# Appendix D

## Analysis of Natural Attenuation as the Preferred Groundwater Remedial Alternative at the DOE UMTRA Site Near Riverton, WY

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# Analysis of Natural Attenuation as the Preferred Groundwater Remedial Alternative at the DOE UMTRA Site Near Riverton, WY

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# 1. Introduction

The Department of Energy (DOE) has responsibility for regulatory compliance at 24 formerly used uranium mill tailings sites around the country. The regulatory requirements are dictated by the Uranium Mill Tailings Radiation Control Act and the U.S. Environmental Protection Agency's Health and Environmental Protection Standards for Uranium and Thorium Mill Tailings (40 CFR Part 192; 60 FR 2854). The DOE's Uranium Mill Tailings Remedial Action (UMTRA) Project has been divided into a Surface Program and a Groundwater Program. Most of the 24 UMTRA sites have been addressed under the Surface Program, with the majority of the sites having completed major tailings removal, relocation and/or disposal actions. The Groundwater Program was begun in earnest some years after the Surface Program to allow for source term removal prior to addressing the potential for adverse groundwater impacts.

The Groundwater Program has identified at least one third of the UMTRA sites as potential candidates for a natural attenuation strategy for compliance with the applicable regulations. This compliance strategy has been discussed in the Programmatic Environmental Impact Statement (PEIS) (U.S. DOE, 1996). A natural attenuation strategy requires that, within a one-hundred year period, concentrations of the contaminants of concern be reduced below regulatory limits, or Maximum Contaminant Levels (MCLs), by natural processes. Several potential natural attenuation processes can be considered:

- hydrodynamic dispersion of the contaminants (e.g., mass spreading and concentration reduction);
- degradation and/or decay (e.g., mass reduction);
- dilution from recharge or infiltration (e.g., areal recharge, stream/irrigation leakage); and/or
- flushing (e.g., discharge to a gaining stream).

For the UMTRA sites, the degradation or decay of contaminants of concern (e.g., uranium) probably has a minimal attenuation effect because the constituents are inorganics and/or

radionuclides with relatively long half-lives. Dilution, dispersion, and especially flushing, are the main processes of interest.

## 1.1 Natural Attenuation Processes

Further discussion of each of the previously mentioned natural attenuation mechanisms and their effects on plume behavior is warranted because of the puzzle that is frequently encountered in attempting to identify the attenuation processes that are occurring and assessing the degree to which each is reducing contaminant concentrations. Stated another way, what one model and its set of parameters may provide as a logical explanation for an observed plume's movement is often totally different from another model's explanation. Because the exact fate and transport processes at a site cannot be determined uniquely, it does help to understand the relative effect that each attenuation mechanism will have on plume behavior, as well as their combined effects. With this understanding it may be possible to eliminate unrealistic or improbable mechanisms from further consideration. The following paragraphs provide a summary of the attenuation processes and their effects on contaminant levels.

Hydrodynamic dispersion is a phenomenon in which dissolved contaminant mass is spread beyond the space it would normally occupy due to average subsurface water movement alone. Transport by average water movement alone is typically referred to as advection, but it is improbable that contaminant transport in the subsurface can occur solely by advection without dispersion occurring as well. Dispersion affects a plume by smearing the contaminant levels along the leading edge of the plume as well as along its side and base edges. Dispersion occurs in contaminant transport in both the unsaturated and saturated zones.

Hydrodynamic dispersion is defined as having two separate components: (1) mechanical dispersion and (2) molecular diffusion. Mechanical dispersion in porous media flow is mixing that occurs as a consequence of local variations in velocity around some mean value of flow

velocity, whereas diffusive transport occurs in response to variations in dissolved concentration of a contaminant. Although both processes cause spreading of a plume, the mixing effects of mechanical dispersion usually dominate those of diffusion. Mechanical dispersion can also be characterized as either being longitudinal or transverse dispersion. Longitudinal dispersion is the mixing that occurs along the direction of flow, whereas transverse dispersion is the mixing that occurs in directions normal to the flow path. On a microscopic scale, transverse spreading of water flow occurs because individual flow paths within the porous medium diverge.

In solute transport, the release of a contaminant for a finite length of time is commonly referred to as a slug release. After a slug release, hydrodynamic dispersion will cause the concentrations within the plume to be less than they were initially during the release.

Sorption is the process in which contaminants leave the dissolved state in water to fixate on the solid particles comprising a porous medium. Several relationships can be used to mathematically describe the relative distribution of a contaminant between dissolved and sorbed states. The most common relationship used in transport modeling assumes linear equilibrium sorption. This relationship allows the propensity for a chemical to adsorb onto solid materials to be described in terms of a soil-water distribution coefficient, or $K_d$. The larger the $K_d$ value, the greater the tendency is for the contaminant to sorb to subsurface media. Sorption retards the movement of a contaminant in groundwater, causing its bulk transport to take place at a rate that is slower than the average groundwater flow velocity. A retardation factor, which measures the ratio of the average groundwater velocity to the average velocity of a sorbing contaminant, can be determined from the contaminant's $K_d$.

Soil-water distribution coefficients are dependent on the dissolved form of the chemical involved in the reaction as well as the materials comprising the porous medium. For certain organic compounds the distribution coefficient is a function of the organic content in the porous materials. Inorganic chemical $K_d$s are strongly affected by soil makeup, particularly clay

content, and can be measured in laboratory experiments or determined through field tracer studies.

Use of a soil-water distribution coefficient and retardation factor implies that sorption is reversible, indicating that the porous material eventually releases the contaminant and allows it to go back into solution. As a consequence, sorption serves not only to delay the arrival of the contaminant, but the temporary storage of the contaminant mass in solid form also causes the peak dissolved concentrations from a slug release to be less than equivalent concentrations without sorption.

Decay refers to the degradation of a contaminant in the environment. There are numerous causes of decay including chemical reactions with water, known as hydrolysis, or the solid materials comprising a porous medium. Organic chemicals may undergo a form of decay called biotransformation. Radionuclides undergo a form of decay wherein mass is converted into radiation. Decay of a radionuclide is characterized by its half-life, which is a constant value. This in turn allows the degradation to be expressed as a first order decay process. Other types of contaminants may also decay in accordance with a first-order process, but, unlike radionuclides, the half-life of one these constituents may vary, depending on pH, oxidizing conditions, or temperature.

Decay influences transport by reducing the total mass of the contaminant, thereby decreasing both its dissolved and sorbed concentration.

Dilution of a dissolved contaminant occurs when clean water mixes with contaminated water. A given quantity of contaminant mass in a larger volume water causes a decrease in the contaminant's dissolved concentration. One form of dilution occurs when infiltrating water from a source that is widespread areally, such as precipitation or flood irrigation water, mixes with

shallow contaminated groundwater. Dilution from areal recharge is manifested in much the same way that decay affects contaminant concentrations.

Water infiltrating from the base of a surface waterway and recharging an aquifer can also cause dilution. Examples of waterways that tend to lose water in this manner include irrigation canals or a stream on the margin of an alluvial basin whose bed lies above local groundwater levels. Dilution brought about by this phenomenon differs from areally distributed recharge because the mixing of waters occurs generally beneath the waterway and not uniformly over the entire aquifer.

Natural flushing from a contaminated aquifer occurs when the contaminated groundwater discharges in whole or in part to a surface waterway such as a river or agricultural drain. Because the flow in a river is generally much larger than the contribution of locally contaminated groundwater, the contaminant levels in the river are highly diluted, often to non-threatening levels. Through this process, the aquifer can eventually purge its contamination to the point where residual contaminant concentrations no longer pose a threat to human or environmental health.

## 1.2 Evaluation Model

Sandia National Laboratories (SNL) has been supporting the UMTRA Groundwater Program for several years in developing an approach and associated computer tool to address groundwater issues at UMTRA sites. This approach is more robust than previous attempts to address natural attenuation concepts in that it explicitly accounts for uncertainty through the use of Monte Carlo simulation techniques. Therefore, the likelihood of success of the natural attenuation strategy can be evaluated with this approach. In contrast, conventional modeling approaches utilize discrete estimates of contaminant fate and transport behavior, which do not address uncertainty. The methodology and associated computer code developed by SNL is embodied in the

Groundwater Analysis and Network Design Tool, or GANDT. This tool was used to perform the analyses presented in this report.

As mentioned, the methodology employed within GANDT to explicitly address uncertainty is the stochastic Monte Carlo technique. With Monte Carlo simulation, the modeler benefits from evaluating the relative influence of model input parameters on model predictions. Parameters that have a profound effect on model results, as identified and evaluated with sensitivity analysis techniques, are often quite uncertain. The uncertainties associated with input parameters may be due to spatial variability, measurement error, an imperfect knowledge base, or other factors. One can statistically estimate the uncertainties associated with key input parameters by collecting data during a site characterization effort. Alternatively, parameter uncertainty may be estimated using literature sources, or with the use of expert judgment. Once the critical input parameters have been approximated by statistical distributions, the Monte Carlo method invokes sampling schemes to combine the suite of input parameters into multiple data sets. Model simulations are performed with all of these sets of input parameters. The combined results of the model runs are then statistically analyzed to form a probabilistic description of the uncertainty in model predictions. Appendix A provides a simplified discussion of the Monte Carlo method in quantifying uncertainties.

An aspect of the GANDT code that enhances its ability to address uncertainties is the use of an efficient, stratified sampling technique to assemble the input parameter sets that fully describe the stochastic nature of the problem. This method is called Latin Hypercube Sampling (Iman and Shortencarrier, 1984), or LHS. By invoking the LHS method, the number of Monte Carlo model runs required to capture the full behavior of model uncertainty is generally many times smaller than the number needed using pure random sampling (Peck et al., 1988). A recommended minimum number of model simulations when using LHS is 4/3 the number of uncertain parameters, whereas pure random sampling may require as many as ten or more times the number of stochastic variables. Thus LHS has a significant advantage over the conventional

sampling approach, making Monte Carlo analysis of groundwater flow and transport problems relatively efficient.

Another advantageous feature of the LHS methodology is its ability to specify correlations between parameters. If two or more input parameters can be demonstrated as having some degree of correlation with one another, such as through a regression analysis, accounting for it within LHS, as compared to allowing a totally random association of the parameters, may help to reduce uncertainty in model predictions.

Other functional aspects of the GANDT code, such as the flow and transport models incorporated in it, are discussed in subsequent sections. More detailed explanations of algorithms within it can be found in several publications regarding the tool and its applications (Knowlton et al., in press; Walker et al., 1996; Metzler et al., 1997).

This report provides a summary of analyses performed by SNL to evaluate the potential success of a natural attenuation strategy at the DOE UMTRA site near Riverton, Wyoming. The format of this report is based on the American Society for Testing Materials (ASTM) "*Standard Guide for Documenting a Ground-Water Flow Model Application*" (ASTM, 1995), with some added sections discussing groundwater flow and contaminant transport aspects of the GANDT methodology. At the direction of DOE personnel, the natural attenuation modeling discussed herein has been performed for two constituents of concern: uranium and molybdenum.

