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QUANTIFICATION OF TRAVEL PATH UNCERTAINTY BY GEOSTATISTICAL SIMULATION

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Introduction

There are many risks associated with the storage of nuclear or other toxic wastes. One of the major risks is the escape of material from the repository. No matter how well a storage facility is engineered, the potential escape of dangerous material must be studied. This kind of study will include some estimation of the "travel path" of the particles. The travel path of a radio-nuclide particle will depend on the geological and hydrological parameters of the surrounding rocks. These parameters must be estimated from a limited number of samples available within the study area. Any estimation will — of necessity — contain a certain amount of uncertainty or "estimation error". This uncertainty will be carried through to the analysis of potential movement of particles, so that the estimated travel path itself will be subject to some error. This paper presents an approach which may lead to a quantification of the uncertainty on the predicted travel path.

A case study is presented, focussing on the Pennsylvanian aquifer in the Palo Duro Basin, Texas. This aquifer underlies a site which has been considered for a potential high level nuclear waste repository. Our discussion centres on one parameter only, the potentiometric level within the aquifer and how this affects the likely travel path. The values of this parameter are estimated over the study area, together with the uncertainty associated with the estimation. Likely deviations from these estimates are analysed using simulation methods. Both estimation and simulation are carried out using geostatistical techniques. This presentation also includes a brief comparison between traditional geostatistical methods and a multivariate estimation including parameters from other aquifers in the same area.

Estimation of Potentiometric Levels

The area of study lies in the northern portion of Texas in the Panhandle region, and includes a minor to the west in New Mexico. 109 boreholes intersecting the deep brine aquifer called the Pennsylvanian were available for analysis. The data are potentiometric or piezometric values from the aquifer which is 8,000 feet below ground surface. These values are expressed as elevation in "feet above sea level" in a well at that location. The locations of the boreholes are shown in Figure 1.

Deaf Smith County in northern Texas was a possible site for a future high-level nuclear waste repository. The Pennsylvanian aquifer underlies the salt bed which would be a host for such a repository (cf. Bair et al 1985). The analysis of the underlying aquifers is a vital component in the characterisation of this site, because a breach of the repository would cause hazardous material to be released into the aquifers. Because fluids tend to flow from areas of higher potentiometric levels to lower level, the study of this parameter is essential to the estimation of potential travel paths. Other parameters must be considered for the estimation of flow rates and travel times. This topic is outside the scope of the present discussion.

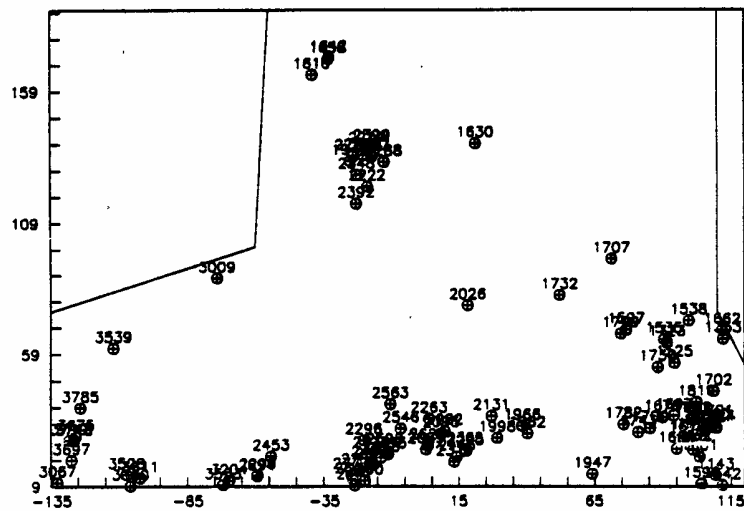


Figure 1 — Locations of boreholes in Pennsylvanian Aquifer

The data used in this analysis were collected and filtered by Stone & Webster Engineering Corporation under contract to the Office for Nuclear Waste Isolation (ONWI). This data is available in the public domain and represents the flow system within the aquifer at steady state conditions before oil and gas production (Bair et al.). The potentiometric level within the aquifer has been treated as a "two dimensional" variable for the purposes of our analysis, with no consideration being given to possible fluctuations within the aquifer in a vertical direction.

