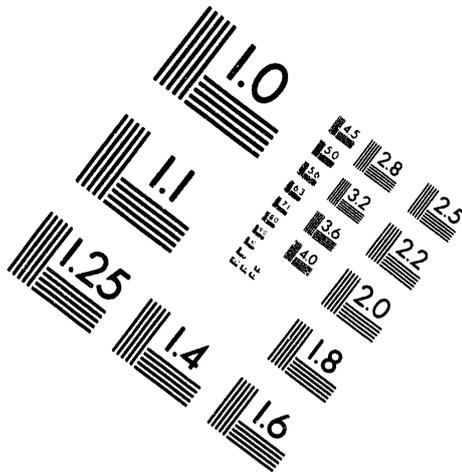
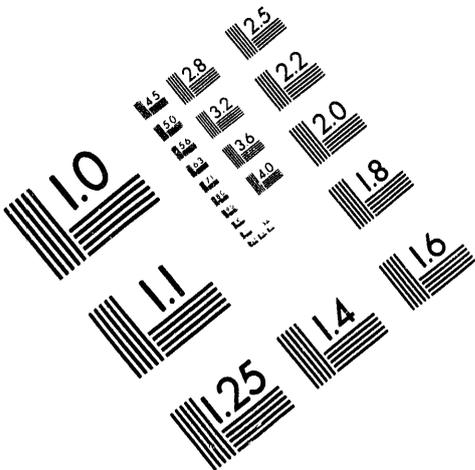




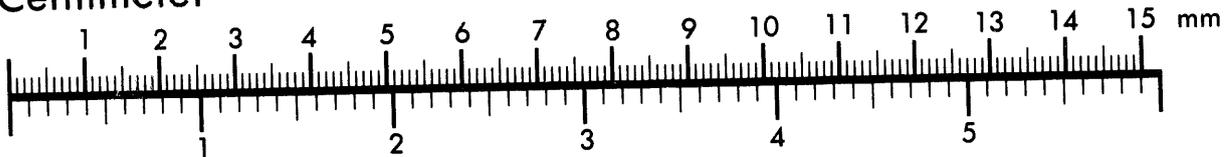
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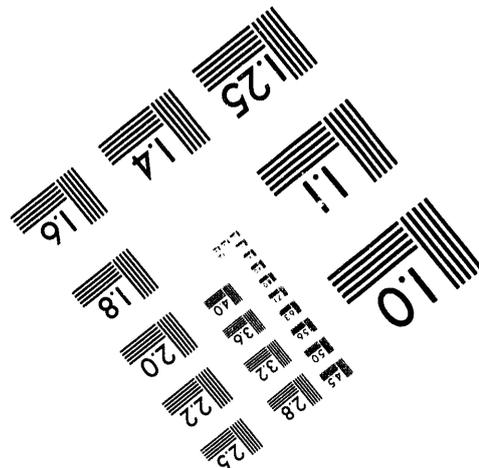
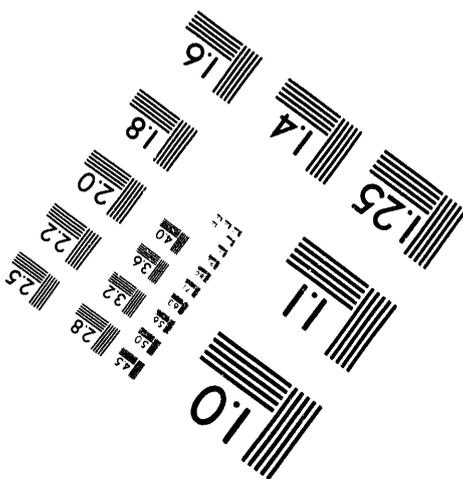
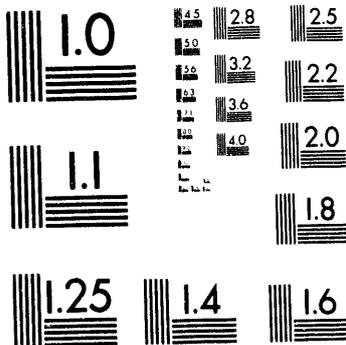
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A Comparison of Geostatistically Based Inverse Techniques for Use in Performance Assessment Analyses at the Waste Isolation Pilot Plant Site: Results from Test Case No. 1

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ABSTRACT

The groundwater flow pathway in the Culebra Dolomite aquifer at the Waste Isolation Pilot Plant (WIPP) has been identified as a potentially important pathway for radionuclide migration to the accessible environment. Consequently, uncertainties in the models used to describe flow and transport in the Culebra need to be addressed. A "Geostatistics Test Problem" is being developed to evaluate a number of inverse techniques that may be used for flow calculations in the WIPP performance assessment (PA). The Test Problem is actually a series of test cases, each being developed as a highly complex synthetic data set; the intent is for the ensemble of these data sets to span the range of possible conceptual models of groundwater flow at the WIPP site. The Test Problem analysis approach is to use a comparison of the probabilistic groundwater travel time (GWTT) estimates produced by each technique as the basis for the evaluation. Participants are given observations of head and transmissivity (possibly including measurement error) or other information such as drawdowns from pumping wells, and are asked to develop stochastic models of groundwater flow for the synthetic system. Cumulative distribution functions (CDFs) of groundwater flow (computed via particle tracking) are constructed using the head and transmissivity data generated through the application of each technique; one semi-analytical method generates the CDFs of groundwater flow directly.

This paper describes the results from Test Case No. 1. Of the five techniques compared, those based on the linearized form of the groundwater flow equation exhibited less bias and less spread in their GWTT distribution functions; the semi-analytical method had the least bias. While the results are not sufficient to make generalizations about which techniques may be better suited for the WIPP PA (only one test case has been exercised), analyses of the data from this test case provides some indication about the relative importance of other aspects of the flow modeling (besides the inverse method or geostatistical approach) in PA. These ancillary analyses examine the effect of gridding and the effect of boundary conditions on the groundwater travel time estimates.

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PREFACE

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**A COMPARISON OF GEOSTATISTICALLY-BASED INVERSE TECHNIQUES
FOR USE IN PERFORMANCE ASSESSMENT ANALYSES AT THE WIPP SITE
RESULTS FROM TEST CASE NO. 1 ***

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ABSTRACT

The groundwater flow pathway in the Culebra Dolomite aquifer at the Waste Isolation Pilot Plant (WIPP) has been identified as a potentially important pathway for radionuclide migration to the accessible environment. Consequently, uncertainties in the models used to describe flow and transport in the Culebra need to be addressed. A "Geostatistics Test Problem" is being developed to evaluate a number of inverse techniques that may be used for flow calculations in the WIPP performance assessment (PA). The Test Problem is actually a series of test cases, each being developed as a highly complex synthetic data set; the intent is for the ensemble of these data sets span the range of possible conceptual models of groundwater flow at the WIPP site. The Test Problem analysis approach is to use a comparison of the probabilistic groundwater travel time (GWTT) estimates produced by each technique as the basis for the evaluation. Participants are given observations of head and transmissivity (possibly including measurement error) or other information such as drawdowns from pumping wells, and are asked to develop stochastic models of groundwater flow for the synthetic system. Cumulative distribution functions (CDFs) of groundwater flow (computed via particle tracking) are constructed using the head and transmissivity data generated through the application of each technique; one semi-analytical method generates the CDFs of groundwater flow directly.