## 2. Modeling Objectives

The main objective of this modeling effort is to evaluate the likelihood of success of a natural attenuation remedial option at the UMTRA site near Riverton, Wyoming. To help meet this objective, a probabilistic modeling approach has been applied, using Monte Carlo methods to quantify uncertainties. Specific objectives include:

- model the transport of constituents within and from a mill tailings source zone, using a pulsed leaching algorithm due to the fact that the tailings have been removed from the site;
- model the fate and transport of constituents through the vadose zone beneath the former tailings area;
- model the fate and transport of constituents in groundwater in the uppermost surficial aquifer at the site;
- perform Monte Carlo analyses to quantify the uncertainty in the distribution of contaminants in the aquifer over a 100-year period (including the utilization of a geostatistical technique to quantify spatial variability in the hydraulic conductivity field);
- condition the Monte Carlo simulation results on known water quality data, i.e., automated calibration based on the concentration data collected from local monitoring wells;
- develop average concentration distributions for the constituents of concern, based on the probabilistic analyses;
- develop probability distributions for MCL exceedance to visually illustrate the likelihood of meeting groundwater standards over a 100-year period;
- develop statistical ranges of water quality data at key monitor well locations over the next 100 years to be used to verify the progress of the natural attenuation processes; and
- develop conclusions/recommendations regarding the likelihood of success for natural attenuation.

## 3. Model Function

For the past several years SNL has been developing the Groundwater Analysis and Network Design Tool, or GANDT, to provide DOE Environmental Restoration programs with a comprehensive system for analyzing groundwater flow and associated contaminant transport, while directly accounting for transport uncertainty and providing decision analysis capabilities for monitor well network design. As a point of reference, GANDT began its development under the name Borehole Optimization Support System, or BOSS, but was changed due to copyright considerations. A draft report (Knowlton et al., in press) detailing the technical attributes of the GANDT code is under development and available for review. A draft user's manual has also been developed and is available from Sandia National Laboratories.

GANDT is a comprehensive groundwater analysis package, providing the following features:

- Utilizes flow and transport models in a probabilistic framework to account for uncertainty in contaminant movement and fate; and
- Simplifies the analysis of natural attenuation potential, providing an estimate of the likelihood of success of this option, thereby possibly avoiding costly and time-consuming pump-and-treat options for groundwater remediation.

The GANDT code contains a number of tools that, when combined, make it a unique modeling system. Some of these items are:

- Simulates leaching from contaminant source term, including a pulsed leaching time to account for source removal;
- Simulates either aqueous- or vapor-phase movement of contaminants in the unsaturated zone, and accounts for contaminant transfer into the underlying aquifer;
- Analytical and numerical solutions for the saturated zone (including FTWORK, a 3-D numerical finite difference code for flow and advective/dispersive transport [Faust et al., 1994]);

- An automatic grid generation module to simplify the numerical model input (and also automatically account for grid orientation when the user specifies uncertainty in the groundwater flow direction);
- Monte Carlo technique employed to propagate input parameter uncertainties into flow and transport uncertainties;
- Latin Hypercube Sampling (LHS) technique (Iman and Shortencarrier, 1984) employed to minimize computational burden by reducing the number of simulation runs required for the Monte Carlo analysis;
- Spatial variability explicitly accounted for using a geostatistical simulator (e.g., Sequential Gaussian simulator), which honors observed hydraulic conductivity estimates;
- Conditioning of simulation results on observed water quality data using statistical methods (e.g., essentially a built-in calibration method to honor water quality data); and
- An intuitive graphical user interface and graphical display of results for ease of use on PC Windows and Macintosh platforms.

GANDT currently has the capability to simulate flushing, dilution, and radioactive decay. The numerical simulation option in the GANDT code is currently set up to perform steady-state flow simulations and transient fate and transport analyses.

In conventional flow and transport simulations a calibration procedure is manually performed to "match" model results with observed site data, such as measured water levels and water quality data. One of the model parameters that is commonly adjusted to achieve a better match between observed and computed values is aquifer hydraulic conductivity. The calibration process can be quite tedious and time consuming. SNL has built an automated calibration capability in GANDT that effectively conditions, or honors, observed concentrations in the saturated zone through use of statistical analysis techniques. Any Monte Carlo simulation with a cumulative measure of the differences between observed and computed concentrations, which are commonly called residuals, that does not meet a specified statistical tolerance is omitted from the probabilistic

analysis. This feature is extremely important when the user is interested in probabilistic (i.e., Monte Carlo) analyses, where many simulations are performed to get a statistical representation of the uncertainty in model results. The user has the ability to choose from a chi-square test (Haan, 1977) for acceptance of a run or a root mean squared error (RMSE) analysis (Anderson and Woessner, 1992). To apply the chi-square method, the residuals must be normally or log-normally distributed. GANDT can graphically display data distributions to evaluate normality, giving the user great flexibility in selecting conditioning criteria.

It is important to note that the version of GANDT used for this study is limited to conditioning on water quality data. That is, conditioning to hydraulic heads (i.e. water levels) has not yet been included in the software due to the fact that, of the possible types of data used for model calibration in groundwater contamination investigations, water quality information is most effective in reducing transport uncertainty. This phenomenon was illustrated by Van Rooy and Rosbjerg (1988), who compared the relative ability of three different parameter estimation approaches - geostatistical conditional simulations of transmissivity, selection of groundwater flow model runs based on observed hydraulic heads, and selection of transport model runs based on measured concentrations - to produce a model that best approximated actual site conditions in a case study. Similar results were reported by McLaughlin et al. (1993), who used three comparable parameter estimation techniques to clearly show that the greatest reduction in model uncertainty was achieved by conditioning on water quality measurements. Though the current version of GANDT does not utilize water levels as calibration targets, SNL's experience with the code shows that it does quite well in matching hydraulic heads at sites characterized by relatively uniform flow fields. In addition, mass balance reports from individual simulations are provided, enabling the user to compare computed groundwater flow quantities with those that are expected for a site.

GANDT has the ability to display the results of probabilistic analyses in a variety of ways. Two-dimensional visualization graphics that the user can observe include hydraulic conductivity

distribution plots, contaminant distribution plots, and probability of exceedance plots. Contaminant distributions can be displayed for all user-specified time steps, and for each of as many as six layers in a numerical simulation. The types of contaminant plots available are:

- Plume concentrations from each Monte Carlo simulation, with user-specified color mapping of the contaminant concentrations, and an optional player mode that cycles the Monte Carlo simulation output in an "animation" format;
- Average plume distribution from all Monte Carlo runs;
- Standard deviation plot;
- Variance plot;
- Coefficient of variation plot; and
- Probability plots, wherein the user specifies a threshold contaminant concentration (e.g., MCL), and the resulting plot displays the probability of exceeding that concentration.

The last plotting option mentioned is extremely important in evaluating the likelihood of success of a natural attenuation approach to remediation.

## 4. General Setting

The former Riverton uranium processing site is located in Fremont County, Wyoming, approximately 2 miles southwest of the city of Riverton, Wyoming (Figure 4.1). The Riverton site encompasses about 80 acres on a level, alluvial terrace between the Wind River and the Little Wind River. The uranium mill operated from 1958 to 1963. The tailings pile and associated contaminated soils were removed in 1988 and 1989. Groundwater at the site occurs in an unconfined surficial aquifer, an underlying semiconfined aquifer, and a deep confined aquifer. The surficial aquifer, consisting of sand and gravel (16-20 feet [ft] thick), and the semiconfined aquifer containing sandstone (16-30 feet thick), are separated by an aquitard of shale and siltstone (6-10 feet thick). The depth to groundwater varies from 5.5 to 7.5 feet. Groundwater flow is generally toward the east-southeast, exhibiting a horizontal gradient of approximately 0.0024. In response to infiltration from a nearby irrigation canal, the flow direction can become more southerly and show a gradient of as much as 0.0034. Pumping tests at and near the site indicate that representative hydraulic conductivities for the surficial and semiconfined aquifers are 56 ft/day and 33 ft/day, respectively (DOE, 1985a). Assuming effective porosities of 0.30 and 0.15, respectively, in the two aquifers, and a hydraulic gradient of 0.0024, average linear groundwater velocities in the two respective units are computed to be 160 and 190 ft/year. Because an aquitard consisting of shale and minor sandstone lenses exists between the semiconfined aquifer and the deep confined aquifer, no hydraulic tests have been performed in the confined aquifer. Additional information on the general setting for the Riverton site, including more detailed discussions of the site hydrogeology, is presented in reports prepared by the U.S. Department of Energy (DOE) (1995a; 1995b).

A DOE Baseline Risk Assessment report (DOE, 1995b) indicated that constituents in the surficial aquifer comprise the greatest concern for groundwater contamination at the Riverton site. This and other previous investigations have suggested that contaminants in this aquifer are flushed out into the Little Wind River by natural groundwater flow.