Since a geostatistical analysis was used to estimate the complete potentiometric surface, a semi-variogram was constructed from the sample data. Investigation in various directions revealed that a strong trend was present on the surface. This is not surprising with this type of variable and indicates a strong flow direction, generally to the north-east within the study area. Removing the trend with a common Polynomial Trend Surface technique, allows semi-variograms to be constructed for the residuals from the trend surface. These are seen to be isotropic, allowing a semi-variogram model to be fitted to the experimental semi-variogram. The model used is a Spherical semi-variogram with a range of influence of 50 miles, a sill on the spherical component of $46,000 \text{ (ft)}^2$ and a nugget effect of $11,000 \text{ (ft)}^2$. This model was confirmed by a cross validation study using Universal Kriging to include the form of the known trend over the study area. A fuller description of this study may be found in Harper et al., 1986.

Once a semi-variogram model has been fitted to the sample data over the study area, this model — combined with the original sample data — may be used to estimate values at selected locations within that area. To produce a map of the area it is usual to estimate values at the nodes of a square grid laid over the area of interest. The size of the grid is usually a compromise between the amount of computer time taken for the estimation and the amount of detail which is necessary on the final map. Figure 2 shows a contour map which was constructed on a 5 mile grid laid across the study area indicated in Figure 1. The map also

shows the approximate site of the planned high level nuclear waste repository. The solid line which has been superimposed on this map is the 'most likely' travel path of a freed radio-nuclide if the repository was breached. That is, this line follows the steepest slope of the potentiometric surface away from the site location. The path comes to a stop in an estimated local low point in the Amarillo basin. This would generally be quoted as the travel path in a report. There are two problems with this prediction which we shall discuss here.

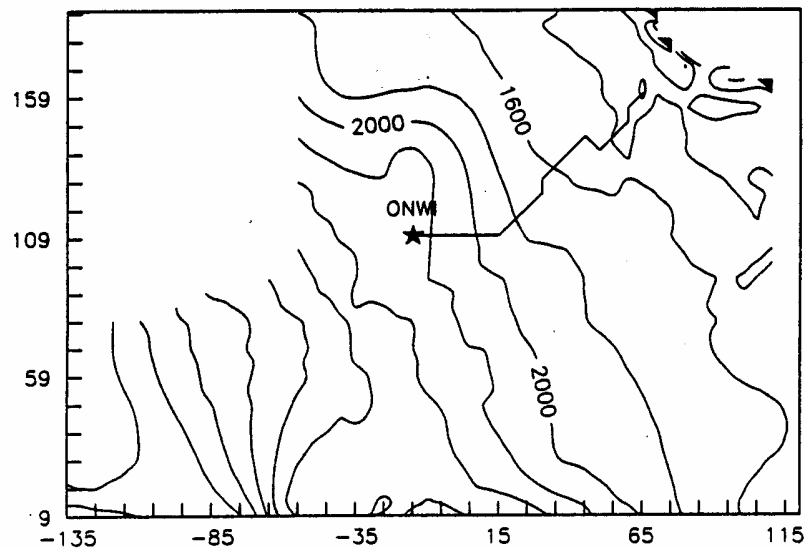
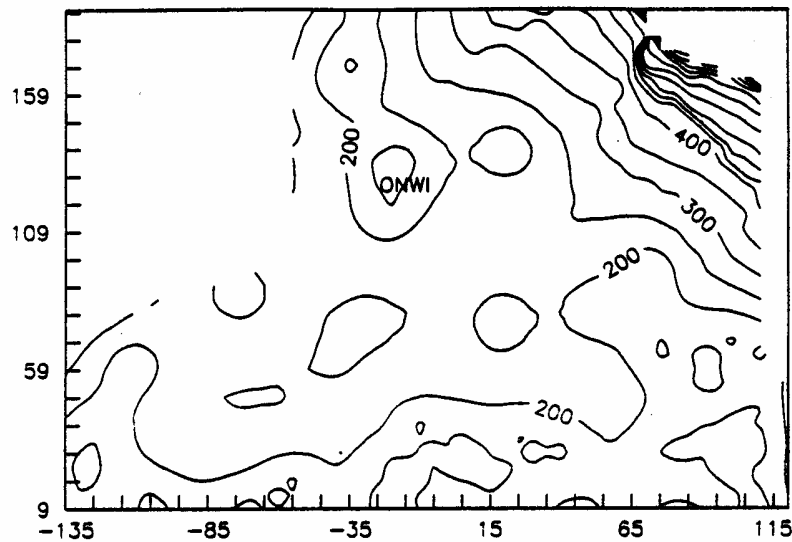