This paper describes the results from Test Case No 1. Of the five techniques compared, those based on the linearized form of the groundwater flow equation exhibited less bias and less spread in their GWTT distribution functions; the semi-analytical method had the least bias. While the results are not sufficient to make generalizations about which techniques may be better suited for the WIPP PA (only one test case has been exercised), analyses of the data from this test case provides some indication about the relative importance of other aspects of the flow modeling (besides inverse method or geostatistical approach) in PA. These ancillary analyses examine the effect of gridding and the effect of boundary conditions on the groundwater travel time estimates.

I. INTRODUCTION

The Waste Isolation Pilot Plant (WIPP) is proposed as a geologic repository for disposal of transuranic radioactive wastes generated by defense programs of the U.S. Department of Energy (DOE). For WIPP to be considered an acceptable disposal site,

performance assessment (PA) analyses must show compliance with the U.S. Environmental Protection Agency's (EPA) 40 CFR 191, Subpart B standard, which regulates the disposal of high-level and transuranic radioactive waste. The EPA standard requires that the analyses account for "uncertainties caused by all significant processes and events" for 10,000 years following disposal. These include uncertainty in models, parameters and the future state of the system. The containment requirements of the EPA standard are, in fact, probabilistically based. The Containment Requirements specify that the probability of the normalized EPA sum of releases of radionuclides to the accessible environment being greater than the limits set in the standard shall not exceed 0.1, and probability of being greater than 10 times the limit shall not exceed 0.001. In accordance with the EPA standard and with safety assessment in general, the analyses used in PA are probabilistically based to account for uncertainty; consequently, the analyses result in a range or distribution of simulation results.

The Culebra Dolomite aquifer of the Rustler Formation above the proposed WIPP repository has been identified as a potentially important pathway for release of radionuclides to the accessible environment¹. Consequently, uncertainties in the models and parameters describing flow and transport in the Culebra need to be addressed in the PA. In March, 1991, a Geostatistics Expert Consultant Group (GXG) was convened to address the issue of characterizing spatial variability and treating uncertainties in the hydrologic and transport processes and parameters in the groundwater flow system at the WIPP site. At that meeting, the recommendation was made to investigate and compare alternative techniques for generating conditional simulations of Culebra transmissivities to evaluate the applicability of these approaches in the WIPP PA. The GXG discussed the development of a "Geostatistics Test Problem" which would be used to compare various geostatistically-based inverse techniques. This paper describes results from the initial phase of the Test Problem investigation.

A. Test Problem Definition

The purpose of the Test Problem is to evaluate various inverse procedures to assist in providing justification for choosing a particular method to use in the final PA of the WIPP. The test will compare the alternative approaches for generating conditional random fields using a series of independent synthetic data sets

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that are intended to span the range of possible conceptual models of the groundwater flow system at the WIPP site. By using a series of synthetic data sets, for which the underlying spatial structure of the parameters and processes are known, the relative robustness of alternative approaches for characterizing the spatial variability in aquifer transmissivity and in treating uncertainty under various conditions can be assessed. The results of the Test Problem should provide guidance to eliminate from further consideration those approaches that consistently perform poorly in terms of simulating system behavior.

The Test Problem analysis approach is to use a comparison of probabilistic groundwater travel time estimates to a known groundwater travel time as the basis for the evaluation. The groundwater travel time performance measure was chosen as a simpler, yet related measure of a site's ability to contain the wastes. The assumption is made that the groundwater travel time is a relative scalar measure of the speed of solute transport for a given model and set of parameters. For a set of simulations using a single model, the distribution of travel times and travel paths reflects uncertainty in the model parameters. By incorporating alternative assumptions into the underlying model, uncertainty in the model can be represented as sets of simulations. The goal of the Test Problem is to incorporate these concepts over the suite of synthetic data sets to evaluate the alternative approaches in way that is consistent with the parameter and model uncertainty observed at the WIPP site.

The Test Problem is based on the generation of a series of independent synthetic data sets that are intended to span the range of possible conceptual models of the groundwater flow system at the WIPP site. That is, the synthetic data sets intend to reflect the type of site characteristics which are thought to possibly exist at the WIPP site (i.e., characteristics either inferred from geological interpretations or conjectured on a weaker yet plausible basis). For example, in the first data set the transmissivity data are generated in such a way that it spans the same degree of magnitude variability and possesses the same type of spatial covariance structure as that estimated from the observed WIPP site data. Other features (e.g., faults, channels, leakage etc.) which may be incorporated into the synthetic data sets are also supposed to reflect plausible geohydrologic characteristics of the WIPP site. Each set may be considered as representing alternative conceptualizations of features that could exist at the WIPP site, with the entire set hopefully spanning the range of possible important features.

Knowledge of both the qualitative and quantitative aspects of the conceptual and mathematical models on which the data sets are built will be limited to a select group of individuals (e.g., hydrologists, geologists), who provide input into the development of each data set. The group of data-set developers may change from set to set, depending on the expertise required to develop each set. Transmissivity and hydraulic head observations are then sampled spatially over an arbitrary domain determined by the data administrator and are then provided to the Test Problem participants without information about the conceptual or mathematical model used in generating the underlying fields. The number of these synthetic field measurements is the same as that collected from the WIPP site. There may or may not be error in the measurements, the scale of the measurements may vary and, in some cases, the data may consist of drawdown measurements at pumping wells and/or observation wells in lieu of sampled

transmissivity values. The Test Problem participants must then analyze the data, develop and implement their respective conceptual and mathematical models, and generate an ensemble conditioned random fields of transmissivity and head using a Monte Carlo or similar procedure. The transmissivity and head simulations are returned to the data administrator, who in turn calculates groundwater travel times and travel paths and compares these to the known travel times and travel paths computed on the synthetic data set. Each stage of the Test Problem repeats this procedure using different conceptual models to generate the synthetic data set. With each stage, the data administrator may go back to the Test Problem participants and request further analyses given more information (e.g., known boundary conditions provided in addition to sampled transmissivity and head).

B. Synthetic Data Sets to Evaluate Alternative Approaches

The conceptual and mathematical models used in PA are, by definition, simplified representations or approximations of the processes occurring at the real site. Consequently, it is not expected that these models will accurately simulate every detail of actual site conditions. Thus, for safety assessment, there must be confidence that model simulations of the relevant processes occurring at the site represent and encompass reality, or, at least, are conservative relative to actual site conditions. In general however, it is difficult to determine *a priori* (except for certain classes of models, parameters and site conditions) whether or not the estimates resulting from these models are, in fact, conservative. Furthermore, because of temporal and spatial scales typical of geologic disposal sites, it is practically impossible to ascertain the accuracy of the model predictions required for regulatory compliance assessment. Because of these practical constraints, analyses necessarily must account for uncertainty.

To evaluate each model's ability to encompass reality, the comparisons in this study are based on *known* groundwater travel times which are each derived from a "synthetic reality." That is, dense synthetic data sets, in which the true groundwater travel time can be determined, can be built using known conceptual and mathematical models. Sparse data can be sampled from these synthetic data sets as it would be for a real site, and using that sampled data, analyses can be conducted in light of uncertainty. The distribution of analysis results can then be evaluated relative to a known system.