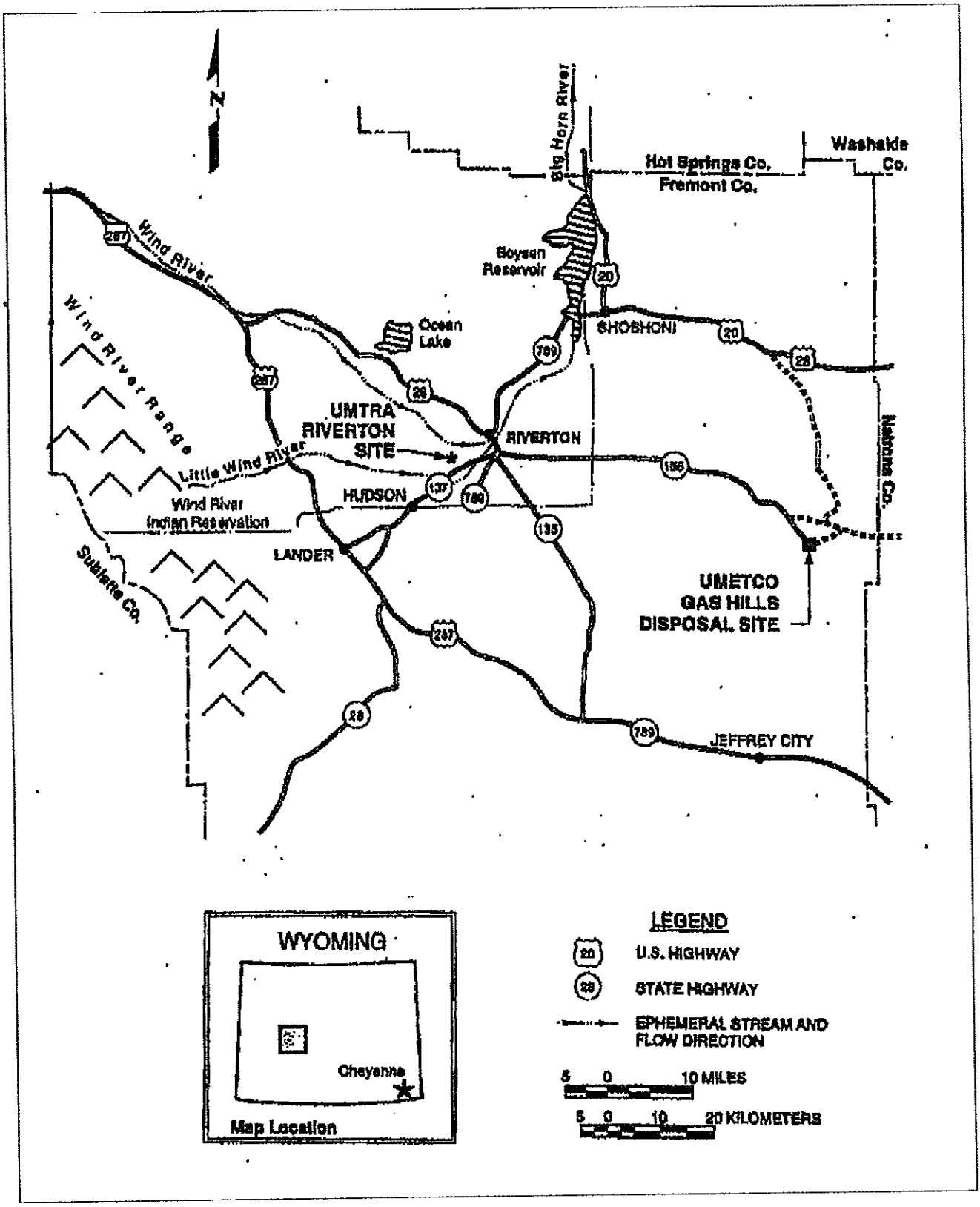



**Figure 4.1 - Riverton, Wyoming, Site Location (after DOE, 1985a)**

## 5. Conceptual Model

Because this investigation focuses on natural attenuation processes, development of a conceptual model for the Riverton site should focus on both general hydrogeologic processes and the phenomena that more specifically help to attenuate contaminant concentrations, including:

- dilution from areal recharge;
- dispersion as part of the transport process; and
- natural flushing to the Little Wind River (i.e., aquifer discharge to the gaining river).

The groundwater system at the site is hydraulically connected to the unsaturated zone, which, at one time, contained the contaminant source in the form of a tailings pile. The GANDT code simulates the leaching of contaminants from the source zone, subsequent transport through the unsaturated zone, and mass flux into and within underlying aquifers. Thus each of these zones must be examined in the conceptual model. In addition, the time frame of interest is approximately 140 years. This is because the facility was established in 1958, monitoring data from 1997 are used for the conditioning of transport simulations, and a 100-year time period after 1997 is considered when analyzing the potential for MCLs to be achieved by natural processes. Given a 140-year time frame of interest, it is assumed that the seasonal, transient behavior of the hydrologic system will be dampened, allowing the system to approximate some average form of behavior. Accordingly, steady-state flow conditions are assumed to be appropriate. Uncertainty associated with the long-term average flow conditions, such as the magnitude of the gradient and the direction of groundwater flow, is taken into account by establishing statistical distributions for these parameters in the Monte Carlo analysis.

### 5.1 Aquifer System

The aquifer system at the Riverton site consists of a surficial, unconfined unit, a semiconfined unit, and a deeper confined aquifer. The main aquifer of interest for groundwater compliance is

the surficial unit. An extensive amount of testing has been performed on this uppermost aquifer and has been documented in DOE (1995a) and SNL (1996). The depth to groundwater is relatively shallow, and ranges from 5.5 to 7.5 feet in the mill tailings area. South and east of the tailings are wetland areas characterized by groundwater discharge and high evapotranspiration potential; these areas are considered to have little impact on overall contaminant fate and transport in the subsurface. The surficial aquifer is 16-20 feet thick and is assumed to be hydraulically connected to the Little Wind River, located downgradient of the tailings. This hydraulic connection is assumed to be one in which the Little Wind River is a gaining stream, with the aquifer discharging to it.

## 5.2 Hydrologic Boundaries

For the purposes of this natural attenuation analysis, a steady-state flow system is assumed. This approach is taken on the premise that, though hydraulic heads change with both sporadic and periodic stresses (e.g., recharge from precipitation, high river conditions, flooding, irrigation, conveyance of water in irrigation canals, pumping), the average, long-term groundwater flow conditions (i.e., flow direction, flow rate) remain generally the same. This assumption corresponds with a state of "dynamic equilibrium" (Freeze, 1969), in which there are no long-term (several years) changes, or trends, in regional and local groundwater levels.

Though there are clear indications of short-term changes in hydraulic head at and near the Riverton site, there is little to no evidence collected thus far to clearly demonstrate that the regional groundwater flow system is undergoing major, lasting alterations. However, there is a distinct possibility that the hydraulic gradient within the groundwater system downgradient of the mill tailings was considerably larger than has been observed in recent years, which could be attributed to the large quantities of moisture that were likely in the tailings when they were first placed onsite. If such a relatively steep gradient existed for several years, it is also possible that the distribution of contaminants observed in today's groundwater system is a vestige of larger

groundwater flows than those occurring recently. Without direct evidence of such conditions, the approach taken in this study has been to use a range of groundwater flow directions and hydraulic gradients representative of recent times.

The assumption of a dynamic equilibrium state is partially supported by an analysis of the variation in head measurements at monitoring wells throughout the site. The analysis was performed by DOE-UMTRA personnel using the SEE.UMTRA database query system. Appendix B gives a summary of this statistical analysis. In short, the analysis showed a maximum observed standard deviation of observed heads in monitoring wells over a 10-year period of about 2 feet; this observation was made for a well adjacent to the Little Wind River, where fluctuations in response to changing river levels are likely to be more prominent than elsewhere. Hydraulic head variations of this magnitude are considered small in the context of transient flow conditions. Further evaluation of water levels at the site shows that the local hydraulic gradient can vary between 0.0024 and 0.0034 (SNL, 1996). This variability can be represented in GANDT using the probabilistic modeling features of the code. In addition, groundwater flow direction can be treated as an uncertain parameter in GANDT; consequently, assigning a probability distribution to this parameter may make it possible to capture some of the influences of temporally-variable flow directions occurring in response to irrigation, river flooding and other system stresses.

The assumption of steady-state flow conditions is made not only with respect to the time period between the mill startup and recent years, but also with respect to future conditions, extending as much as 100 years hence. It is true that it may not be possible to assure that such a system will continue for this length of time, as future land use and other regional trends may influence local groundwater flow. However, without direct knowledge of land-use plans for this area, the focus of this study was on the potential for natural flushing of site contaminants with conditions as they exist today.

In GANDT, steady-state flow is established by controlling boundary conditions in the code's flow simulator. The user specifies the hydraulic gradient (or a distribution representative of a range of gradients) and the groundwater flow direction. The code's automatic grid generator constructs a finite-difference grid oriented along the longitudinal axis of flow. Initially, the upgradient and downgradient ends of the model domain are set as constant head boundaries such that the specified hydraulic gradient is maintained. If a gaining stream is located downgradient of the contaminant source, the river trace is used to establish and replace the model's downgradient boundary condition. In such a case, the river is assigned constant heads, which are based on the prescribed gradient and an estimate of the head loss attributed to phenomena such as convergent flow, vertical flow across alluvial strata, and flow across semipermeable streambed materials (Peterson and Wilson, 1988) The boundaries parallel to the flow direction are set as no-flow boundaries.

Because the Little Wind River is assumed to be a gaining stream downgradient of the tailings area, the river is treated as a boundary, with flow from the aquifer entering the river. The river is assumed to act as a sink for all groundwater flow intersecting it, and no flow or contaminant transport occurs beyond the river. As previously mentioned, surface water levels in the river are specified using hydraulic heads initially established with the grid generation package and additional data provided by the user reflecting the degree to which local head losses are expected to reduce groundwater levels from those expected on the basis of the regional gradient. Treatment of the river in this manner has an effect on hydraulic heads upgradient of the river.

The Wind River flows in a west-to-east direction approximately two thirds of a mile north of the Riverton site. If a regional model was constructed for the flow simulations, this river would likely constitute the location for a model boundary. However, the simulations performed in this study are mainly focusing on flow and transport from the former milling site downgradient to the Little Wind River, and, consequently, do not directly account for the Wind River. The previously-mentioned GANDT methodology for prescribing constant head boundaries and

uncertainty distributions for the hydraulic gradient and the direction of groundwater flow should account for the relative effects of the Wind River on flow through the area of interest.

The assumption that the Little Wind River downgradient of the site is a gaining stream may be questioned due to the lack of conclusive evidence demonstrating such a phenomenon. However, in addition to the DOE analyses mentioned above, there are reasons to believe that the river is indeed gaining in the subject area. In particular, it is typical of perennial streams like the rivers in this region to benefit from groundwater inflows due to topography effects (Freeze and Cherry, 1979). Groundwater typically flows from higher areas, where recharge is relatively significant and water levels are elevated by the recharge, to lower areas, where streams are commonly found. Consequently, surface water bodies in the forms of streams, rivers, lakes, and wetlands tend to act as discharge sites for the upland recharge. For this natural recharge-discharge mechanism to be upset, in which a river begins losing its water to the subsurface rather than gaining from it, very large withdrawals of groundwater on a regional scale are quite often necessary (Peterson and Wilson, 1988). On the basis of data presented in the DOE reports (1995a; 1995b), there is no indication that such a reversal in flow has occurred at the Riverton site, especially not within the surficial aquifer.

## 5.3 Hydraulic Properties

Numerous field and laboratory tests have been performed to estimate hydraulic properties for the surficial, unconfined aquifer. Slug tests, aquifer pumping tests, tracer tests, and sorption tests are some of the key data collection activities that have taken place. Results of these analyses are summarized in DOE (1995a) and SNL (1996). Estimated hydraulic conductivities span several orders of magnitude, illustrating the importance of considering uncertainty and spatial variability in a modeling study of this nature. It should be pointed out that such a large range of reported conductivity values may reflect biases occurring in the methods used to estimate this parameter. This is mostly due to the fact that slug tests provide measures of material properties over

relatively small zones of influence (e.g., Domenico and Robbins, 1998), whereas long-term pump tests gauge aquifer response over distances spanning as much as hundreds of feet. Both types of data have been collected at the Riverton site, and are being employed in the model runs in the interest of using as much information as possible.

## 5.4 Sources and Sinks

There are no major pumping or injection wells in the model domain selected for the site. Several sources and sinks which may have minor effects on the flow model have been assessed. For example, a number of irrigation canals just north of the former milling site likely contribute recharge to the surficial aquifer. Detailed data describing the transient flows in and hydraulic characteristics of these canals were not available to this modeling study. In addition, little to no groundwater level data has been collected in the vicinity of the canals that would indicate groundwater mounding or more regional influences on general groundwater movement in the study area. Consequently, the GANDT analyses presented herein were based on the assumption that the influence of canal losses on long-term groundwater flow was insignificant. Dilution from recharge occurring as a result of irrigation water applied to local fields fed by the canals is accounted for in GANDT through the use of an assumed areally-distributed recharge rate, which can be considered uncertain in the model.