Figure 2 — Estimation of Potentiometric Level

Uncertainty on the estimated surface

When a value is estimated by a geostatistical method, like Universal Kriging, two figures are produced. A Kriging technique produces an estimator formed from a linear combination of the surrounding sample values. The particular linear combination used is that which minimises the "estimation variance" associated with the prediction. This quantity is the variance of the difference between the "actual" value at that location and our estimate of it — given our model of the parameter semi-variogram. This estimation variance may be related, through its square root, to the traditional notion of "standard error" of an estimation. In short, then, each estimate is accompanied by a second value measuring the potential error or uncertainty at that location. If we produce a grid of values, such as the one which was used to construct Figure 2, then we also produce a grid of standard errors. Thus a second map may be constructed showing the uncertainty of the first estimated map. Figure 3 shows the standard errors associated with the construction of the map of potentiometric levels in Figure 2. We have used the term "standard error" here to denote the square root of the estimation variance produced during the Universal Kriging estimation process.

Figure 3 — Standard Errors Associated with Universal Kriging



It can be seen from Figure 3 that the errors are lower in the area around the proposed repository, but rise sharply away from this location. In particular, they rise precipitously towards the north-east – the very direction in which we expect a freed particle to move. The uncertainty associated with the travel path in this case rises almost proportionally to its distance from the proposed repository. The solid line in Figure 2, then, can be seen to be merely a "best estimate" subject to a great deal of potential error. We seek some way to relate the standard error on the predicted potentiometric levels to the uncertainty on the direction of travel of a radionuclide particle.

It has been proposed that simulation may hold the key to the problem of quantifying the uncertainty on the travel path. Two major approaches have been proposed. Several previous papers (cf. Clifton & Neuman (1982), Dagan (1985), Devary et al. (1985)) suggests that simulation of the fluctuations around the surface can be carried out using the standard errors as shown in Figure 3. This approach would restore the "stochastic" roughness of the surface to the smooth kriged grid and allow a travel path to be calculated. If many simulations are carried out, many possible travel paths will result producing a "fan" of possible destinations for a freed particle. This process requires a simultaneous multivariate simulation of the errors at each point on the estimation grid. A covariance matrix must be constructed between the errors at each node of the grid and a realisation from this covariance matrix simulated. A direct implication of this approach is that the errors at the grid points must be multivariate Normal. This approach may also prove unwieldy in operation, since the simulation of a 12 by 12 grid of points requires the simulation of a multivariate Normal from a 144 by 144 covariance matrix.

An alternative approach is to simulate the complete surface at all grid points with the spatial structure of the original parameters and the actual borehole values at those locations. This is known in geostatistics as "conditional simulation" and is well documented in the geostatistical literature (cf. Journel and Huijbregts (1978) and (1979)). The underlying assumptions to geo-

statistical conditional simulation are of Normality for the original variables and of a particular model for the semi-variogram of this data. In a case such as the Pennsylvanian, where a strong trend exists, these assumptions apply to the residuals from the trend surface. Should the data be non-Normal, it is simple to a transformation on the original data, construct the semi-variogram on this and then back-transform once simulation has been carried out. A comparison of the two approaches to simulation is in preparation (Harper & Clark, 1989) and will not be discussed here. This paper discusses the latter "traditional" conditional simulation approach — that is, we simulate a surface which has the same spatial and statistical structure as the original data and takes the actual data values at the actual sample locations. The simulated surface will have the same roughness as the original parameter data. If many surfaces are simulated, an idea of the sensitivity of the travel path may be gained.

