi) = \exp(\mathbf{R}_\phi h_\phi) \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2)$$

where ϕ denotes a lag in the direction ϕ, and $\mathbf{R}_\phi$ denotes a transition rate matrix

$$\mathbf{R}_\phi = \begin{bmatrix} r_{11,\phi} & \cdots & r_{1k,\phi} \\ \vdots & \ddots & \vdots \\ r_{k1,\phi} & \cdots & r_{kk,\phi} \end{bmatrix} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (3)$$

with entries $r_{jk,f}$ representing the rate of change from category j to category k (conditional to the presence of j) per unit length in the direction ϕ (Krumbein, 1968). The transition rates are adjusted to ensure a reasonable fit between the Markov Chain model and the observed transition probability data.

The transition rate matrix has some important theoretical properties useful in model development. The transition rate corresponds to the *slope* of the transition probability as it approaches lag zero:

$$r_{jk,\phi} = \frac{\partial t(h \to 0)}{\partial h_\phi} \quad \dots (4)$$

The diagonal entries are negative ($r_{jj,f} < 0$), and the off-diagonal entries are non-negative ($r_{jk,f} \geq 0$), which ensures that $0 \leq t_{jk}(h_\phi) \leq 1$. The diagonal entries $r_{jj,f}$ are related to $\overline{L}_{j,z}$, the mean length of category j in the direction ϕ by

$$r_{jj,\phi} = \frac{1}{\overline{L}_{j,\phi}} \quad \dots (5)$$

Furthermore, the row sums must equal zero:

$$\sum_{k=1}^{K} r_{jk,\phi} = 0 \quad \dots (6)$$

and the column sums must obey

$$\sum_{k=1}^{K} p_j r_{jk,\phi} = 0 \quad \dots (7)$$

where p_j is the proportion of the total material corresponding to category j. This ensures that the transition matrix converges on the specified proportions, $t_{jk}(h_\phi \rightarrow \infty) = p_k$ as expected for a stationary Markov chain.

Once the Markov chain is developed for the vertical (z) direction from the borehole data, models of spatial variability are developed for the lateral (x and y) directions. Borehole data are typically not sufficiently dense in these directions. However, x and y-direction transition rate matrices for Markov chain models can be developed by assuming lateral vertical ratios of mean lengths, geologically plausible juxtapositional tendencies and the same proportions assumed in the vertical model. The x, y, and z Markov chain models are converted into a continuous 3D Markov chain model using the MCMOD utility within T-PROGS.

In the final phase of setting up a transition probability analysis using T-PROGS, the modeler creates a grid, specifies the number of realizations (N), and launches the TSIM utility. The TSIM code uses the 3D Markov chain to formulate both indicator cokriging equations and an objective function for simulated annealing. It generates stochastic simulations using a combination of modified versions of the GSLIB codes SISIM and ANNEAL (Deutsch and Journel, 1992).

The output from the TSIM code is a set of N arrays of indicator values, where each value specifies the material id for the corresponding MODFLOW grid cell. These indicator

value arrays can be used to define parameter zones in MODFLOW 2000. Each indicator

type inherits the hydraulic properties (k_h, k_z) from the list of parameter zones. A sample

MODFLOW grid generated via transition probability geostatistics is shown in Figure 2.

Hydrogeologic Unit Flow Package

Using transition probability geostatistics with MODFLOW models presents two basic

limitations. First, the underlying stochastic algorithms used by the T-PROGS software are

formulated such that the MODFLOW grid must have uniform row, column, and layer widths.

The row width can be different from the column width, but each row must have the same

width. This results in a uniform orthogonal grid. While MODFLOW grids are orthogonal in

x and y, the layer thickness is allowed to vary on a cell-by-cell basis. This makes it possible

for the layer boundaries to accurately model the ground surface and the tops and bottoms of

aquifer units. If a purely orthogonal grid is used, irregular internal and external layer

boundaries must be simulated in a stair-step fashion either by varying material properties or

by activating/inactivating cells via the IBOUND array. A second limitation is that in order to

get a high level of detail in the simulated heterogeneity, the grid cell dimensions are

generally kept quite small. This can result in difficulties in the vertical dimension. The large

number of layers with small layer thicknesses near the top of the model generally ensures

that many of the cells in this region will be at or above the computed water table elevation

(for simulations involving unconfined aquifers). As a result, these cells will undergo many

of the numerical instabilities and increased computational effort issues associated with cell wetting and drying.