A water supply well is located at the St. Stephens facility situated southwest of the former milling site. The pumping rate at the well is considered negligible relative to the flow occurring within the model area of interest, and is assumed to have little to no influence on GANDT results. This conclusion is supported by the DOE (1995a; 1995b) reviews of concentration distributions for the contaminants of concern, and the fact that contaminant plumes have shown no tendency to diverge toward this well (DOE, 1995a).

## 5.5 Water Budget

Water budget considerations for the steady-state model used to simulate the surficial aquifer flow include (1) infiltration of water through the mill tailings source area, (2) groundwater discharge to the Little Wind River, and (3) areally-distributed recharge throughout the site. The first of these is assumed in GANDT to influence contaminant transport from the tailings but have no appreciable effect on the general hydraulic gradients and flow directions currently occurring in the model area. Reasons for this latter assumption were discussed previously as part of the rationale for adopting steady-state flow conditions (see Section 5.2). The second component, groundwater discharge, is determined in GANDT as a result of boundary conditions established in the code's automatic grid generation package, and is included in mass balance reports produced by the groundwater flow model. The third, areal recharge, comprises an input parameter for the Monte Carlo simulations. It has been assumed in this investigation that this latter component, like water seepage through mill tailings, is not substantial enough to influence general groundwater flow conditions and velocities. However, GANDT does account for the effects of areal recharge on contaminant dilution. This is accomplished through a version of the numerical groundwater model in the code that specifically addresses water-mass conservation in the solute transport equation (Voss, 1984; Knowlton et al., in press).

Water budget results will vary with each Monte Carlo run conducted with the GANDT code. Because each simulation makes use of a local finite difference grid of unique size and containing unique hydraulic properties, total cumulative flow volumes cannot be predicted a priori. What can be estimated prior to the Monte Carlo analysis, however, is the range of flows per unit width of the model. On the basis of reported hydraulic conductivities, hydraulic gradients, and aquifer thicknesses (see Chapter 4 and Section 7.2), these per-unit-width flows are expected to range from 1 $ft^2$/day to 7.5 $ft^2$/day (365 $ft^2$/yr to 2750 $ft^2$/yr).

An additional concern regarding water balances is found in the transient nature of overbank flooding from the Wind River and Little Wind River. These episodic events are not easily handled and cannot be predicted over a 139-year time window employed in the simulations for this study. Again, treating the hydraulic gradient and flow direction as uncertain is believed to be a method for simulating the long-term effects of occasional stresses such as those associated with flooding. If the objectives of this modeling study were aimed at ascertaining short-term system effects, influences like flood events would likely need to be addressed explicitly.

## 5.6 Contaminant Source Term

As previously mentioned, two contaminants of concern at the Riverton site are examined in this study: uranium and molybdenum. Other contaminants exist at the site, but most of them have been discounted from the list of contaminants of concern in the DOE Baseline Risk Assessment (DOE, 1995b). A contaminant of interest that does exist at the site in elevated concentrations is sulfate. Though no regulatory standard exists for sulfate at this time, assessment of its transport would be useful, as it is likely that this constituent will flush from the aquifer system more quickly than uranium or molybdenum due to its low sorption potential. Such analysis, however, is hampered due to the Koch sulfur producing plant which lies directly upgradient of the old tailings area, and is a continual source of sulfate leakage into the surficial aquifer. Accounting for the effects of the Koch operations is beyond the scope of work required for this investigation, and is not likely to be a concern for DOE UMTRA.

Concentrations of the contaminants of concern in the mill tailings source area when the tailings were present are very uncertain. The concentration distribution is generally established on the basis of expert judgment and trial and error in the modeling process. This also holds true for the overall physical dimensions of the source area, which are uncertain. The source term dimensions are established on the basis of measurements of the site layout and from information in the

SOWP (DOE, 1995b). Each of these types of source-term variables are treated as uncertain in the GANDT analyses.

5.7 Fate and Transport Properties

Model fate and transport properties are derived from field and laboratory testing (e.g., sorption tests), as well as literature values. Experimental data are available, for instance, on sorption coefficients for uranium and molybdenum (e.g., Yu et al., 1993; DOE, 1993). There is a fairly wide range of sorption coefficient values reported for each of these contaminants.

Geochemical processes that may have occurred, or are still occurring, at the site, are not easily accounted for in GANDT or any conventional groundwater modeling system. Specifically, when the tailings were emplaced at the site, the pH of the tailings and its leachate was relatively low, reflecting acidic conditions (personal communication, S. Morrison, MACTEC-Environmental Restoration Services). As a result, the effective sorption coefficients of uranium and molybdenum were likely lower than would be observed under today's more chemically-basic conditions. As the contaminants leached and migrated through the unsaturated zone soils and surficial aquifer, it is likely that additional geochemical interactions took place away from the source area whose net effect may have been to effectively increase the respective constituents' sorption potential. This in turn may signify faster contaminant movement in the early years during and after tailings emplacement than is currently taking place downgradient of the tailings area . Sufficient data do not exist to support extensive modeling of this transient scenario. However, because the GANDT model provides a mechanism for honoring water quality data, as discussed earlier in this report, it will attempt to approximate the effects of a transient phenomenon of this nature through adjustment of fate and transport parameters other than those based on the geochemical phenomena mentioned above.

## 6. Computer Code Description

The GANDT code can be used to analyze flow and transport of contaminants from a source area in the unsaturated zone, through the unsaturated soils underlying the source material, and subsequently into and within the saturated zone. Uncertainty analyses are directly addressed in GANDT through probabilistic simulations based on the Monte Carlo method in conjunction with Latin Hypercube Sampling (LHS) of stochastic model parameters. Probabilistic results from the code can help to provide estimates of the likelihood of occurrence of specific transport scenarios. GANDT contains options for simulating subsurface contaminant movement using screening level, analytical solutions of advective-dispersive transport. A numerical, three-dimensional, finite-difference groundwater flow and transport solution based on the public-domain code FTWORK (Faust et al., 1994) can also be employed. The numerical simulator is used for this study because of its ability to account for groundwater discharge to a river, including a sinuous waterway. Spatial variability of hydraulic conductivity is accounted for through the use of geostatistical conditional simulation (Peck et al., 1988) , the algorithms for which are taken from the GSLIB system of codes (Deutsch and Journel, 1992). GANDT is relatively unique because of its ability to automatically condition model runs on observed water quality data, which essentially provides the model user with a built-in calibration technique. The code employs an automatic grid generator for ease of use in setting up a finite- difference grid when employing FTWORK. Data input and the examination of results from probabilistic analyses are handled easily through an intuitive user interface.

Versions of GANDT exist for both on PC-Windows and PowerPC Macintosh platforms. A draft reference report detailing the algorithms used in GANDT is currently undergoing revision (Knowlton et al., in press), but is available for review. A draft user's manual for GANDT is also available.

## 6.1 Assumptions

The reader is referred to the draft reference manual for GANDT (Knowlton et al., in press) for a complete description of the flow and transport models and geostatistical algorithms employed in the software. Many of the assumptions upon which both the analytical and numerical simulators in the code have been developed are also provided in the reference manual. More detailed explanations of the FTWORK model are presented in Faust et al. (1994).

## 6.2 Limitations

Potential limitations of the modeling software that may be relevant to this natural attenuation evaluation include:

- Steady-state flow conditions - The current version of the code does not simulate transient groundwater flow.
- User-defined boundary and initial conditions - Boundary conditions within the model are currently established through an automatic grid generator within the code, thus limiting the ability of users to define their own boundary and initial conditions.
- Honoring of hydraulic head information - Water levels and hydraulic heads are now available for display in the model's graphical output, but the user does not have the ability to calibrate to the flow conditions of the site.
- Single time frame for conditioning - At this time, the user can only specify one time to be used for conditioning of model results on measured groundwater concentrations.
- Single source term - Currently, the GANDT user is limited to specifying a single source area for each transport simulation.

## 6.3 Solution Techniques

As mentioned above, both analytical and numerical models of subsurface flow and transport are provided in GANDT, discussion of which is presented in the draft reference manual (Knowlton et al., in press).

## 6.4 Effects on Model

Perhaps the biggest concern regarding the application of GANDT to this evaluation of natural attenuation is the model's utilization of steady-state flow solutions, as developed within the code using the automatic grid generation package in conjunction with the numerical simulator. However, as discussed in earlier report sections, utilization of steady-state conditions in the current study appears to be a legitimate approach to assessing the long-term prospects for natural attenuation at the Riverton site.

## 7. Model Construction

The GANDT system is designed to be user friendly and minimize work associated with data input. As a consequence, many of the groundwater flow and transport modeling steps that are necessary for conventional model construction have been simplified or automated. Some of these features are identified in the next few sections.

### 7.1 Model Domain

A local model domain is generated within each Monte Carlo simulation conducted with the numerical flow and transport model; the size of the domain and the quantity and size of the finite-difference blocks depends on parameters used to define the simulation. Prior to conducting a probabilistic analysis, a global domain must be established that encompasses an area significantly larger than the area of contamination and any region that is expected to be affected by future plume movement. The code's automatic grid generator uses the parameter set sampled for a given model run and employs algorithms to design a local grid that is appropriately sized and properly oriented. Other checks and balances are made by the automatic grid generator to assure that mass balance is conserved and phenomena such as numerical dispersion are minimized (Knowlton et al., in press).

### 7.2 Hydraulic Parameters

Hydraulic parameters used in this study were derived from Site Observational Workplans (DOE, 1995a; SNL, 1996). Figure 7.1 provides a plot of hydraulic conductivity values used in the numerical simulations. These data were derived from either aquifer pump test analyses or slug tests. As mentioned in Section 5.3, aquifer test data are representative of a larger portion of the aquifer than is tested with slug tests. In addition, the aquifer system is stressed for a longer duration under an aquifer test, making it possible to identify nearby hydraulic boundaries.

Although both types of analyses are used in this study, more emphasis is placed on aquifer test data than on slug test data at locales where both exist. Two slug test values associated with wells 717 and 722, as well as a value from a tracer test well, 785, were left out of the analysis of the spatial distribution of hydraulic conductivity because they either: 1) did not compare well to the aquifer test data; or 2) did not allow the transient contaminant plume simulations to honor the water quality data due to impeding effects (i.e., conductivity values were too low). As this figure indicates, the range of hydraulic conductivity values is quite large, spanning several orders of magnitude. The mean hydraulic conductivity used for the geostatistical simulations of spatial variability was 57 feet per day (ft/d). Values of hydraulic conductivity from the combined results of aquifer test and slug test analyses ranged from 1 to 178 ft/d.