The Travel Path Fan

In addition to the "statistical" uncertainty on the travel path of a freed radionuclide, we would like to discuss another source of uncertainty which does not seem to have been considered in the literature. The most likely travel path has been illustrated in Figure 2 - as a single solid line leading down the steepest slope on the potentiometric surface. A simple intuitive analogy would be that of water in a stream, which always follows the steepest path open to it. However, this may be a simplistic analogy. All we know for certain is that flow will take place from a higher potentiometric level to a lower one.

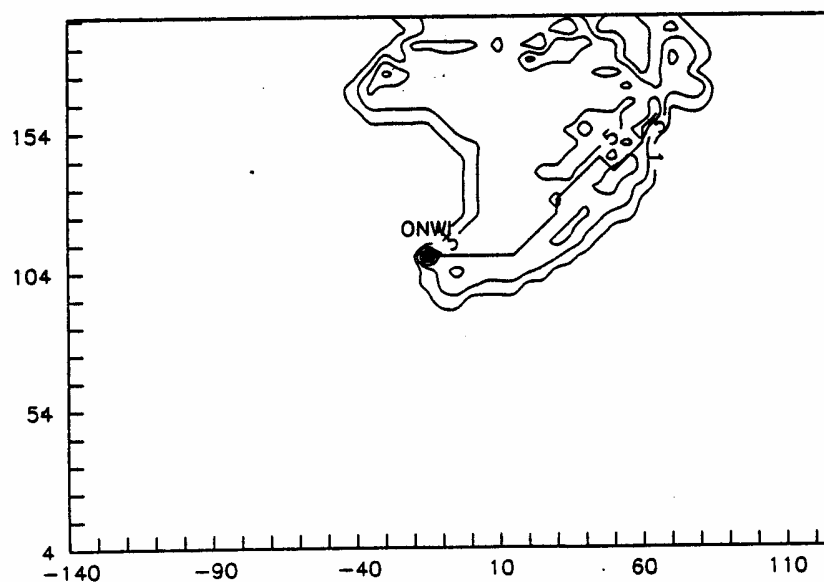


Figure 4 — Travel Path Fan for Pennsylvanian

Then is no certainty that a particle will follow the path of least resistance - it may flow to any lower level which is available for it. Given a fixed starting point, the path of a freed radionuclide may be any one of several potential paths. Taking this (admittedly simplistic) analogy, the likely travel path of a particle is in the form of rather irregular fan spreading out

from the original location. Figure 4 shows such a fan for the Kriged potentiometric for the Pennsylvanian aquifer. The contours represent the number of ways that a particular grid point (on Figure 2) can be reached. That is, a value of '3' implies that this point is lower in potentiometric level than three neighbouring points in potential travel paths.

The 'most likely' path has been superimposed on this map. It can easily be seen that the uncertainty on the most likely path is not, symmetrical around it but is related to the dip on the estimated surface itself.

This simplistic approach has been based on the assumption that all paths downward are equally likely to be taken by the particle. This is fundamentally unrealistic and will be the subject of further research. However, for the purpose of a visual representation of the 'travel fan' this approach is extremely useful since it shows all of the locations which could be reached by a freed radionuclide particle.

Simulated Travel Fans

In Figure 4, we saw that the most likely travel path of a freed radio-nuclide particle actually covered an area to the north-east of the proposed repository. The area which could be reached by a particle forms an irregular fan with its apex at the storage site and following the general trend of the potentiometric levels as estimated by the Universal Kriging method. This fan taken no account of the uncertainty inherent in the estimation of the parameters at the grid points. This uncertainty has been illustrated by mapping the standard errors for each estimated point (Figure 3). For a more realistic idea of the potential travel "fan" we must include this uncertainty in the analysis.