Of course the synthetic data sets are constrained by the complexity (or lack thereof) of available mathematical models, computing power, and the imagination of the data set developer. However, an attempt can be made to develop synthetic data sets that represent important characteristics of a given site. While each synthetic data set is not expected to represent, by itself, the extreme complexity of the real world, the analysis of a series of multiple synthetic data sets can provide a means of assessing how robust an approach to modeling the system is for a specified set of conceptualizations. The analysis of these data sets also provides a means of assessing how accurate model simulations of certain site characteristics are likely to be, and, consequently, whether or not the model predictions are likely to be conservative. In addition, we believe that this comparison exercise will provide useful information about the *modeling process* itself which may help guide PA activities in a manner consistent with the goals of PA.

One of the primary objectives of the Test Problem is to evaluate the accuracy of the model predictions relative to the synthetic site, and to determine whether or not they are conservative across various flow system conceptualizations. Another objective is to assess the treatment of uncertainty by the various techniques (i.e., the spread in the output distributions). The former evaluates where the known travel time falls relative to the simulations, whereas the latter evaluates how well the approach encompasses the known travel time in light of uncertainty.

The results of the Test Problem (a series of test cases) are intended to provide evidence as to which inverse techniques are more likely to perform well for the purposes of the WIPP PA. Consequently, the synthetic data sets must "adequately" reflect the type of site characteristics known or thought to possibly exist at the WIPP site. Secondly, the performance measures computed in these test cases must directly relate to the regulatory compliance criteria. And third, the manner of comparing the results from the various methods must be fair, objective, and meaningful for the stated purpose (e.g., comparing transmissivity field estimates, while interesting, is not relevant to PA, whereas comparing travel paths is). Without a doubt, the first of these is the most difficult and challenging aspect of this work. We do not propose that the initial data set, in itself, is an adequate or complete representation of the Culebra Dolomite aquifer properties or Rustler Formation flow system processes. Rather, this first test case represents one conceptualization of how the system may operate. In addition, the first stages serves as a "trial exercise" which we are using as a learning experience for dealing with the type of difficulties that will be encountered in attempting to achieve the stated overall objectives of this work.

II. GENERATION OF THE SYNTHETIC DATA SET FOR TEST CASE NO. 1

The exhaustive data set, or the "synthetic reality," was developed using a model of the Culebra transmissivities which was based on a geostatistical analysis of the WIPP site transmissivity data. The \log_{10} -transmissivity field was modeled as an isotropic process having an exponential covariance structure with a mean $\log(T)$ of -5.5 and as low a variance as the data could reasonably be interpreted to exhibit, a $\log(T)$ variance of 1.5 . The correlation length (i.e., correlation parameter of the exponential covariance model) was 3905 meters, the same as that interpreted from the geostatistical analysis of the WIPP site data. The field was generated on a very fine mesh (over three million nodes for a 40km by 40km square area) using the Turning Bands code TUBA². Figure 1 shows the $\log(T)$ field over the local model area (the inner 20km by 20km region).

The boundary conditions for the regional model were generated using a combination of linear trend surface and spatially correlated residuals. An anisotropic exponential model with zero nugget, a sill of 50m^2 , and range of 5km and 15km in the north-south and east-west directions respectively, were used to model the hydraulic head residuals (these were the parameter values and covariance model type estimated from the WIPP site head data). TUBA was used to generate a mean-zero random field having these semivariogram properties and then the trend surface was added to arrive at the boundary conditions.

The regional model head solution was obtained via a multigrid solver. Dirichlet boundary conditions were imposed



Figure 1. \log -transmissivity field over the local model region; dark = low value, white = high value.

along all four boundaries. The solution was verified by performing a mass-balance analysis independently from the solver program. The regional model head solution is shown in a three-dimensional view in Figure 2; the anisotropy in the correlation structure of the head field is obvious. The local model (central) region is relatively uniform, thus, not likely to cause problems for any of the inverse methods including the linearized techniques. A contour plot of the local model head field along with the hydraulic head sampling locations is shown in Figure 3.

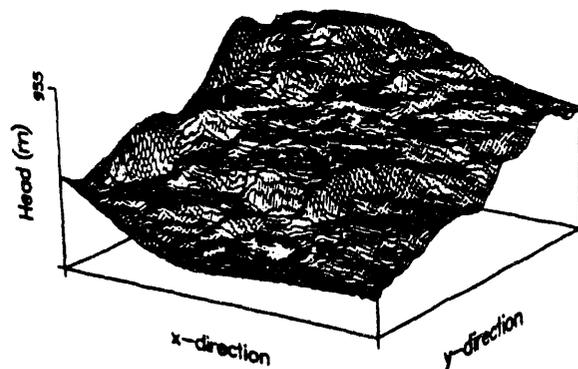


Figure 2. Three-dimensional view of the regional model head solution.

The sampling locations for the $\log(T)$ and head observations were "modeled" after the WIPP site data, i.e., the sampling points for the synthetic site exhibit the same type of geometrical pattern. The sampled data were taken as point measurements without error (a point being the area of one grid block of the synthetic site model). There were 41 $\log(T)$ measurements and 32 head measurements, the same as that collected at the WIPP site.

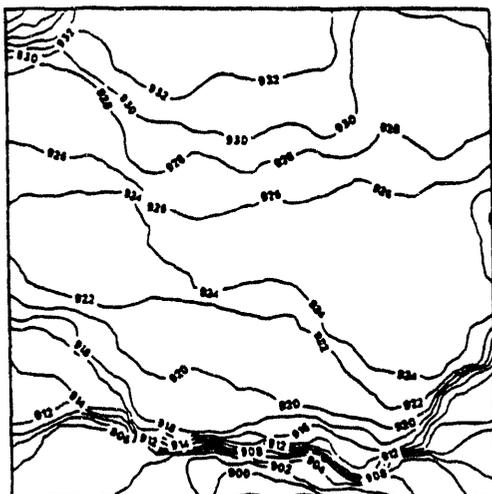


Figure 3. Contours of local model heads and locations of sampling observation points.

Tables 1 and 2 below show that the sampled values reflect the variability of the $\log(T)$ and head fields reasonably well.

Table 1. Statistics of the $\log(T)$ field and sampled $\log(T)$ data.

	Log(T) Field	Sample Data
Minimum	11.1	-8.40
Maximum	0.60	-1.35
Mean	-5.84	-5.30
Variance	1.56	1.36

Table 2. Statistics of the local head field and sampled head data.

	Head Field	Sample Data
Minimum	898.1	917.2
Maximum	940.6	932.8
Mean	922.9	925.4
Std. Dev.	7.9	3.1

III. DESCRIPTION OF TECHNIQUES APPLIED

At least seven geostatistical inverse techniques are planned to be tested, however, to date, only five have provided results for Test Case No 1. It should be understood that the techniques are more general than the codes that embody them. For example, the inclusion of variable density or transient effects may be possible for a particular technique, but the currently available codes may not incorporate these capabilities. A brief description the techniques, as they are currently implemented in the computer codes, follows.

Pilot Point Inverse⁴: The pilot point inverse methodology begins by generating a conditional simulation of the transmissivity field. The flow field is then modeled based on the transmissivity simulation and subjectively determined boundary conditions. If the error in the modeled pressures relative to the observed

pressures falls below a specified least square error criterion, then the initial transmissivity field is retained as a conditional simulation. If the error is too large, synthetic transmissivity data (i.e., pilot points) are added to the transmissivity field to improve the calibration of the groundwater flow field. Adjoint sensitivity analysis is used to determine the locations where additional transmissivity information should be included. The method searches the entire model domain to find potential locations. Once the most sensitive location for improving the calibration is identified and a pilot point is added (using a least square optimization procedure), the flow model is run again, and the error in pressures is recalculated. The iteration of adding pilot points is continued until the least-squared error criterion is met or the addition of more pilot points does not improve the calibration further. The entire procedure is repeated for the number of conditional simulations desired.