The hydraulic conductivity data were subjected to a variogram analysis (Deutsch and Journel, 1992) so that input for GANDT's geostatistical simulation tool could be prepared. The variogram is used in the geostatistical simulator to approximate the spatial trends in the hydraulic conductivity data. A variography package known as Variowin (Pannatier, 1996) was employed to determine variogram descriptors. Prior to performing the variography analysis, the data were log-transformed, as hydraulic conductivity values from a study area are typically log-normally distributed (e.g., Domenico and Schwartz, 1998). Figure 7.2 illustrates the variogram that was ultimately selected to perform the conditional simulations. The variogram parameters were: spherical variogram model; nugget = 0.467; sill = 1.0; range = 1200 feet.

A Sequential Gaussian conditional simulation tool in GANDT was used to generate hydraulic conductivity values for each model block in each Monte Carlo run. Figures 7.3 and 7.4 show two examples of the variability that the geostatistical model can produce while honoring each of the hydraulic conductivities derived from field-tested wells. Figure 7.5 shows the average hydraulic conductivity distribution from all the simulations used in the uranium analysis.

Additional model parameters (e.g., porosity) were selected from publications that specifically discuss site characteristics (DOE, 1995a; DOE, 1995b; DOE, 1996) and from other literature sources, both pertaining to the site (e.g. Narasimhan et al., 1986) and those of a more general nature. The resulting parameter values, including the distribution descriptors for uncertain parameters, are listed for the contaminant source term, the unsaturated zone, and the saturated in Tables 7.1, 7.2, and 7.3, respectively. These tables also list the data sources used to justify the parameter values selected.

## 7.3 Sources and Sinks

As stated previously, no point sources or sinks (e.g. pumping wells) are considered in the Riverton analysis. The Little Wind River represents the sole discharge site within the groundwater flow model.

## 7.4 Boundary Conditions

As stated above, the flow model in GANDT is set up for steady-state conditions. The user-specified gradient is used to establish constant head boundaries on the upgradient and downgradient ends of the local domain for each Monte Carlo run. Side boundaries of each local domain are treated as no-flow boundaries.

## 7.5 Selection of Calibration Targets and Goals

As discussed in Section 5.2, the GANDT methodology relies on calibrating, or honoring, water quality data. This is accomplished through what is termed a post-conditioning exercise, which occurs after the Monte Carlo simulations have completed. At this time, GANDT does not specifically honor head data. Consequently, it cannot be used to perform a conventional flow field calibration on the basis of observed hydraulic heads. The current version of the model is

limited to conditioning on groundwater contaminant concentrations, as water quality data provide the means for effecting the greatest reduction in uncertainty of plume movement and contaminant fate (Van Rooy and Rosbjerg, 1988; McLaughlin et al., 1997).

The current GANDT code is capable of performing a conditioning analysis only on the basis of one time period. Thus groundwater water quality data from a single point in time are desired to perform the calibration. The year chosen for the data conditioning in this investigation was 1997. Figures 7.6 and 7.7 show the 1997 water concentrations for uranium and molybdenum, respectively, at each Riverton site monitoring well. These groundwater concentration data essentially comprise the model calibration targets.

Two types of tests are available in the GANDT code for honoring water quality data through a post-conditioning statistical test. The first is a chi-square distribution test (Haan, 1977) on the transport model residuals (i.e., differences between measured and simulated concentrations). For a chi-square test to be valid, the residuals must be either normally or log-normally distributed. Such a requirement was not met in the preliminary model runs made with GANDT. Consequently, a second method of assessing the differences between simulated and measured concentrations, the root mean squared error (RMSE) approach (Anderson and Woessner, 1992), was employed. A trial-and-error methodology, in which various parameter choices are tested to determine their effect on model residuals, was required to establish an appropriate RMSE value. Generally, an RMSE value on the order of the observed calibration targets (i.e., water quality concentrations) is typical. The RMSE criteria ultimately selected for the uranium and molybdenum simulations were 0.35 parts per million (ppm) and 0.45 ppm, respectively.

## 7.6 Numerical Parameters

The input parameters and distributions used in these simulations are shown in Tables 7.1, 7.2, and 7.3, for source term, unsaturated zone, and saturated zone parameters, respectively. A

parameter not included in the tables is the half-life of uranium, which is assumed to be $1 \times 10^9$ years. The data presented in these tables was derived from several sources: 1) site specific data and analyses, when available; 2) literature information; and 3) expert judgment, including trial and error in the modeling runs. Tables 7.1, 7.2, and 7.3 contain an annotation on the source of the information used for each of the parameters.

**Table 7.1 - Source Term Parameters**

| TYPE OF PARAMETER | NAME OF PARAMETER [UNITS] | VALUE OR DISTRIBUTION | JUSTIFICATION FOR DATA |
|---|---|---|---|
| **Geometry** | Center of mass, X coord. [ft] | Uniform, min = 7440, max = 7570 | Based on measurements at site, DOE (1985a). |
| | Center of mass, Y coord. [ft] | Uniform, min = 10100, max = 10200 | Based on measurements at site, DOE (1985a). |
| | Length [ft] | Uniform, min = 1540, max = 1670 | Based on measurements at site, DOE (1985a). |
| | Width [ft] | Uniform, min = 1180, max = 1310 | Based on measurements at site, DOE (1985a). |
| | Thickness [ft] | Uniform, min = 1.6, max = 4.9 | Based on information in DOE (1985a). |
| **Flow** | Infiltration rate [ft/yr] | Uniform, min = 0.26, max = 0.36 | Expert judgment; model trials. |
| | Saturated hydraulic conductivity [ft/d] | Lognormal, min = 3.5, max = 18.0 | Based on information in DOE (1985a) and SNL (1996). |
| | Porosity | Normal, $\mu = 0.3$, $\sigma = 0.02$ | Based on information in DOE (1985a) and general literature. |
| | Residual water content | Normal, $\mu = 0.05$, $\sigma = 0.002$ | General literature. |
| | van Genuchten n factor | Normal, $\mu = 3.9$, $\sigma = 0.5$ | General literature. |
| **Fate & Transport** | Initial Soil Concentration [ppm] | Uranium: Normal, min = 0.5, max = 4; Molybdenum: Normal, min = 2, max = 8; | Expert judgment; model trials. |
| | Solubility of contaminant [ppm] | Uranium: 100; Molybdenum: 100 | General literature. |
| | Distribution coefficient [cc/g][1] | Uranium: Uniform, min = 0.05, max = 0.1; Molybdenum: Uniform, min = 0.05, max = 0.1; | DOE (1983) and general literature. |
| | Dry bulk density [g/cc][1] | 1.7 | General literature. |
| | Time since waste release [y] | 39 | DOE (1985a). |
| | Pulse duration [y] | Uniform, min = 10, max =15 | Expert judgment; model trials. |

[1]Common unit of expression

**Table 7.2 - Unsaturated Zone Parameters**

| TYPE OF PARAMETER | NAME OF PARAMETER [UNITS] | VALUE OR DISTRIBUTION | JUSTIFICATION FOR DATA |
|---|---|---|---|
| **Geometry** | Thickness [ft] | Uniform, min = 5.2, max = 8.2 | DOE (1985a). |
| **Flow** | Saturated hydraulic conductivity [ft/d] | Lognormal, min = 3.5, max = 18.0 | DOE (1985a) and SNL (1996). |
| | Porosity | Normal, $\mu = 0.3$, $\sigma = 0.02$ | Based on information in DOE (1985a) and general literature. |
| | Residual water content | Normal, $\mu = 0.05$, $\sigma = 0.002$ | General literature. |
| | van Genuchten $\alpha$ coefficient [1/ft] | Normal, $\mu = 0.1$, $\sigma = 0.015$ | General literature. |
| | van Genuchten n factor | Normal, $\mu = 3.9$, $\sigma = 0.5$ | General literature. |
| **Fate & Transport** | Longitudinal dispersivity [ft] | Uniform: min = 1.6, max = 3.3 | Expert judgment and general literature. |
| | Distribution coefficient [cc/g] [1] | Uranium: Uniform, min = 0.05, max = 0.1; Molybdenum: Uniform, min = 0.05, max = 0.1; | DOE (1983) and general literature. |
| | Dry bulk density [g/cc] [1] | 1.8 | General literature. |

[1]Common unit of expression

**Table 7.3 - Saturated Zone Parameters**

| TYPE OF PARAMETER | NAME OF PARAMETER [UNITS] | VALUE OR DISTRIBUTION | JUSTIFICATION FOR DATA |
|---|---|---|---|
| **Geometry** | Thickness [ft] | Uniform, min = 5, max = 6 | DOE (1985a). |
| **Flow** | Down gradient flow direction (counterclockwise from due east) [degrees] | Uniform, min = 310, max = 315 | DOE (1985a) and expert judgment. |
| | Hydraulic gradient (horizontal) | Normal, $\mu = 0.0028$, $\sigma = 0.0003$ | DOE (1985a) and expert judgment. |
| | Recharge rate [ft/y] | Normal, $\mu = 0.07$, $\sigma = 0.01$ | Expert judgment and general literature. |
| | Mean saturated hydraulic conductivity [ft/d] | 57 | DOE (1985a), SNL (1996) and model trials. |
| | Hydraulic conductivity anisotropy (H/V) | 100 | Expert judgment and general literature. |
| | Porosity | Normal, $\mu = 0.3$, $\sigma = 0.02$ | DOE (1985a) and general literature. |
| **Fate & Transport** | Longitudinal dispersivity [ft] | Uniform: min = 160, max = 230 | Expert judgment and general literature. |
| | Dispersion anisotropy [long./trans] | Uniform: min = 10, max = 20 | Expert judgment and general literature. |
| | Distribution coefficient [cc/g] [1] | Uranium: Uniform, min = 0.1, max = 0.2; Molybdenum: Uniform, min = 0.1, max = 0.3. | DOE (1983) and general literature. |
| | Dry bulk density [g/cc] [1] | 1.8 | General literature. |
| | Tortuosity | 0.39 | General literature. |