Conditional simulation, in the geostatistical sense, introduces the correct stochastic component back into the predicted surface and shows a more realistic potentiometric surface — in terms of 'roughness'. This statement does not imply that a simulated surface is a better estimator than a Kriged surface. This is simply one possible which honours the data values at the sampled locations and has the same spatial and statistical structure as the original data. This type of simulation has been fully described elsewhere (cf Harper & Clark, 1988) and will be only briefly here. Basically, such a surface is constructed in three stages:

- (i) A Kriging exercise is carried out on the original parameter data to produce a grid of estimated points.
- (ii) Values are simulated at each sample location. The Kriging exercise is repeated for the same grid.
- (iii) Values are simulated at each grid point.

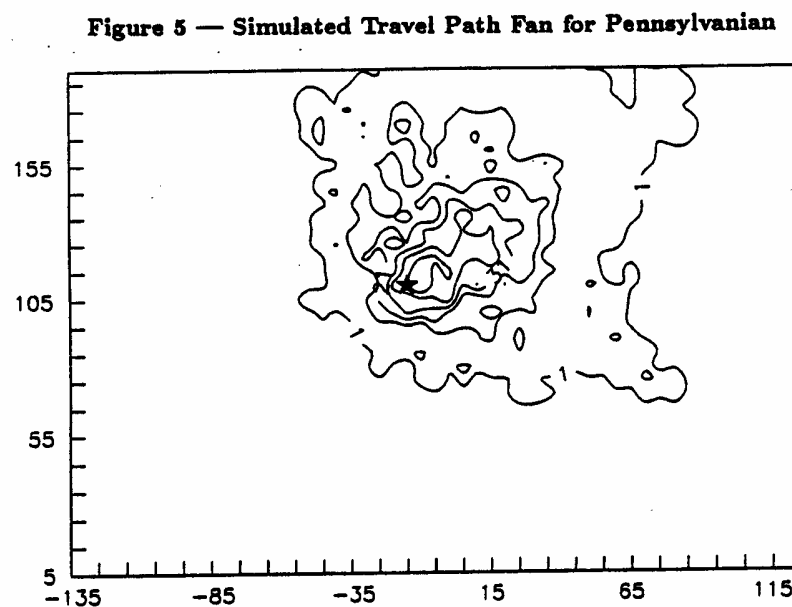
The conditional simulation is produced by subtracting (ii) from (iii) and adding the result to (i) for each grid point. Provided the simulated data followed the semi-variogram and distribution as the original data, this will produce a simulated surface which honours the data values and has exactly the same characteristics as the original surface. In the case of a surface such as the

Pennsylvanian potentiometric data, the semi-variogram and distribution referred to are than of the residuals from the trend surface.

In practice, the Kriging weights in stage (i) are stored and used in stage (ii) to save computation time. In this way, the actual Kriging only has to be carried out once for any particular surface — no matter how many simulations are required. For each simulation, the travel path can be calculated and accumulated.

The Pennsylvanian Aquifer

The Kriged surface in Figure 2 was produced on a five mile grid. Taking the same mesh size, 25 conditional simulations were produced and the travel fans from each were stored. A study of individual simulations revealed that some travel paths were extremely short with the particle becoming trapped in a local depression very soon after leaving the repository. However, some fans were much larger. Figure 5 shows the accumulation of 25 such simulated travel fans.



Comparison with Figure 4 shows that the spread of the simulated fan is much greater than that on the Kriged surface — as should be expected. One interesting feature of the simulated fan is that there are possible paths to the south and west of the repository. On the kriged map these directions are estimated to be "uphill". This behaviour illustrates neatly one of the valuable contributions of the simulation approach. Figure 2 shows the "best" estimation of the potentiometric level at each one of the 5 mile grid points. However, the true surface is much more irregular than this smooth kriged surface. The simulation reminds us that there may be directions of travel which would not even be considered if only the estimated surface is considered.