The new Hydrogeologic Unit Flow (HUF) package (Anderman & Hill, 2000) released with MODFLOW 2000 makes it possible to overcome both of these limitations resulting in a powerful mechanism for incorporating transition probability geostatistics in MODFLOW simulations. The HUF package is an alternative to the Block-Centered Flow (BCF) and Layer Property Flow (LPF) packages (McDonald and Harbaugh, 1988; Harbaugh, et al., 2000). Each of these packages is used to compute cell-to-cell conductances from the layer geometry and aquifer properties. With the HUF package, the modeler is allowed to input the vertical component of the stratigraphy in a grid-independent fashion. The stratigraphy data are defined using a set of elevation and thickness arrays. The HUF arrays are identical to the MODFLOW grid in plan view (same number of rows and columns) but are independent in the vertical direction. The first HUF array defines the top elevation of the model. The remaining HUF arrays define the thicknesses of a series of hydrogeologic units, starting at the top and progressing to the bottom of the model. For each array of thicknesses, many of the entries in the array may be zero. This makes it possible to simulate complex heterogeneity, including pinchouts and embedded lenses that would be difficult to simulate with the LPF and BCF packages.

We have developed a computer algorithm for integrating transition probability geostatistics results with the HUF package. The algorithm approach overlays a dense

background grid on the MODFLOW grid and runs T-PROGS on the background grid. A set of HUF arrays is then extracted from the background grid for use with the MODFLOW model. The main steps of the algorithm are as follows:

Step 1 - Create the MODFLOW Grid

The first step is to create a MODFLOW grid with the desired number of layers and to interpolate the layer elevations to match the aquifer boundaries. The row and column widths are uniform but the layer thicknesses may vary from cell to cell. A simple approach is to uniformly distribute the layer thicknesses from a set of top elevations corresponding to the ground surface to a set of elevations corresponding to the bottom of the aquifer as shown in Figure 3a. Alternatively, the thicknesses can be biased such that the top layer is thicker, resulting in less cells undergoing wetting and drying.

Step 2 - Create a Background Grid

The second step is to create a background grid that encompasses the MODFLOW grid. The rows and columns of this grid match the MODFLOW grid but the layer thicknesses are uniform and relatively thin, resulting in a much greater number of layers than the MODFLOW grid. The top of the grid must be above the highest elevation in the MODFLOW grid and the bottom of the grid must be below the lowest elevation in the MODFLOW grid.

Step 3 - Run T-PROGS

Once the MODFLOW grid and the background grid are both constructed, the next step is to perform a T-PROGS simulation to obtain a set of indicator arrays for the background grid. This will result in a series of indicator arrays or "realizations" on the background grid as illustrated in Figure 3b.

Step 4 - Convert the T-PROGS Output

The final step is to convert T-PROGS output of indicator arrays onto the background grid into a set of HUF elevation/thickness arrays. This is a difficult process to automate since the heterogeneity in the background grid can be quite complex. We use the following algorithm to accomplish the conversion:

1) The HUF top elevation array is set equal to the top of the MODFLOW grid.

2) Each row/column combination in plan view represents a vertical sequence of cells in the background grid and the MODFLOW grid and a vertical sequence of hydrogeologic units in the HUF arrays. The HUF thickness arrays are developed by traversing the vertical sequences and performing the following for each sequence.

   a) Starting at the top of the corresponding sequence of cells in the background grid, work downward through the vertical sequence until the cell is found that contains the HUF top elevation. The indicator value corresponding to this cell represents the first

hydrogeologic unit in the sequence. The thickness of the unit is found by continuing down the set of cells in the background grid until a cell with a different indicator value is found. This process is repeated for each of the units defined by the background grid. The search is stopped when the cell in the background grid containing the bottom elevation of the MODFLOW grid is found. This represents the bottom of the hydrogeologic units.

b) For each hydrogeologic unit found in the previous step, we must modify the proper entry in the HUF thickness arrays. To do this, we first traverse the set of units found in the vertical sequence from top to bottom and assign an *index of occurrence* to each unit. For example, if a unit represents the third occurrence of a particular indicator (e.g. clay) in the sequence, the unit is assigned an index of occurrence of *three*. Once the indices are assigned, we traverse the units once again, starting at the top. For each unit, we check to see if there is an entry in HUF thickness arrays with a corresponding index of occurrence. For example, for the third clay unit in the sequence, we locate the third clay unit in the HUF thickness arrays and assign the appropriate thickness to the cell in the array corresponding to the current row/column. If a corresponding thickness array does not yet exist, we create one and assign a zero thickness to all cells except the cell in question. This process is repeated for each vertical sequence of cells/hydrogeologic units.