[1]Common unit of expression

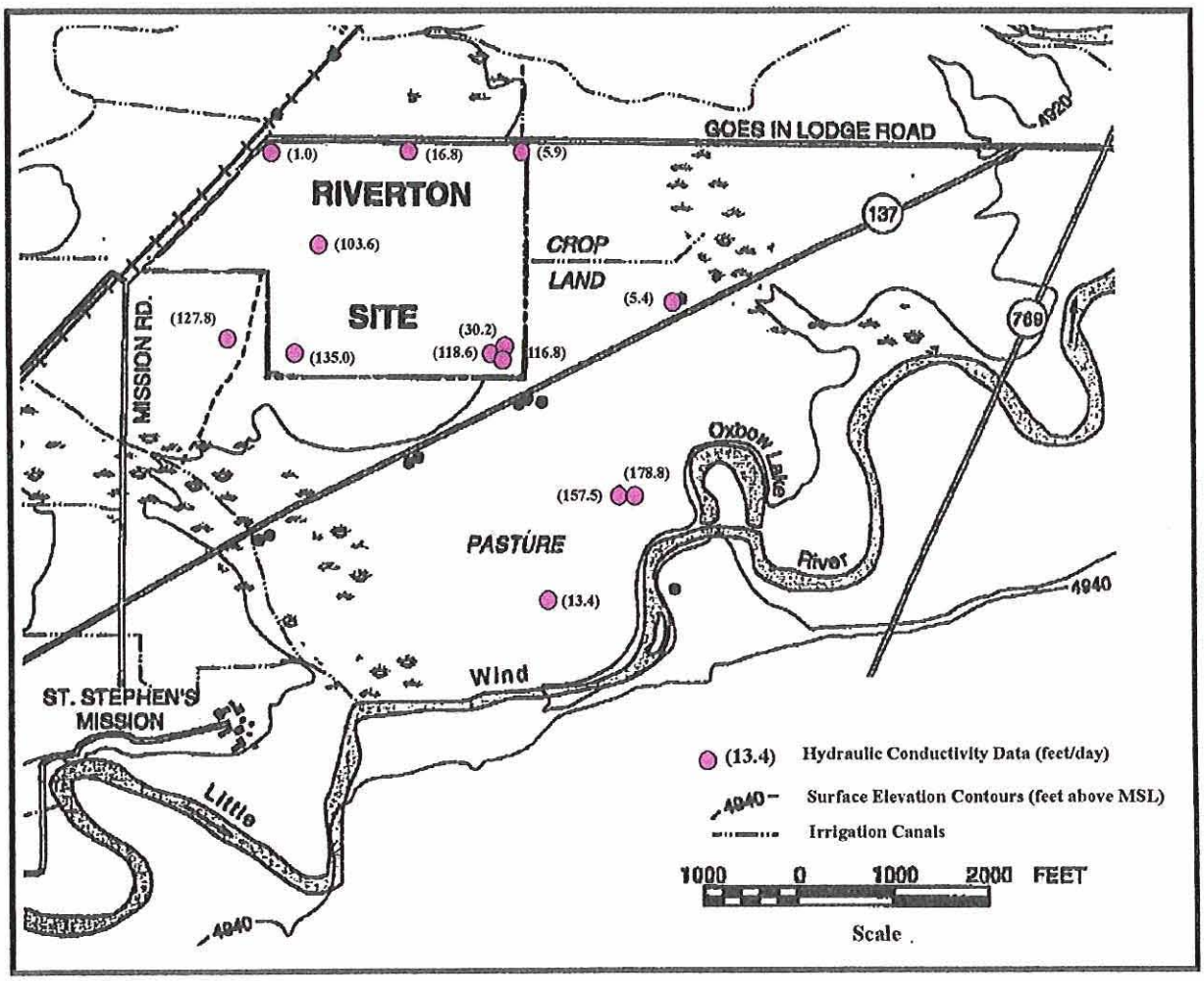



**Figure 7.1 - Hydraulic Conductivity Data Used in Geostatistical Modeling of Spatial Variability, From DOE (1985a)**

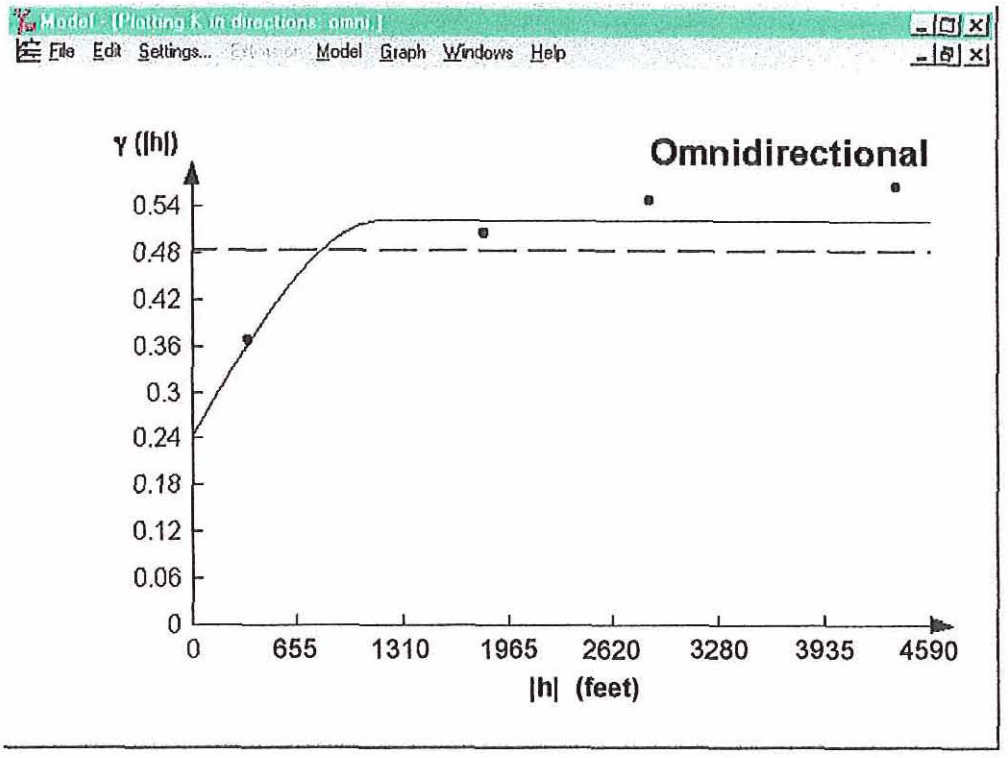



**Figure 7.2 - Variography Results for Hydraulic Conductivity Data**

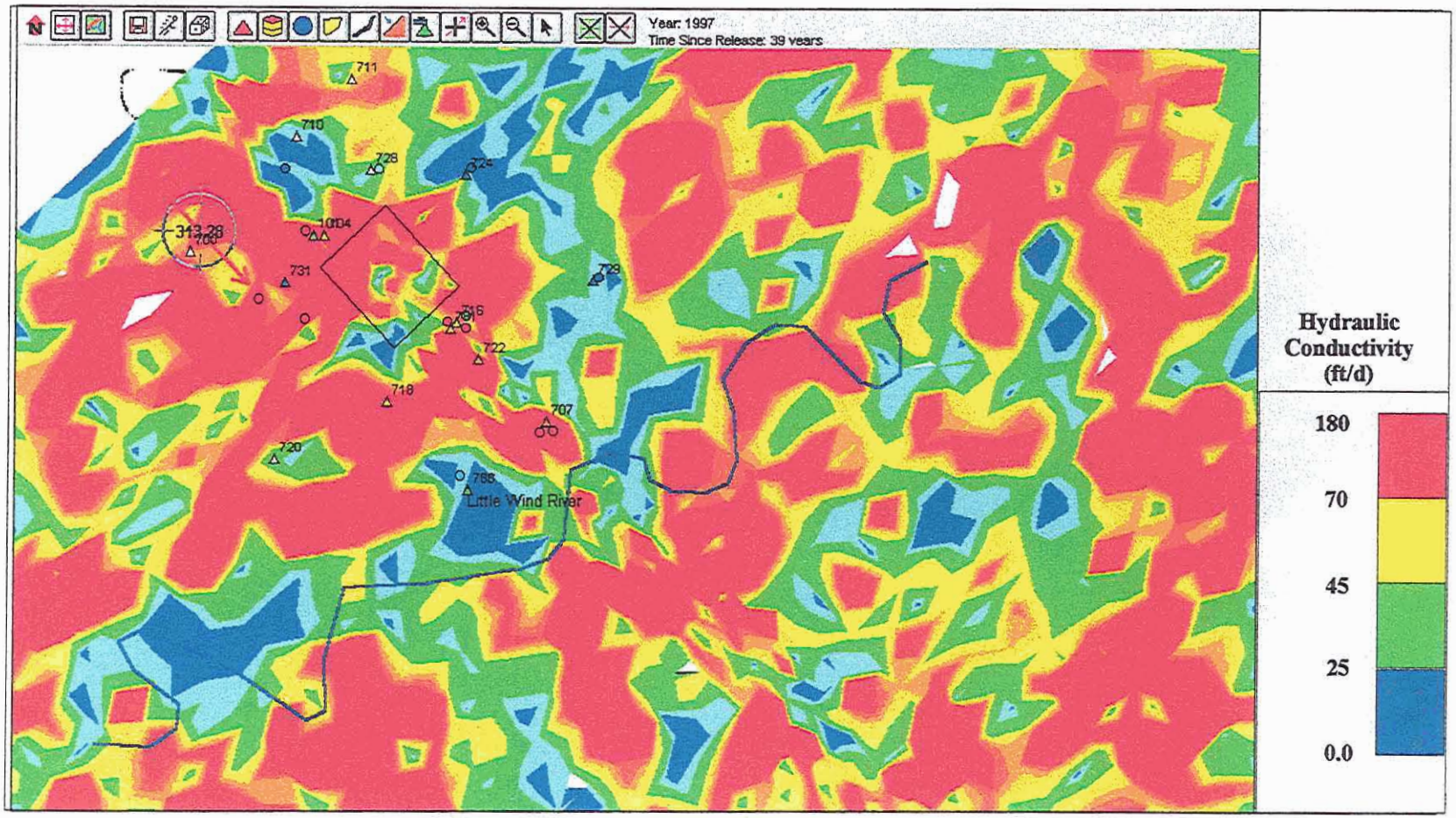



Figure 7.3 - Sample Hydraulic Conductivity Distribution From Geostatistical Simulator