Linearized Cokriging⁵: This approach cokriges the transmissivity and head fields and conducts conditional simulations using covariance/cross-covariance models based on field measurements of both transmissivity and head. In the approach, exponential covariance functions are assumed to describe the log-transmissivity and boundary head spatial variability. Cross-covariance between the transmissivity and head fields is developed through linearization of the steady-state flow equation. Linearization is achieved by separating the head and log-transmissivity parameters into deterministic (expected value) and stochastic (perturbation) components, expanding the resulting equation, and neglecting the second order terms (products of perturbations) in the equation. Measured data and the linearized flow equation are used to fit the covariance and cross-covariance parameters using maximum likelihood parameter estimation. Cokriging of the transmissivity and head data is conducted using the resulting covariance models. Simulations conditioned on measured transmissivity are conducted using Cholesky decomposition of the log-transmissivity covariance matrix. Corresponding head simulations are attained through solution of the flow equation using the conditionally simulated transmissivities and prescribed boundary heads. Boundary conditions are constrained to be fixed head, although uncertainty in the boundary conditions can be incorporated.

Linearized Fast Fourier Transform⁶: This approach also uses the linearized form of the steady-state flow equation. However, in the Fast-Fourier Transform approach, the head and transmissivity perturbation components, assumed mean-zero second order stationary, are represented in the spectral domain as Fourier integrals in two-space. The covariances and cross-covariance are also represented in the spectral domain, being functions of the spectral and cross-spectral densities. Independent, mean-zero measurement error (i.e., nugget) can also be incorporated into the model. Fast Fourier Transform is used to calculate the random fields for the transmissivity and head fields. Conditioning is conducted in the classical manner by adding the difference between the unconditional simulation and kriged estimate of the unconditional simulation to the kriged estimate of the field at the data points. Both the transmissivity and head fields are conditioned directly on the observed data. For large fields (large number of prediction points), relatively few calculations are required, making the approach very efficient.

Linearized Semi-analytical Cokriging⁷: This is a semi-analytical approach also uses the linearized form of the steady-state flow

equation to develop cross-covariances. The approach assumes a uniform flow field and an infinite model domain. Covariances and cross-covariances are given analytically. Transmissivity and steady-state head are co-kriged using the analytical covariance models and well-observation data. This approach can treat non-uniform flow by fitting and removing a quadratic trend to the observed mean head field. The approach can similarly treat transient flow if the head field is assumed to change linearly with time.

Self-Affine Fractal Simulation⁴: This approach assumes that the transmissivity field can be described as a statistically self-affine fractal field. That is, the variogram for the two-dimensional transmissivity field is given as a simple power law relationship in which $\gamma(h)$ is proportional to the separation distance h taken to the power $2D$ [$\gamma(h) = h^{2D}$, $D \in (0,1)$]. Using the fractal approach, smaller and smaller scale details can be incorporated in the model by scaling down the observed inter-well spatial variability in a self-consistent, nonlinear manner. Unlike kriging, which generates a smoothed representation of the field and adds variability through addition of random components, the fractal approach directly generates non-smooth realizations using the scaling relationship of spatial variability derived from the data. Because of the nonlinear incorporation of variability over a range of scales, the fractal approach commonly results in channelling of flow and non-Fickian dispersion. The numerical code AFFINITY generates the statistically self-affine transmissivity realizations using the observed data, solves the groundwater flow problem, and conducts tracer injection and tracking. The fractal fields can be generated using either spectral theory with fast Fourier transform, or via iterated function schemes.

IV. RESULTS AND DISCUSSION OF TEST CASE NO. 1

The data received from the participants consisted of multiple (conditional) simulations of transmissivity, the corresponding head fields, and a description of the field geometry and discretization. Groundwater travel times were computed via a particle tracking procedure using the PATH3D code³. The code uses a fourth-order Runge-Kutta solution capable of automatic stepsize adjustment to achieve a specified level of accuracy. The groundwater travel times were computed for ten release points within each realization. The ensemble of realizations was used to construct cumulative distribution functions (CDFs) of groundwater travel time for each release point. In the semi-analytical approach, these CDFs (for only four of the ten release points) are generated directly, hence no transmissivity or head fields are produced.

The one "true" groundwater travel time was computed from the release point out to a distance of 5km in radius using the exhaustive (synthetic) data set (and a constant porosity of 0.16). The objective was to compare the distribution of travel times obtained from each technique with the known travel time. Three characteristics of the travel time CDFs were used for the comparison: 1. accuracy (or bias), 2. precision (or spread), and 3. peakedness (or kurtosis). Accuracy is a measure how close to the true value the estimates lie while the precision, or spread, measures the degree of uncertainty in the estimates. The peakedness measure reflects exactly that - how peaked the probability density function (PDF) is; the more peaked the distribution, the greater percentage of the time the predictions will fall within a narrow range of travel times (relative to the range of the

PDF). It is desirable to have the bias measure close to zero and the measure of spread as small as possible. For example, it would be more desirable to have a precise (narrow) distribution exhibiting a small amount of bias, than an imprecise but "accurate" (centered on the true value) distribution. Similarly, the more peaked of two distributions, each having roughly the same amount of spread and a relatively small amount of bias, would be the more desirable one.

The accuracy was assessed by using the Tukey tri-mean (the sum of the .25 quantile plus twice the median plus the .75 quantile, divided by four) as a measure of central tendency and comparing that to the true travel time. A non-dimensional measure of accuracy (or bias) was computed by subtracting the true travel time from the Tukey tri-mean statistic and dividing by the true travel time. Thus, a negative bias implies shorter travel times and hence, a conservative result. A dimensionless measure of the spread in the CDFs was computed by subtracting the .05 quantile from the .95 quantile and dividing by the true travel time. By chopping the tails off the distributions in measuring the spread, we may be introducing some bias into the comparison, however, at the time this analysis was performed, we did not have estimates for the extreme tails from one of the techniques. The peakedness was assessed as the quotient (interquantile range) / (.95 quantile minus .05 quantile). Hence, the smaller the peakedness measure, the more peaked the distribution is.

In Figure 4, the bias is plotted on the abscissa and the spread is plotted on the ordinate. The numerical values on the graph are unitless and only serve to show the relative performance among the techniques. Each point on the graph of Figure 4 represents the bias and spread measures of the CDF for a particular release point. The bottom plot reveals more detail where the data are tightly clustered.

The results from this test case appear to show that the linearized techniques (linearized cokriging, linearized FFT, and semi-analytical) generally exhibit less bias than the methods that do not invoke the assumptions in the linearized approach (uniform flow, stationarity, small perturbations etc.). Because the data are not sufficient to draw definitive conclusions based on this one test case, we can only conjecture as to whether this is a general result and why this might be true. It is true that the synthetic data set was developed using geostatistical and flow model perfectly consistent with those used in the linearized techniques. The question which comes to mind is, would we have found the opposite result if the synthetic site were developed using non-stationary models with higher variability?