At the end of this step, the hydrogeologic units defined by the background grid are now represented by the HUF arrays as shown in Figure 3c. The hydrogeologic units are properly trimmed to the top and bottom of the MODFLOW grid. The total number of HUF thickness arrays required to represent the hydrogeologic units for a particular model instance can be determined from the following equation:

$$n_{ta} = \sum_{j=1}^{n_i} b_i \quad\text{..}(8)$$

where n_{ta} is the number of thickness arrays, n_i is the number of indicators, and b_i is the maximum number of occurrences of indicator i in a single vertical sequence.

The end result of this conversion process is N sets of HUF input arrays, each array corresponding to one 3D indicator array from the T-PROGS simulation. These sets can then be used as input to a Monte Carlo simulation.

Sample Application

To test the technique described above, we performed a Monte Carlo simulation using a model of the Aberjona aquifer in Woburn, Massachusetts. In the early 1980's a group of citizens in Woburn, Massachusetts filed a lawsuit against three corporations located near the Aberjona Valley. The lawsuit contended that illegal disposal of TCE by the companies resulted in the deaths of several children from ingestion of contaminated ground water

pumped from two municipal wells in the Aberjona aquifer. The story of the resulting jury trial was featured in a non fiction novel entitled "A Civil Action" (Harr, 1995) and was later made into a major motion picture of the same name.

A conceptual representation of the Aberjona model is shown in Figure 4. The model boundaries are similar to the boundaries used in a MODFLOW model developed by the USGS (Lima & Olimpio, 1989). The north and south boundaries correspond to parallel flow boundaries and the east and west boundaries correspond to ground water divides. The Aberjona River runs down the center of the model, flowing from north to south. Wells G & H are just to the east of the Aberjona River. These municipal wells are no longer in use but played a central role in the case since the plaintiffs argued that drinking water produced by the wells was contaminated. The properties belonging to two of the defendants in the case, W.R. Grace and Beatrice, are also shown on the map.

Our goal was to run a T-PROGS simulation on the Aberjona site and use the resulting indicator arrays to perform a stochastic simulation. Using the results of this simulation, we can perform a probabilistic capture zone analysis. The first step in this process is to import the borehole data and analyze the measured transition probabilities. The borehole data were taken from a site investigation performed by the NUS Corporation (NUS Corp. 1986). The original borehole data consist of 27 holes and the borehole logs indicate that the site composed of a complex mixture of clay, sand, silt, and gravel representing glacial sediments

from the Late Wisconsin glaciation which receded approximately 14,000 years ago. More recent alluvial deposits overlay the glacial deposits in some areas.

A large number of different types of soil were listed on the borehole logs. By combining similar soil types, we simplified the number of types to a total of four materials: sandy clay, silt, sand, and sandy gravel. The boreholes were then analyzed using the GAMEAS utility in TPROGS, resulting in the measured transition probability curves for the vertical direction shown by the dashed lines in Figure 5. We prescribed a transition probability rates matrix to produce the Markov Chain model illustrated by the solid lines in Figure 5. The mean lengths (thicknesses) in the vertical direction varied from seven to eleven meters. We assumed a horizontal to vertical length ratio of ten in both the X and Y directions and generated the Markov Chains in the horizontal directions. We then ran the T-PROGS software to generate 100 sets of indicator arrays on a background grid consisting of 100 rows, 100 columns, and 20 layers. This background grid was used to generate 100 sets of HUF input arrays, each of which corresponds to an equally probable hydrogeologic model. A sample set of East-West cross-sections through one of the model instances is shown in Figure 6.