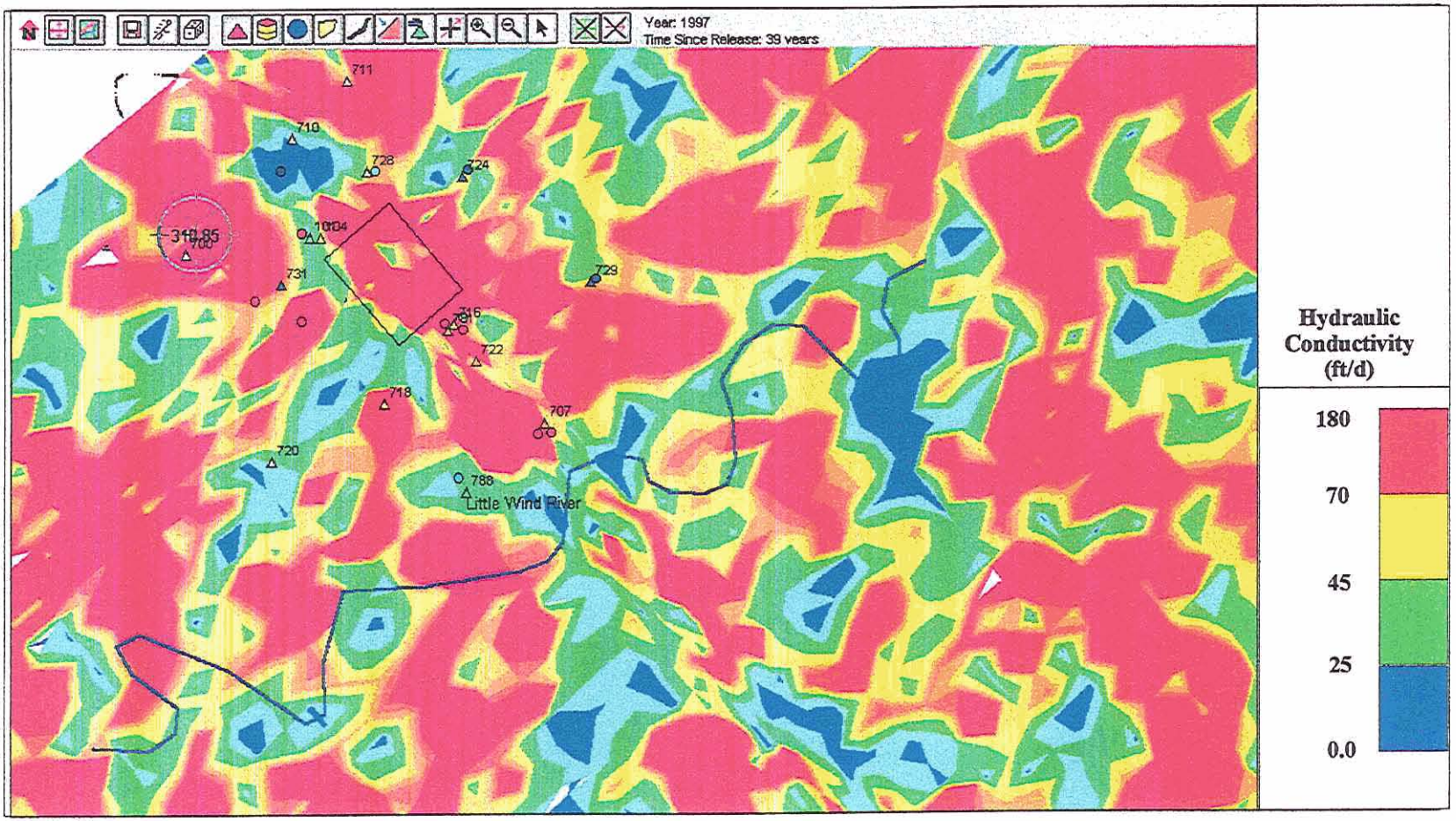



**Figure 7.4 - Sample Hydraulic Conductivity Distribution From Geostatistical Simulator**

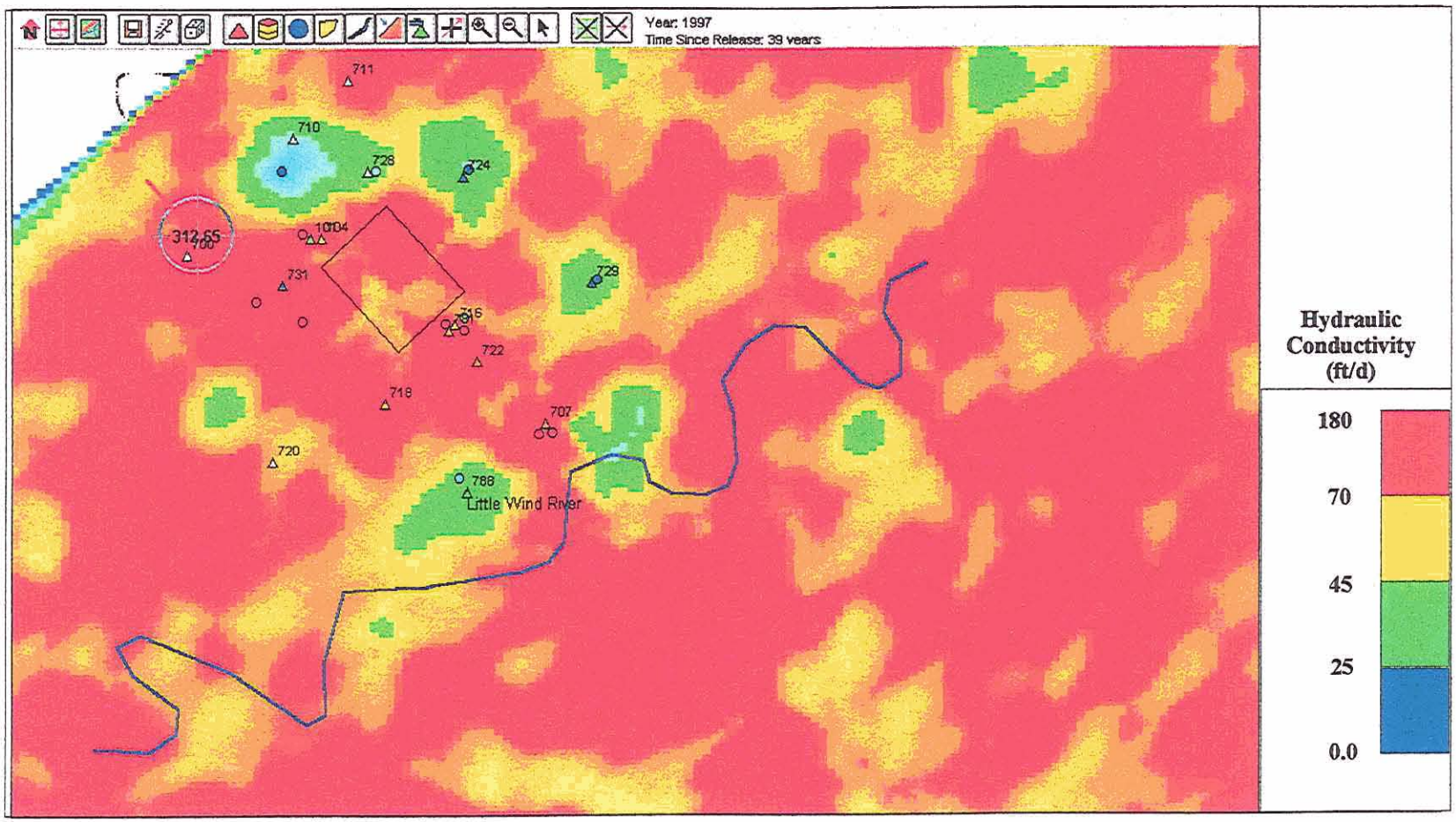



**Figure 7.5 - Average Hydraulic Conductivity Distribution From Geostatistical Simulator for all Monte Carlo Runs**

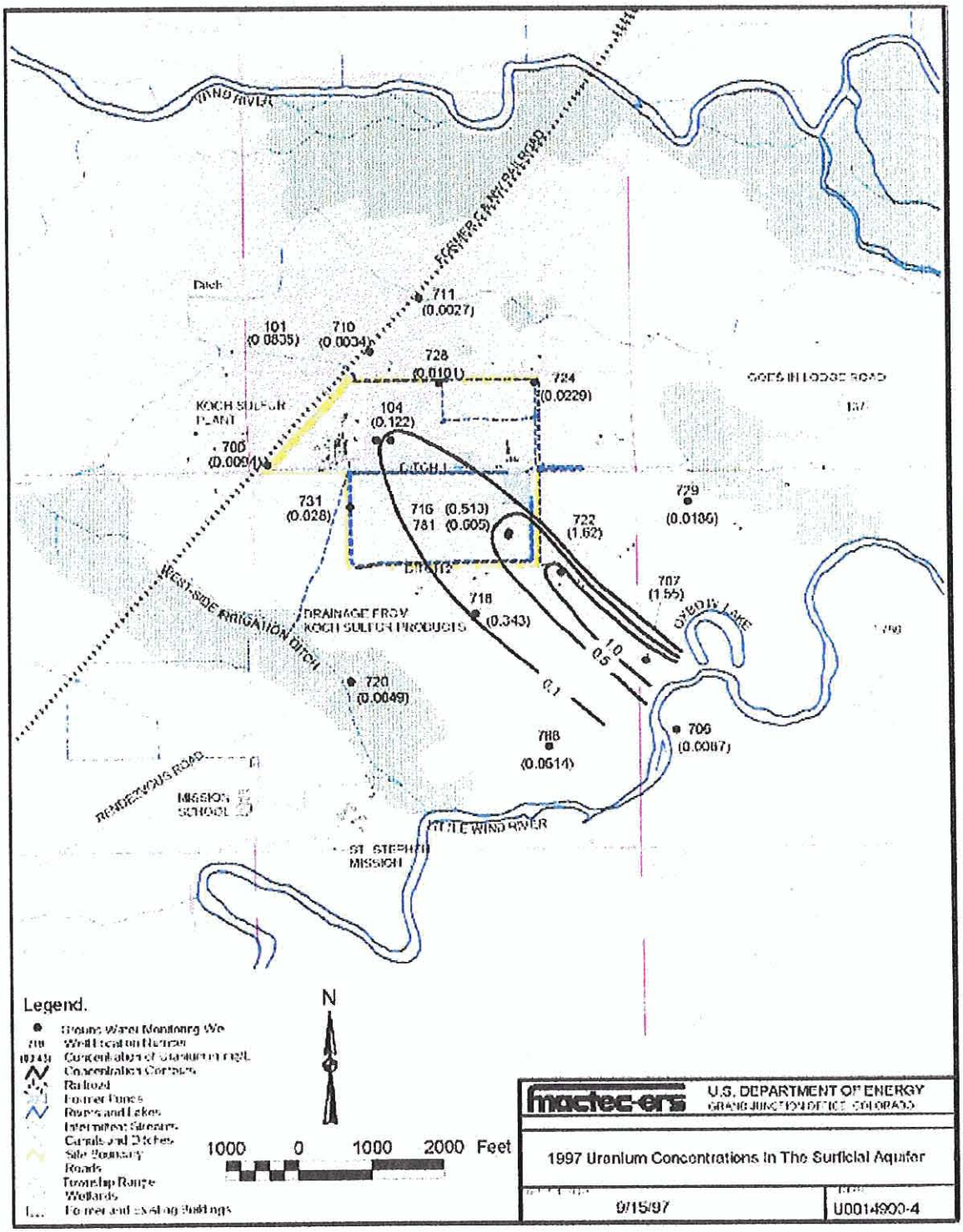



**Figure 7.6 - Water Quality Data for Uranium From 1997 Sampling**

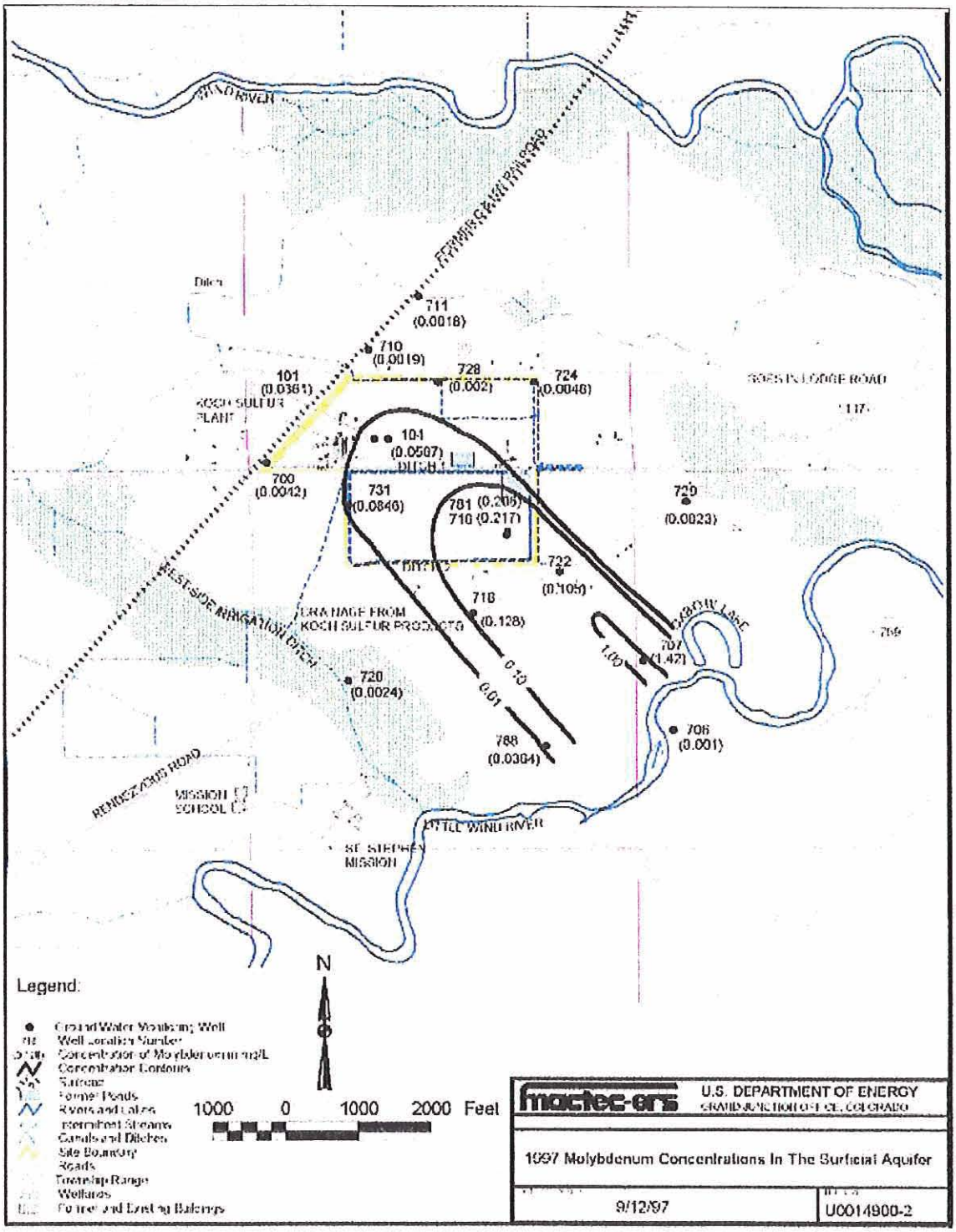



**Figure 7.7 - Water Quality Data for Molybdenum From 1997 Sampling**

## 8. Calibration

As mentioned above, the procedures used in GANDT to assume that model runs perform reasonably well in matching site conditions is quite different from traditional flow model calibration techniques based on matching observed hydraulic heads. Specifically, GANDT employs a post-conditioning algorithm that is based on the comparison of observed and simulated water quality data. The post-conditioning exercise is automated in the Monte Carlo simulation framework.

### 8.1 Qualitative/Quantitative Analysis

Post-conditioning results are somewhat a reflection of the appropriateness of available water quality data. Occasionally, when limited field data or inappropriate data (e.g., laboratory data that does not reflect field conditions) are used, few, if any, simulations meet the conditioning criteria. If the collected concentration data are representative of site contamination, one would expect a greater number of model runs to honor these data and pass the conditioning tests.

In a Monte Carlo analysis that incorporates LHS, it is theoretically possible to quantify uncertainties in the modeling results with as little runs as 4/3 times the number of uncertain variables. In practice a factor of 2 to 4 is recommended. There are 30 uncertain parameters in the analyses performed here for the Riverton site. Therefore, a minimum of 60 runs passing the conditioning test is desired. Using the flow, fate, and transport parameters listed in Tables 7.1, 7.2, and 7.3, and the RMSE criteria prescribed in Section 7.5, 68 runs out of 100 total met conditioning criteria in the uranium analyses, and 63 passed for the molybdenum analyses. The results of these analyses are presented in a subsequent section.

In an early review of this work, a concern was raised regarding the ability of the GANDT code to approximate the hydraulic head distribution generally observed at the Riverton site. To help

address this concern, GANDT was modified under this study to output hydraulic head information in ASCII format. The simulated heads form selected model runs were processed and compared with observed data, both numerically and graphically, to evaluate the appropriateness of the hydrologic information used in the simulations.