Actual quantification of the risk associated with any particular destination for a freed particle is a subject for more extensive research than we have been able to cover in this study. However, we feel that this approach would form a solid basis for developing the refinements required to determine relative probabilities for all of the possible paths revealed by the present study.

Practical Aspects of Simulation

During the analysis which has been described above, various factors were investigated as relevant to the final results. In particular, the size of the grid which was simulated appears to be a definite influence on the size and shape of the final travel fan. The fan on the Kriged surface, of course, remains the same — with minor refinements along the outer envelope. However, the simulated travel fans are heavily influenced by the size of mesh which is studied. All of the results above were produced on a five mile grid. Similar studies were also carried out for 2.5 mile grids and for a one mile grid. The fans tended to be similar in shape but widely different as regards size. Figure 6 shows a comparison between the envelopes around 25 simulations on each of the different size grids. At first sight there seems to be a direct relationship between the refinement of the grid and the area covered by the fan envelope. More detailed study reveals that the areas covered also become more symmetrical around the repository site as the size of the grid diminishes. This effect seems to be rather puzzling until we recall the structure which is being simulated.

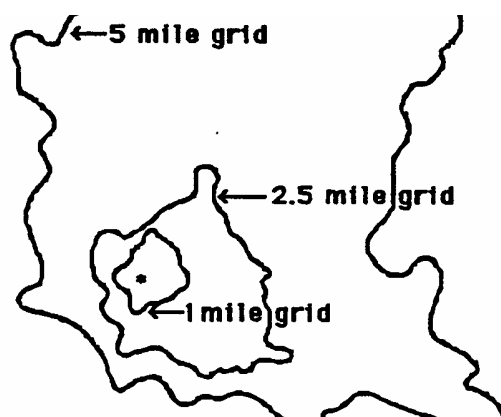


Figure 6 — Envelopes of Simulated Travel Fans

The conditional simulation is producing a surface which is composed of three components: a very large scale trend, dropping to the north-east; a Spherical semi-variogram stochastic component, in which values are related up to 50 miles apart; and a completely random component measured by the nugget effect. At the five mile scale, both trend and spherical components become reasonably strong so that the travel paths are highly influenced by the trend and continuity on the simulated surface. At the smaller scales, the nugget effect becomes stronger than the continuity components resulting in more "depressions" apparently trapping the freed particles. The one mile simulation is almost symmetric around the site of the repository because the simulated surface is almost entirely random — and therefore no preferred directions exist.

The major implications of this scale effect are that the existing sample data is inadequate for this scale of investigation. There are very few borehole pairs within five miles of one another. This means that any geological variability on the one mile scale is being lumped into the 'completely random' nugget effect. Quantification on this scale would require much more detailed sampling to split this supposed nugget effect into its proper spatial structures.

Multivariate Conditional Simulation

We have seen that there are two main components to the potential travel paths of a freed particle. The general structure of the surface as revealed by the Kriging estimation gives the best estimation of the potentiometric surface. This can be used to produce a fan of possible travel paths available to a radionuclide. It may be possible to quantify the relative probabilities of the various final destinations making up the envelope around the travel path fan. The second component is, paradoxically, the easier to quantify — being the stochastic variation which has been smoothed out by the Kriging process, the uncertainty on the actual estimated surface. This is measured by the standard error on the estimation. More "realistic" surfaces may be simulated and the deviation from the "best estimated" fan investigated.

We have discussed how that second component may be quantified and simulated. The Kriging process produces the smallest standard error, and hence the least amount of stochastic variation to simulate. However, this last statement is only true if we consider only the data available within the Pennsylvanian aquifer. It can be seen from Figure 1 that the north-east corner of the study area is particularly badly sampled for values in the Pennsylvanian aquifer. What we cannot see from this Figure is that a companion aquifer, the Wolfcamp, which lies above the Pennsylvanian is well sampled in this area. In addition, there is a high correlation between the Potentiometric levels in the Wolfcamp and those in the Pennsylvanian. An estimation method which could take advantage of this extra information must (surely) be better than a simple Universal Kriging on a single parameter.