Once the HUF arrays were generated, the next step was to assign a vertical and horizontal hydraulic conductivity to each hydrogeologic unit. The vertical hydraulic conductivities were assigned relative to the horizontal values using a vertical:horizontal anisotropy ratio of 0.3. To determine an appropriate set of values for the horizontal conductivity, we utilized a parameter estimation approach. We marked each of the four K_h values as parameters and ran

the automated parameter estimation utility PEST (Doherty, 2000) to find a set of calibrated

conductivities. We calibrated to heads measured at 32 observation wells and an observed

flow rate of -1100 m^3/day in the Aberjona River (Myette, et al. 1987). We ran PEST in

inverse mode for 29 randomly selected model instances. We then computed the mean of the

optimized hydraulic conductivity values and utilized these values for all model instances.

Wells G & H were turned off during the calibration stage since they were not on when the

field measurements were taken.

Using the selected K_h values, we ran all 100 models in steady state mode with wells G and H

turned on. After running all 100 MODFLOW models, we then performed a probabilistic

capture zone analysis using the technique described in Jones, et al. (2003). For each model

instance, we performed a forward particle tracking analysis using MODPATH (Pollock,

1994) and determined which particles were captured by wells G & H. The results were used

to determine the probability of capture for each cell in the grid. The probabilities were

adjusted to give greater weights to the results from model instances with lower residual errors

(sum of the squared weighted residuals). This resulted in a 3D array of capture probabilities.

These probabilities were then converted to a 2D map by taking the maximum probability of

capture in each vertical sequence of cells. The resulting capture probability contours are

shown in Figure 7.

Conclusions

The techniques described in this paper make it possible to utilize transition probability geostatistics for MODFLOW-based stochastic simulations. Utilizing the new HUF package in this process results in model grids with a reasonable number of layers, yet it preserves the complex heterogeneity produced by the transition probability method. It also makes it possible to use model grids with non-uniform layer thicknesses. Combining a Monte Carlo stochastic approach to hydrogeologic modeling such as T-PROGS with the MODFLOW HUF package has enabled both (1) probabilistic estimation of bulk hydraulic conductivities, and (2) probabilistic assessment of contaminant plume capture at a heterogeneous field site.