Most noticeable are the plotted points from the Fractal approach, most of which are nonconservative, and the Pilot Point approach, all of which are nonconservative. It should be understood that this is but one test case and the results should not be considered as applying in general. While time for investigative analyses was limited, we did attempt to look at these cases a little further to examine why this result occurred. One difference between the linearized methods and these approaches is the assumption of stationarity used in the linearized methods. Because of that assumption, those variogram models have a sill; this limits the amount of variability the estimates will have as the estimation point moves further away from observation points. The Fractal approach uses a power-law variogram and, in the Pilot Point method, an IRF-0 (linear variogram) was used; these

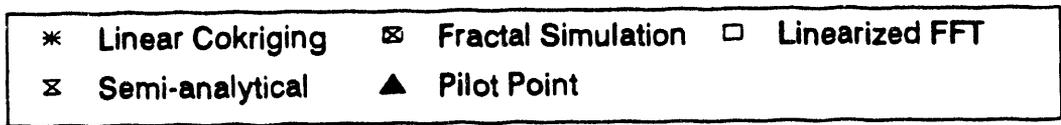
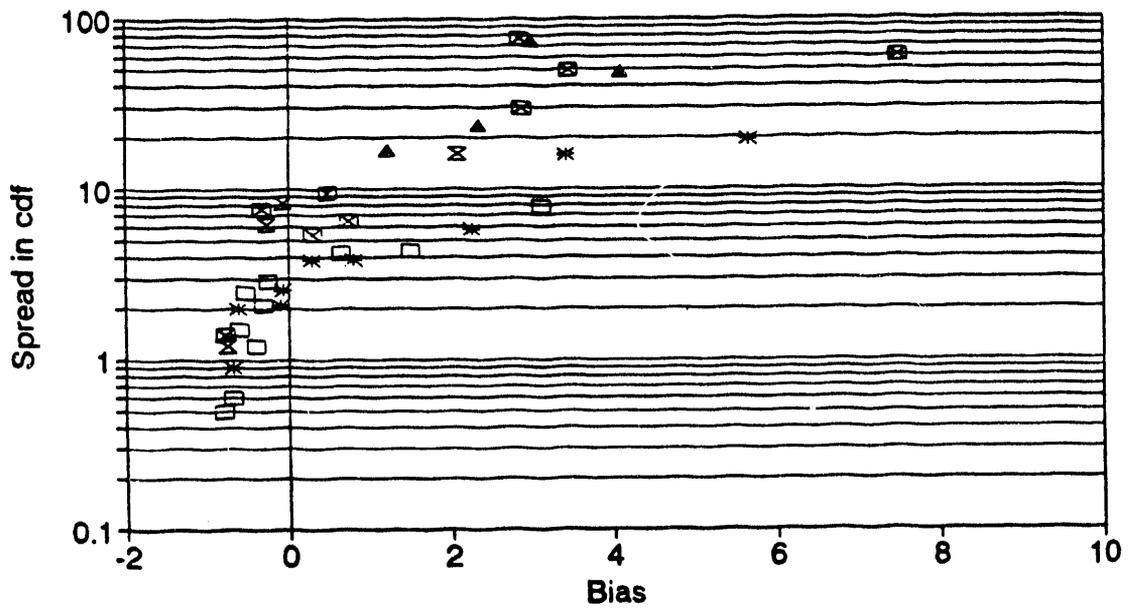
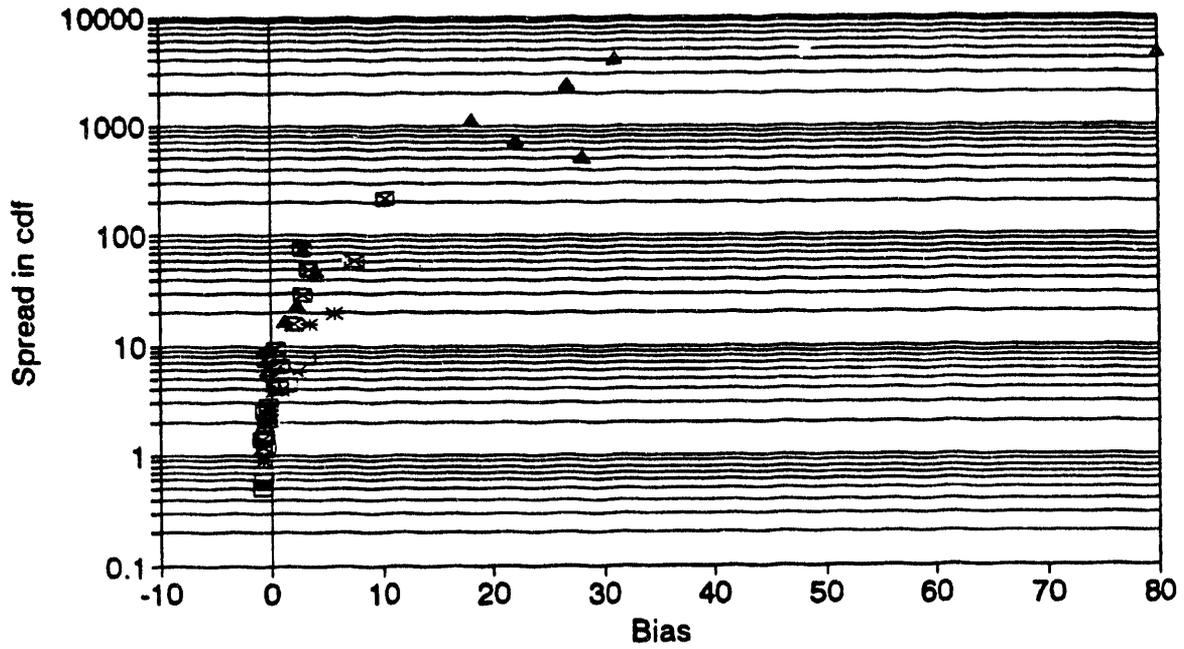


Figure 4. Bias and spread measures of the groundwater traveltime cdfs. Each point represents the bias and spread characteristics of the cdf for a particular release point and inverse method.

models will allow a trend to continue without bound^o thereby possibly leading to divergent estimates in areas lacking in nearby observation points. This could partially explain the higher spread in the CDFs associated with the Fractal and Pilot Point results, but does not explain the systematic bias in those results. Table 3 shows the number of paths with positive versus negative bias for each technique (excluding the Semi-analytical approach which estimated travel times at only four points).

Table 3. Number of travel paths with negative versus positive bias measures.

Technique	Negative	Positive
Linear-Cokriging	4	5
Linearized FFT	6	4
Fractal Simulation	2	8
Pilot Point	0	10

It would be reasonable to expect flow paths occurring in areas far removed from observation points to be associated with travel time CDFs having more spread, however, we did not find this to be true. We replotted the graph of Figure 4 (not shown here) along with an additional label at each point, the label being a measure of "proximity of particle flow path to nearby observation points." We used the kriging error (from the Linearized Cokriging approach) at the release point for this measure; thus, small kriging error implies close proximity while a larger error implies it's in an area of sparse data. We did not find any relationship between "location of travel path relative to observation points" and either spread in the travel time CDF or bias in the CDF estimate. While the number of, and proximity to, observation points certainly aids the estimate of the transmissivity field, this finding suggests that it is aspects of the flow modeling other than data-control points and spatial variability model that leads to the result shown in Figure 4. We can only surmise that perhaps boundary conditions or gridding may be partially responsible. We did investigate the effects of the boundary conditions and gridding scheme on the CDF estimates; these analyses are described in the sections below.