An alternative to univariate Kriging is a multivariate technique, generally known as Co-kriging. With sample data such as that available in this study traditional Co-Kriging cannot be applied. An alternative approach, which has been dubbed Multivariate Universal Co-Kriging (MUCK) has been expounded in detail in Clark et al. (1988). It is sufficient to say here that the technique is exactly analogous to Universal Kriging except that the cross-correlation between samples in the Wolfcamp and values in the Pennsylvanian may be included in the analysis. The ultimate impact is to reduce the size of the estimation variances on the Pennsylvanian estimates by a factor of up to 60%. The simulation process which results includes a multivariate factor, since both Wolfcamp and Pennsylvanian must be simulated, but in principle is similar to the univariate.

25 simulations were made on the MUCKed five mile grid on the Pennsylvanian aquifer. The travel path fans were accumulated and we illustrated in Figure 7. Visual comparison of this envelope with that in Figure 5 shows the reduction in uncertainty associated with the estimation error on the potentiometric levels within the Pennsylvanian aquifer. This improvement more

than compensates for the minor increase in computer time associated with the MUCK estimation method. In fact, if both aquifers were to be simulated and studied in the investigation, the computer time is considerably reduced over two completely separate studies.

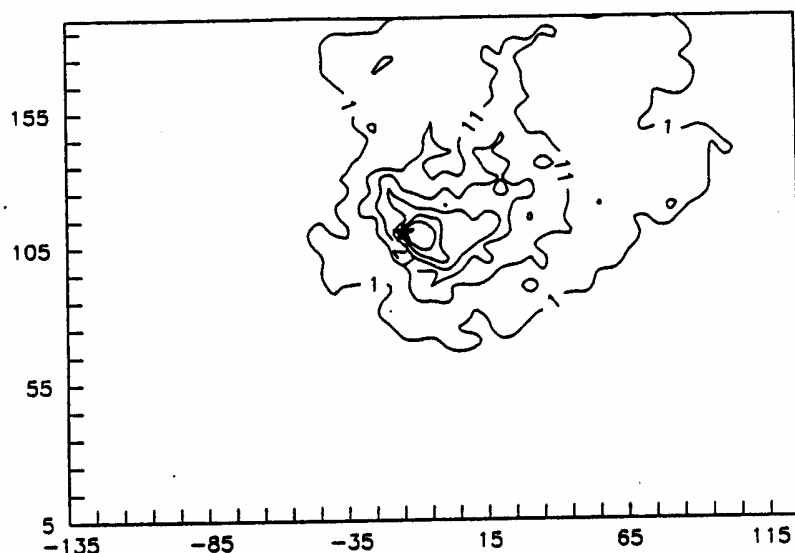


Figure 7 — Multivariate Simulated Travel Fans for Pennsylvanian

Summary of Discussion

In this paper we have considered how geostatistical methods may aid in predicting the likely travel path of a freed radionuclide from a high-level nuclear waste repository. Traditional geostatistical estimation methods allow the prediction of the 'best' or most likely values for hydrological parameters at grid points over the study area. From these the most likely travel path of a freed particle may be calculated. In addition a fan of possible paths may also be produced.

With the addition of geostatistical simulation, fluctuations on the likely travel paths - as indicated by the smoothed Kriged surface - may be studied. We have illustrated this paper with only 25 simulations. Many more would be required for a definitive study, but the principles are clearly illustrated. The possible destination of hazardous material is seen to be a much larger area than would be expected from a non-geostatistical study.

We have also shown that the uncertainty on the travel path or fan can be reduced by introduction of other parameters correlated to that one which is currently under study. Any number of associated parameters can be included in such an investigation, provided that sufficient data is available on each.

Whilst this case study has considered the release of radio-nuclide particles, it should be obvious that these results are equally valid for any toxic or hazardous material which has been stored close to a source of mobile groundwater.

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