Acknowledgements

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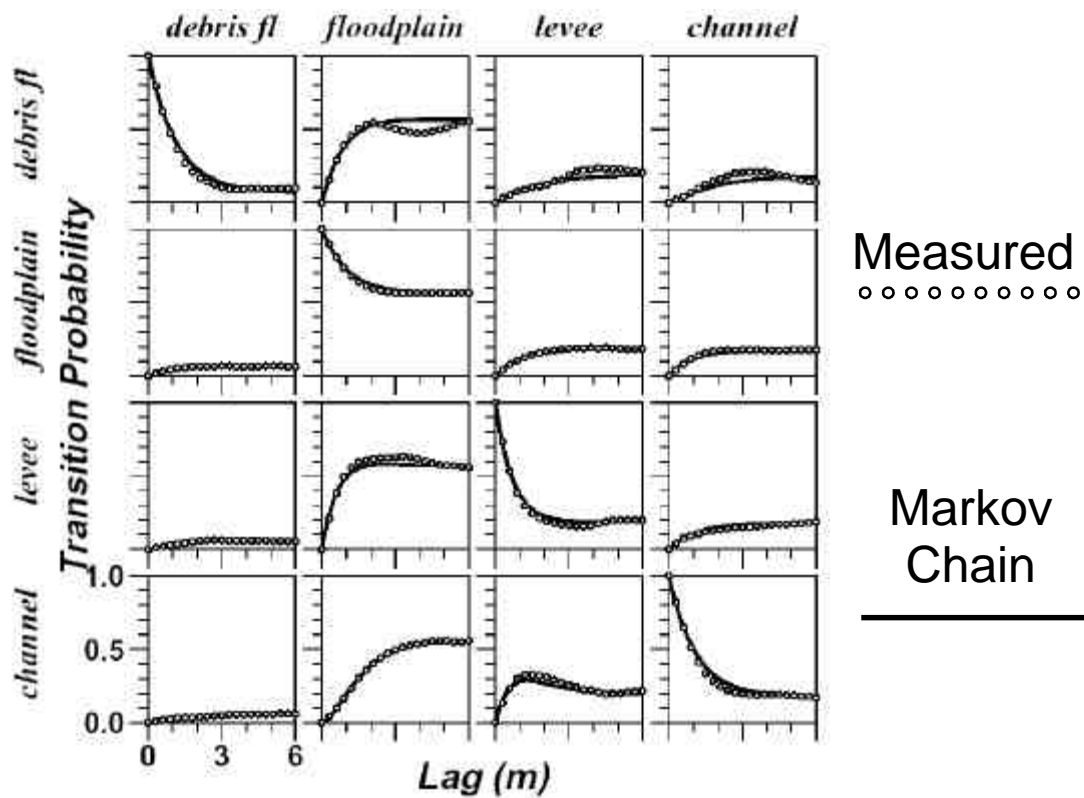
Figure 1 **Sample measured transition probabilities (circles) and Markov chain model (solid lines) for a set of borehole data with four categories (Carle, 1999).**