We did find a strong correlation between the log-transmissivity of the simulated fields at the particle release points and the groundwater travel times. We plotted, in Figure 5, the

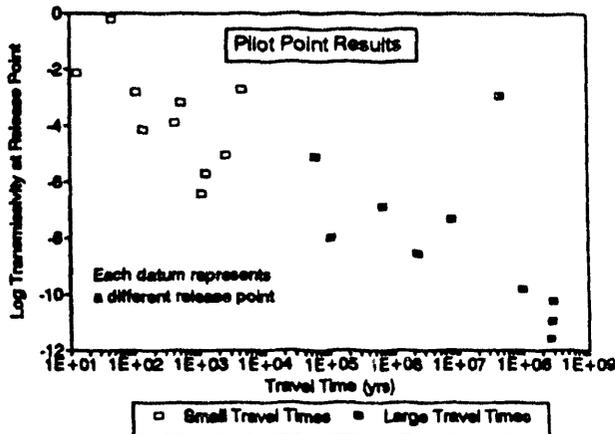


Figure 5. Relationship between release-point transmissivity and groundwater travel time.

Pilot Point log-transmissivity value at the particle release points versus the groundwater travel times for those simulations corresponding to the shortest and longest travel times at each release point. Not surprisingly, the travel time increases as the transmissivity at the release point decreases. Does this imply (together with Figure 4) that "most of the time" the Pilot Point log-transmissivity estimate at the particle release points is too low? If so, why does this occur?

If the geostatistical model and its relationship to the distribution of sample points versus the estimation point (e.g., the extension of a trend in the IRF-k modeling approach) were responsible for this "errant behavior," then one would expect to find that the particle release points were mostly located in preferentially low-transmissivity zones (in the synthetic site model). However, we did not find this to be true. Five of the release-point transmissivities were above the median value of the exhaustive data set for the local model region, and five were below; all of the release-point transmissivities were contained within the interquartile range of the exhaustive data set. This finding supports the idea that it may be aspects of the flow modeling other than data-control points and spatial variability model that leads to the result shown in Figure 4. This hypothesis could be tested as the Pilot Point methodology is not restricted to using only Generalized Covariance models.

Because the bias and spread measures vary dramatically from point to point, we decided to look at the ranks of the bias and spread measures to compare the overall performance of each technique across the entire field (over all release points). Using the data in Figure 4, we converted the bias and spread measures for each release point to ranks and then plotted, in Figure 6, the average rank values. These results show that the Semi-analytical approach had the least bias and the Linearized FFT the lowest uncertainty. The reader should be reminded that these are the results from one test case, and in particular, a case which has characteristics that favor the linearized methods. No generalizations regarding the superior or inferior performance of one technique over another should be construed from these results.

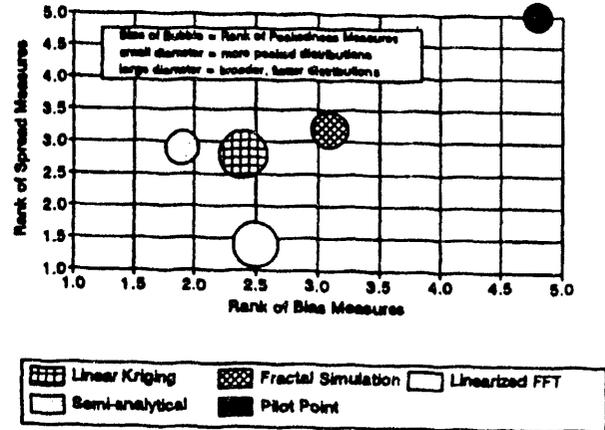


Figure 6. Average ranks of bias and spread measures.

A. Other Factors That Contribute to Groundwater Travel Time Error

While the Test Problem was developed to compare methods of conditional simulation of the Culebra transmissivities, the manner of testing the efficacy of the various techniques in generating these fields involves procedures (e.g., gridding, generation of boundary conditions, etc.) which affect the performance measure in some way. The analysis is thus more complicated than simply comparing one travel time against another. It is possible that the results from this comparison study may show that other aspects of the modeling process are equally or more important than transmissivity field characterization. For example, what is the relative importance between the correct boundary condition specification and the correct transmissivity field description? And how important is it to account for leakage, faulting, three-dimensional or non-equilibrium effects? We began to investigate some of these questions using the results from Test Case No 1.

In this first test case, all of the conceptual models were described by two-dimensional, confined, steady-state flow; all of the numerical methods used Dirichlet boundary conditions all around their model domains. Thus, the error in groundwater travel time estimates can arise from primarily three sources: 1. incorrect transmissivity field specification, 2. incorrect boundary condition specification, and 3. the resolution of the grid. We examined all three of these sources as described in the sections that follow.

Grid Resolution: The modeling domain was left to the discretion of the modeler; all of the participants modeled a region covering approximately 320 square kilometers. The gridding used in the models varied from as coarse as 32 x 38 to as fine as 128 x 128. The grid block sizes varied from 125 meters on a side to as large as 900 meters. In contrast, the grid block size used in the synthetic site model was 22 meters on a side. The error introduced from estimating average properties and computing flow velocities over larger grid blocks was assessed as follows.

Early in the analysis, we noticed what was thought to be an anomalously long travel time (214000 years) in one realization from the Linearized Cokriging simulations. So we chose that realization to examine the effect of gridding on the travel time estimate. We superimposed a fine mesh of size 705 x 833 over the original coarse mesh which was 32 x 38 in size, yielding nodes of the same size as that used in the synthetic site model. We then assigned the transmissivity of the fine mesh the value at the corresponding location in the coarse mesh (An alternative approach would be to go from the fine mesh of the exhaustive data set to a coarse one, but this would have involved finding an appropriate average for all the fine grid blocks falling within one of the larger coarse grid blocks, i.e., it would be a different problem being solved, hence the ability to evaluate the effect of gridding alone would be lost.). We did the same for the corresponding head solution and used those values for the boundary conditions. The multigrid solver was used to obtain the solution on the 705 x 833 grid and the particle tracking was carried out as before.

The normalized travel times for these two cases are plotted in Figure 7; the cross-hatched vertical bars are nearly the same height for all of the release points indicating only minor

differences in the travel time estimates. We found that the difference in travel times ranged from 2 to 25 percent (using the fine grid solution as the base value) with an average of 8.8 percent. Some differences were small, some were large; the large errors were almost always associated with shorter travel times on the fine grid. This is because in the finely discretized model, the particles will follow the high permeability channels, finding their way around the low conductivity regions - a more tortuous, yet faster movement through the system.

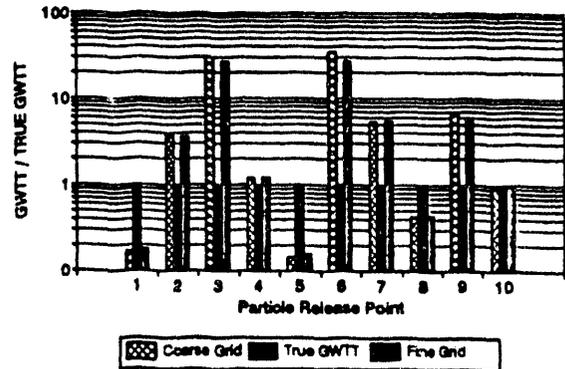


Figure 7. Normalized groundwater travel times for coarse and fine grid discretization.