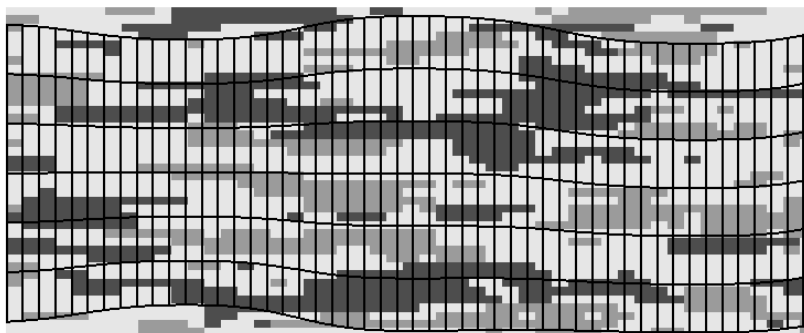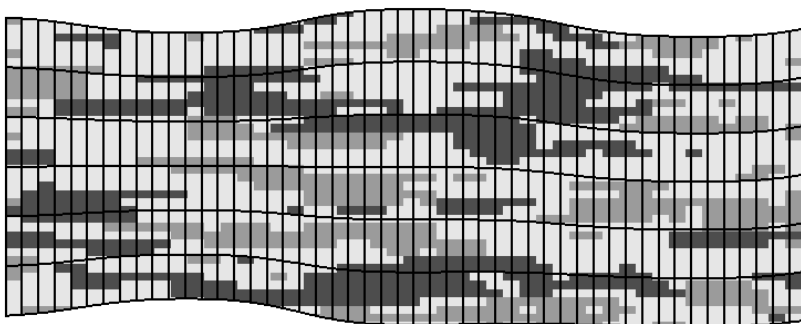
Sand w/ fines
Clay
Clean sand
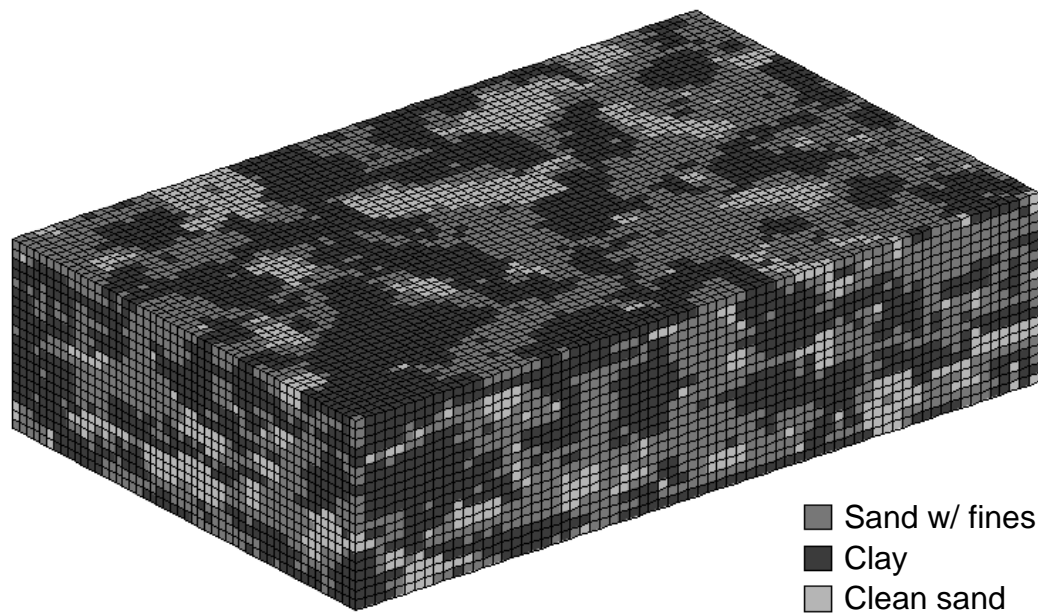
Figure 2   **MODFLOW grid (513 by 305 m by 80 m) with hydraulic property data**