Incorrect Transmissivity Field: We took the same, highly discretized (705 x 833) transmissivity field described in the previous section, and applied the head solution values from the synthetic site model as the boundary conditions. Thus, this case corresponds to the same grid resolution and the exact same boundary conditions as the synthetic site model; the only difference is in the transmissivity field. We reran the multigrid solver and carried out the particle tracking as before and found errors in travel time ranging from -2125 percent to 84 percent. Thus, even with known boundary conditions specified all around the boundary, incorrect transmissivity field characterization can lead to significant travel time errors. These results are plotted in bar graph form along with the results of the "opposite case" (where the exact transmissivity is used with incorrect boundary conditions) as described in the next section.

Incorrect Boundary Conditions: Here we used the "true" (the synthetic site's) transmissivity field and applied the boundary conditions from the Linearized Cokriging realization described above in the section on grid resolution. Thus, for this case, both the grid resolution and the transmissivity field are specified exactly as in the synthetic site model - the only difference comes from the boundary conditions. We reran the multigrid solver and carried out the particle tracking as before and found that the errors in travel time ranged from -100 to 6355 percent. Thus, even when the transmissivity field is characterized perfectly, without the appropriate boundary conditions specified, the travel time estimates can be significantly in error. Both of these cases (true transmissivity field with incorrect boundary conditions and true boundary conditions with incorrect transmissivity field) are plotted together in Figure 8. The plot appears to indicate that knowledge of boundary conditions (for a case like this with Dirichlet boundaries prescribed along all boundaries) is more

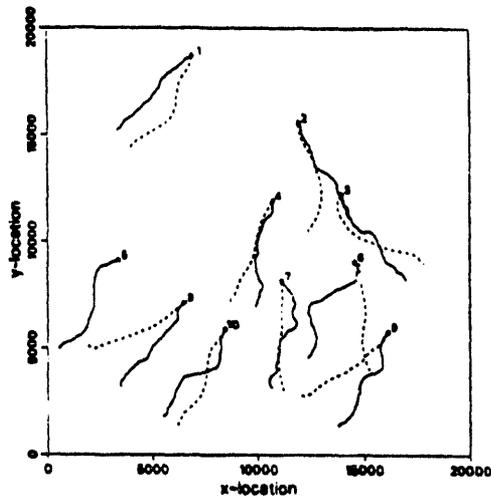


Figure 11. Travel paths - Linearized Cokriging.

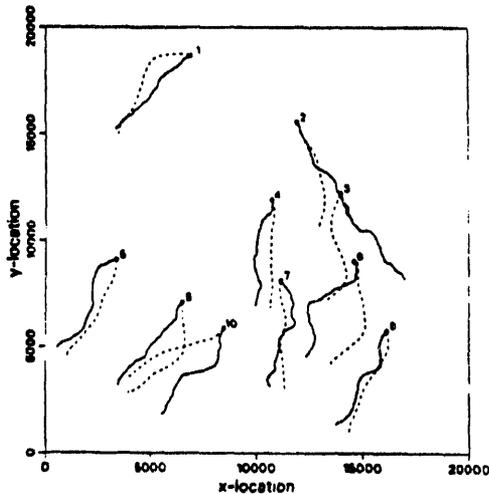


Figure 12. Travel paths - Linearized FFT.

V. SUMMARY AND CONCLUSIONS

A Geostatistics Test Problem is being developed to evaluate a number of inverse techniques that may be used for flow calculations in the WIPP PA. The Test Problem analysis approach is to use a comparison of probabilistic groundwater travel time estimates produced by each technique to a known groundwater travel time as the basis for the evaluation. The Test Problem is actually a series of test cases, each being developed as a highly complex synthetic data set; the intent is for the ensemble of these data sets span the range of possible conceptual models of groundwater flow at the WIPP site.

The first synthetic data set was developed as a very finely-discretized field of hydrologic properties (transmissivity and hydraulic head) exhibiting characteristics similar to those that have been observed, interpreted or inferred from data taken at the WIPP site. Observations of these properties of the synthetic site were sampled using the same number of observations and

similar geometric arrangement as those taken at the real site. The Test Problem participants analyzed these data as they would data from a real site and developed models to simulate groundwater flow across the synthetic site. Five different geostatistical-inverse techniques were used in the analysis of this first test case. Three were based the linearized form of the groundwater flow equation and used stationary models to characterize the spatial variability of hydrogeologic properties; the other two did not have this restriction and used non-stationary models to characterize the variation in hydrologic properties. With the exception of one technique, all produced multiple conditional simulations of transmissivity and then solved the groundwater flow equation to obtain the corresponding head fields.

A particle tracking technique was used to compute groundwater travel times from 10 release points; the ensemble of travel times computed for each release point was used to construct a CDF of groundwater travel time for that release point. The "true" groundwater travel time was calculated using the exhaustive (synthetic) data set. The Tukey Tri Mean was used as a measure of central tendency and a non-dimensional measure of the bias in the CDF was computed by subtracting the true travel time from the Tukey Tri Mean and dividing by the true travel time. Additionally, a non-dimensional measure of spread in the CDF was computed by dividing the range of travel times between the .05 and .95 quantiles of the CDF by the true travel time.

The bias and spread measures for each technique over the 10 release point locations were plotted on a single graph. The plot showed that, in general, the three linearized techniques exhibited less bias and less uncertainty (spread) than the methods which do not invoke the assumptions used in the linearized approach. The reason for this *may* be due to the fact that the synthetic site model was generated to exhibit characteristics perfectly consistent with those used in the linearized methods (approximate uniform flow, low variance, stationary log-transmissivity field). However, the data are insufficient to determine if this is a general result.

Analyses were performed to investigate possible causes of the systematic bias in the CDFs from the Pilot Point approach. The analyses did reveal a strong (negative) correlation between the estimated groundwater travel time and the transmissivity at the particle release point. An unresolved question is why [does it appear that] the estimated transmissivity at the particle release points is preferentially low? While no particular cause for the bias was identified, the analyses did provide some indication of what was probably *not* the cause. The results from these analyses suggest that it is something other than the geostatistical approach used to model the spatial variability; to determine whether this is true, the Pilot Point technique could be rerun using an alternative geostatistical model.

Additional analyses were performed to investigate the significance of other factors that may contribute to error in the groundwater travel time estimates. Three primary sources of error were noted: i) incorrect transmissivity field characterization, ii) incorrect boundary condition specification, and iii) the grid discretization. Of these three, the magnitude of the travel time error resulting from differences in grid mesh density was determined to be the least significant, relative to the bias and the range of differences in the travel time estimates among the techniques. The errors associated with not having specified the boundary conditions correctly were found to be greater than the errors associated with

important than correctly characterizing the transmissivity field. At particle release point No 8, the groundwater travel time for this case (not visible in the plot) is three orders of magnitude lower than the true value.

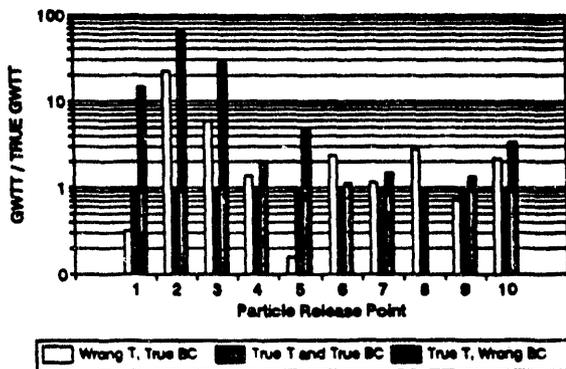


Figure 8. Normalized travel times for: i) wrong transmissivity and true boundary conditions and ii) true T with wrong BC.