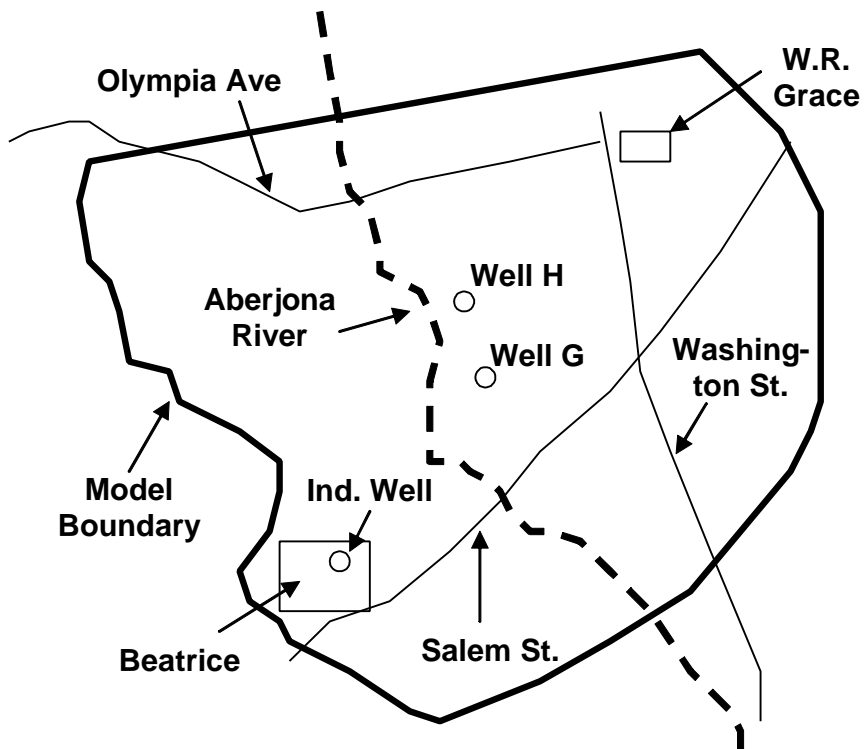**populated by T-PROGS. Z scale magnified by a factor of 5.0.**
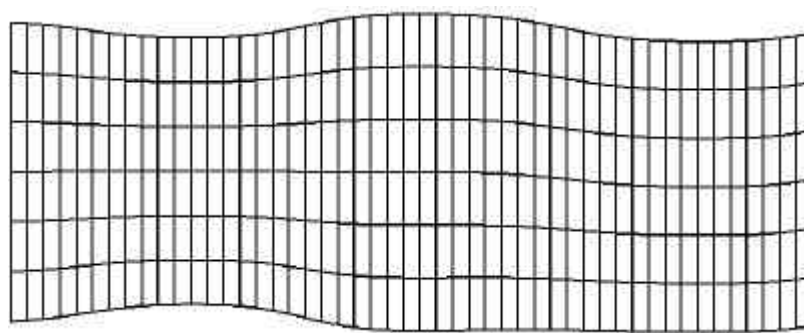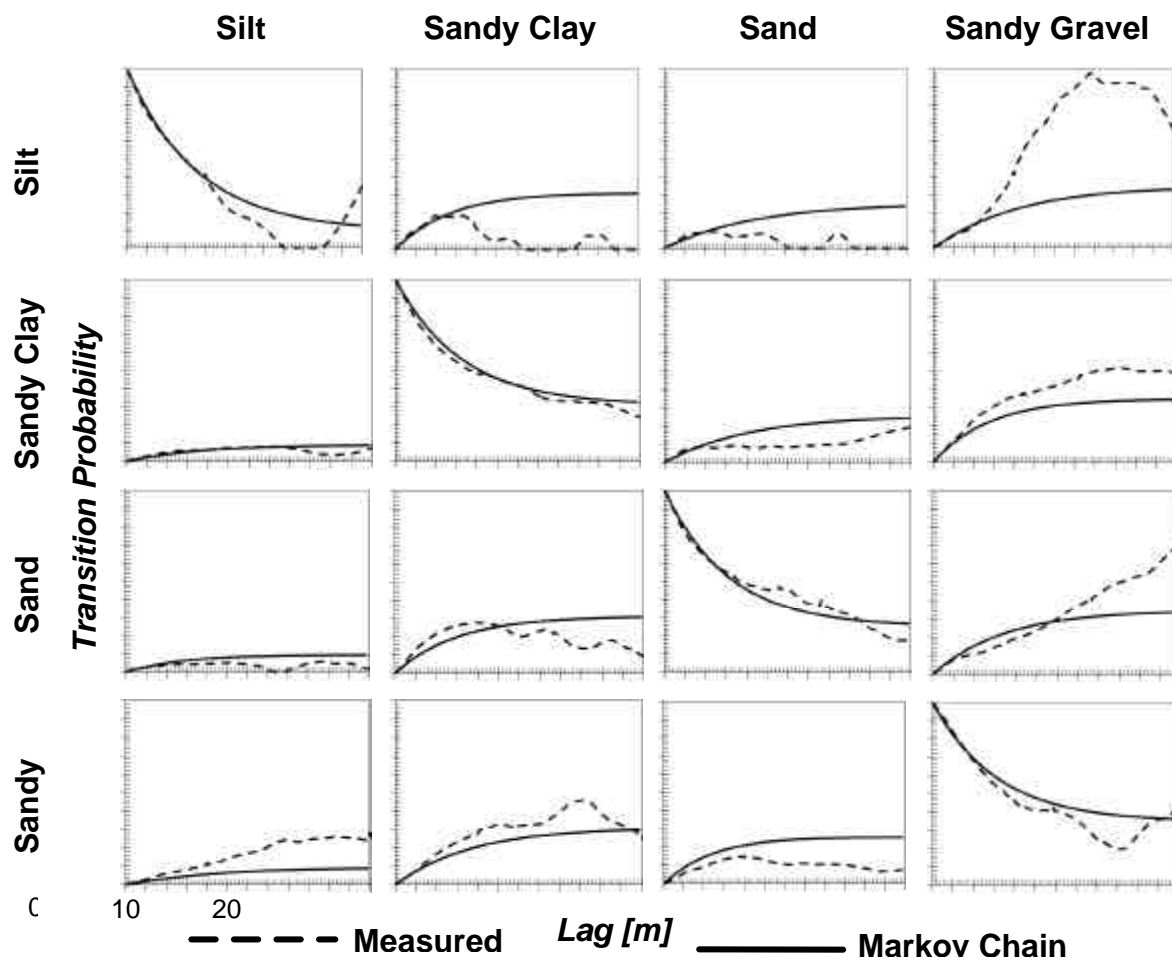
(a)