To further investigate how knowledge of boundary conditions can affect the travel time results in the modeling that is typically done (coarse grids), we reran the suite of Monte Carlo simulations for two of the inverse methods (Linearized Cokriging and Fractal Simulation) using the correct boundary condition information from the reference model. That is, we computed an arithmetic average of the true-solution head values over all fine-grid nodes falling within each boundary-node block of the coarse grid and reran the inverse procedures using those boundary conditions. In the Linearized Cokriging method, the transmissivity field is conditioned on the heads directly using the boundary condition information. In the Fractal Simulation approach, the transmissivity field is conditioned only on the observed transmissivities, and then the boundary conditions are derived using an optimization algorithm. The results for these two techniques are shown in Figures 9 and 10; as before, each point in these plots represents the bias and spread measures for a groundwater travel time CDF at one particle release point.

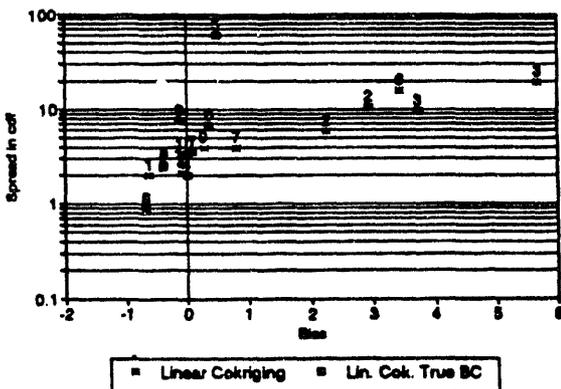


Figure 9. Reduction in bias and spread with application of true boundary conditions - Linearized Cokriging method.

The numbered label above each plotted point designates which particle release point that datum describes. Note that, in both Figure 9 and Figure 10, in almost every case, the absolute value of the bias decreases and the spread decreases for the case with the known ("true" as defined on the coarse grid) boundary conditions applied. This result is most obvious for release points 3, 6 and 8 in Figure 9 and points 5, 7, 8 and 10 in Figure 10; in some of these cases the uncertainty (spread) increased when the known boundary conditions were applied. For both methods, the boundary condition uncertainty has been reduced, so the reduction in spread is expected. The corresponding reduction in bias shows the significance of properly characterizing the boundary conditions.

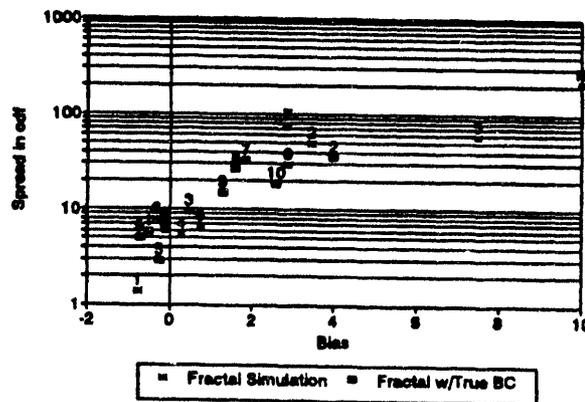


Figure 10. Reduction in bias and spread measures with application of true boundary conditions - Fractal Simulation method.

B. Particle Pathline Analysis

The plot of Figure 4 shows errors in travel time estimates up to two orders of magnitude (in units of "true travel time"). The question which comes to mind is, what is the correspondence (if any) of the particle pathline error to the travel time error? To determine if there is any correlation between accuracy in the travel time estimate and accuracy in the travel path, we computed, for each release point, the travel path from that realization having the closest travel time to the true travel time. These pathlines are plotted in Figures 11 through 14 (the dashed lines) along with the true travel path (solid line).

Note that each plot displays particle pathlines from 10 different realizations. It appears that the pathline error for all of the approaches is approximately the same; all perform reasonably well over most of the domain with the exception of a few outliers. The Linearized Cokriging pathlines are very close to the true paths except for release points 1, 3, and 5; the dashed line ends at the boundary of grid for point No 5 (short of the 5km radial distance).

The travel times of those paths which deviate markedly from the true path are very close to the true travel time. The median travel paths were also plotted (not shown here); those travel paths appear to be about as accurate as the ones plotted in the figures below. These results suggest that accurate travel times do not imply accurate travel paths and vis-a-vis.

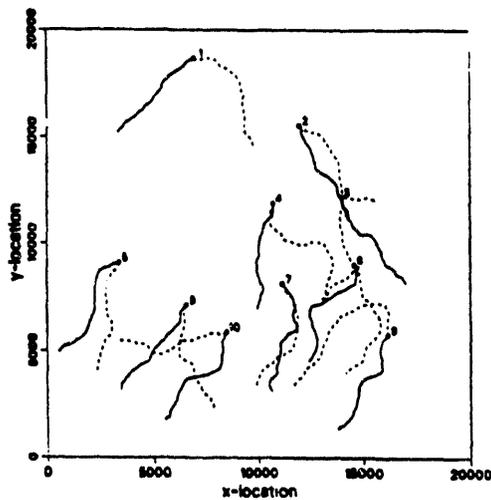


Figure 13. Travel paths - Fractal Simulation.

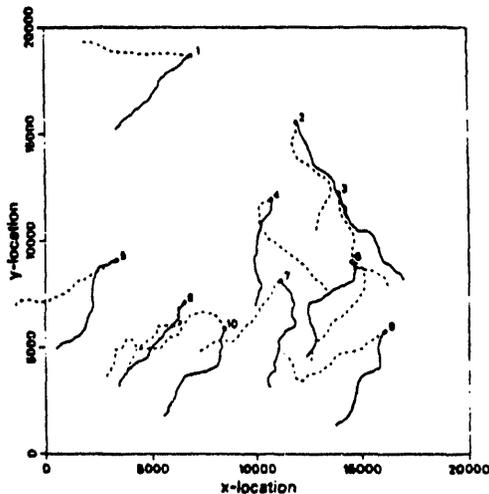


Figure 14. Travel paths - Pilot Point.

incorrectly characterizing the transmissivity field (for one particular field).

A cursory examination of the travel paths showed no correlation between travel time accuracy and travel path accuracy. The results of all of these analyses suggest that relying strictly on "head matching" for calibrating these flow models is not sufficient for ensuring "a likelihood" of accurately predicting either the flow paths or the travel times. All of the techniques are designed to reproduce the observed heads with a minimum of error, yet all exhibit large errors in both travel time and travel path.

At this stage, it would be premature to begin making conclusions or even generalizations based on the limited amount of data analyzed (one test case). Furthermore, this first test case has served more as a learning experience in which mistakes are made and problems had to be overcome. For example, in attempting to adhere to the plan of developing the synthetic site data in a manner that reflects characteristics of the WIPP site, it was

somehow overlooked that the correlation length of the exhaustive log-transmissivity field was large. If the correlation scale of all the simulated fields were much smaller, it might be reasonable to invoke the ergodic hypothesis and consider the results for these 10 particle paths equivalent to those that would be obtained over an ensemble of such fields. However, the correlation scale is large relative to the area covered by the particle pathlines, thus, it is difficult to quantify the magnitude of the errors that might be expected "on average."

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