(b)

(c)

Figure 3   **HUF data generated by T-PROGS for a vertical cross-section (length =**

513 m). (a) Background grid with indicators. (b) MODFLOW grid with

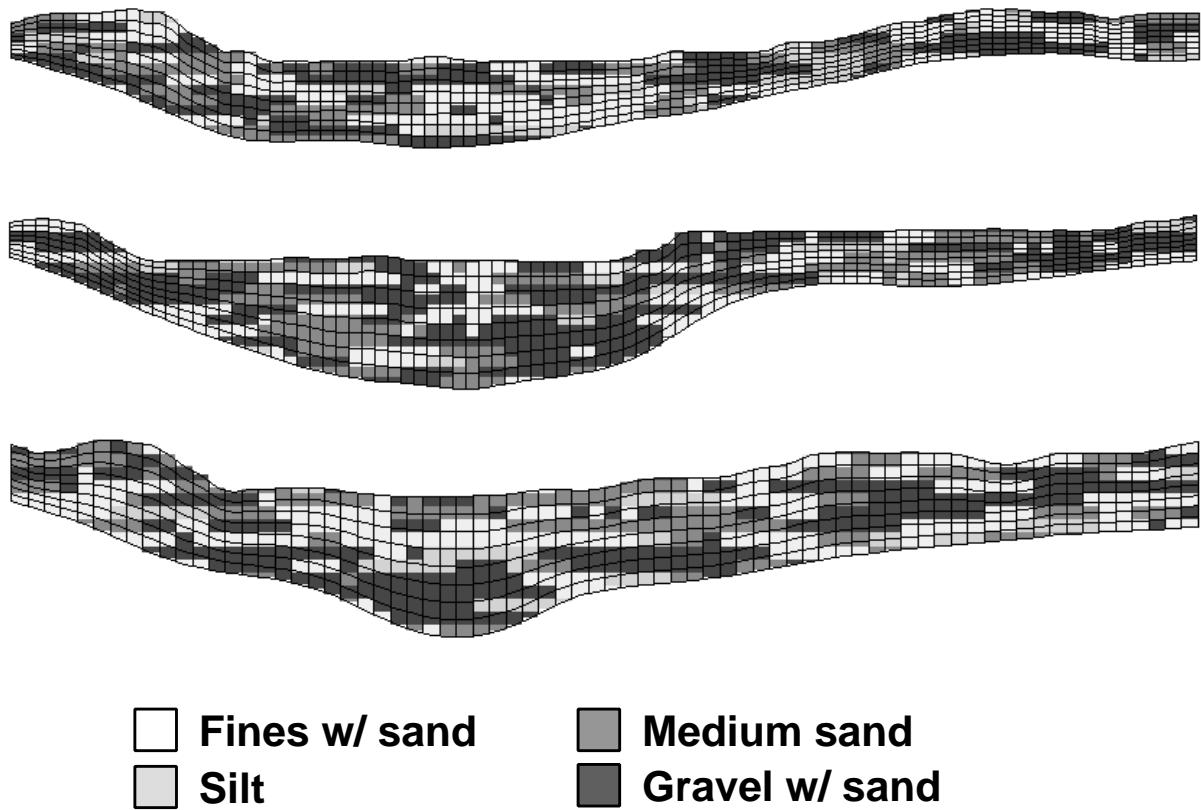variable cell thickness (solid lines) superimposed on background grid. (c)

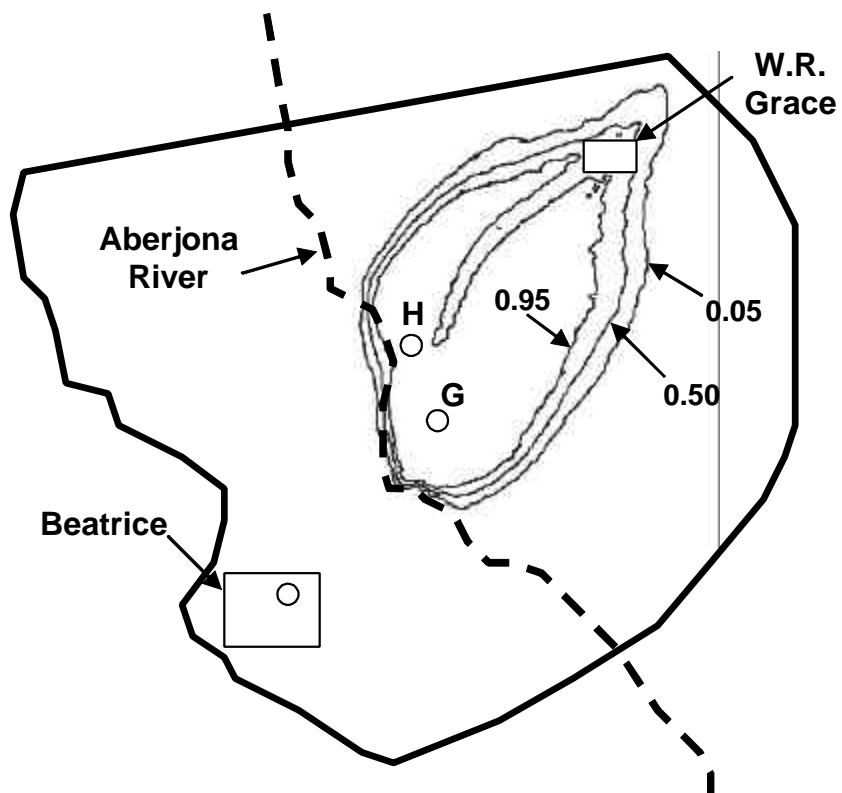MODFLOW grid with HUF arrays extracted from background grid.

Figure 4　　**Conceptual Model of Woburn-Aberjona Site.**

Figure 5 **Measured and Simulated Transition Probability Curves for Woburn Data.**

Figure 6   Sample East-West Cross-Sections Through Woburn Model Instance.

Vertical Scale Exaggerated by a Factor of 5.

Figure 7 **Combined Probabilistic Capture Zones for Wells G&H for 14.5 Years Travel Time.**