As a brief demonstration of the appropriateness of the model-produced hydraulic heads, results from several model runs are presented here. Each model run in the Monte Carlo suite was analyzed to compare simulated heads at representative monitoring wells with the observed hydraulic head elevations from the 1997 monitoring data. The comparison of simulated and measured heads for each run made use of a Root Mean Square Error (RMSE) analysis. Of all the Monte Carlo runs, the simulation with the best fit to observed data had an RMSE of 1.73 feet, whereas the simulation with the largest RMSE had a value of 2.95 feet. Figure 8.1 shows a contour plot of hydraulic heads developed from sampling data taken during 1997. These can be compared to the hydraulic head elevations from the simulation with the largest RMSE, shown in Figure 8.2. Figure 8.3 shows the head distribution for the model run with the smallest RMSE.

Other comparisons also help to assess the ability of the Monte Carlo simulations to represent groundwater flow conditions. The monitoring data depicted in Figure 8.1 are indicative of a groundwater flow system with a hydraulic gradient of about 0.0024. Heads from a Monte Carlo model run that exhibited a hydraulic gradient approximating 0.0024 are shown in Figure 8.4 for comparison. This model run had an RMSE of 2.25 feet. Finally, the head elevations from all model runs in the Monte Carlo suite were averaged and plotted in Figure 8.5. When compared with measured water levels, the average head distribution had an RMSE of 2.13 feet. It is concluded from all of these comparisons that the Monte Carlo simulations do reasonably well in replicating existing flow conditions, and that traditional flow calibration methods applied to this flow system would not necessarily provide better matches with existing data.

The computed rate of groundwater discharge to the Little Wind River in the Monte Carlo simulations that met conditioning criteria varied depending on saturated zone parameters such as spatially varying hydraulic conductivity, hydraulic gradient, and aquifer thickness. Though no detailed analyses of these discharges were carried out, cursory examination of several of the simulations' mass balance results indicated that the groundwater discharge rate to the river generally ranged between 1200 and 1700 $ft^3/yr$ per foot of stream length.

## 8.2 Sensitivity Analysis

A formal sensitivity analysis with the Riverton simulations was not performed. The GANDT analysis resulted in a quantitative expression of the flow and transport uncertainty, which is a higher order step than intended by a conventional sensitivity analysis in terms of addressing variability or reliability in the results.

## 8.3 Model Application Verification

No additional time steps were evaluated against observed data for a verification analysis. The built-in conditioning/calibration step is considered adequate in defending the representativeness of the simulations.

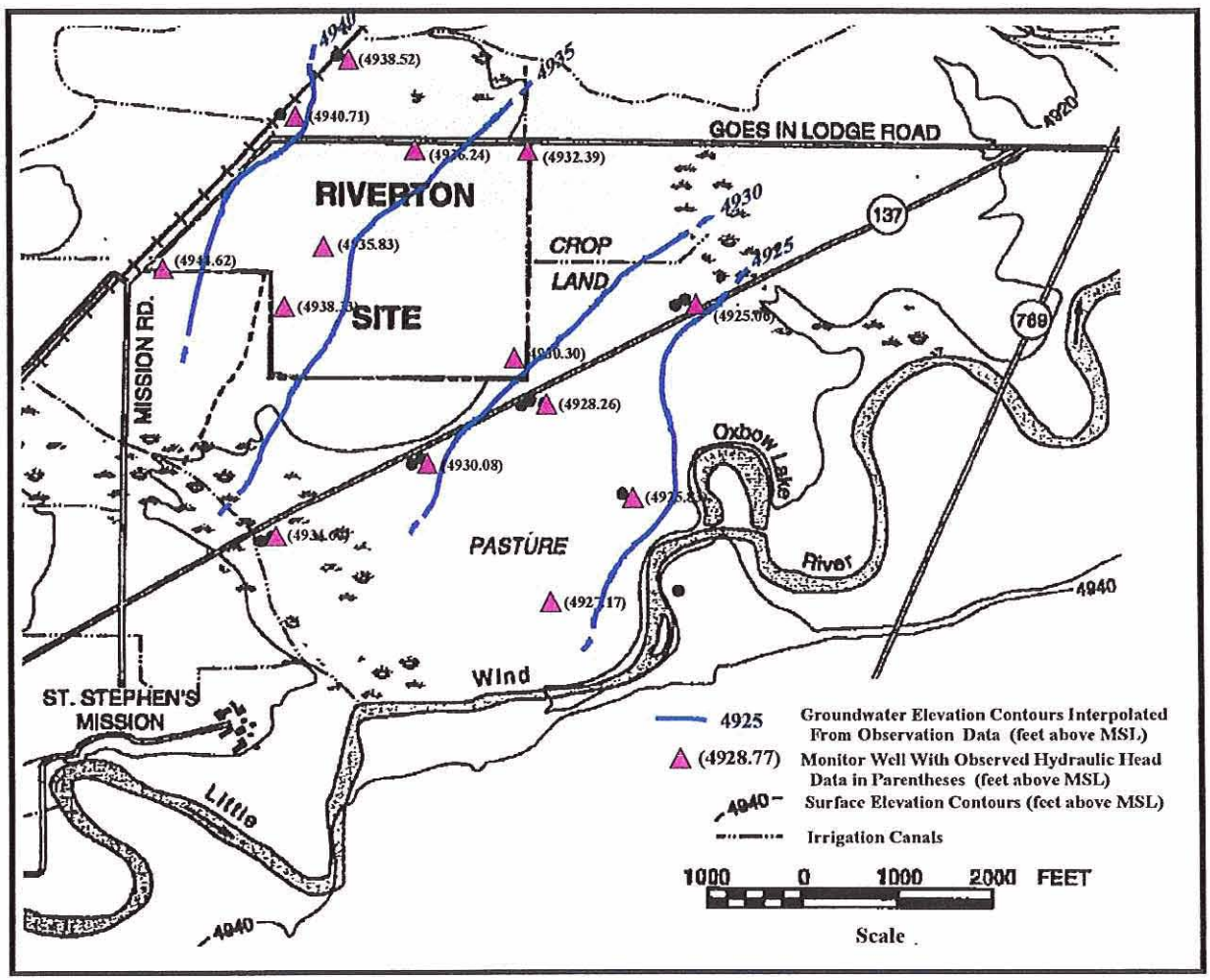



**Figure 8.1 - Groundwater Elevations From 1997 Observed Hydraulic Head Data**

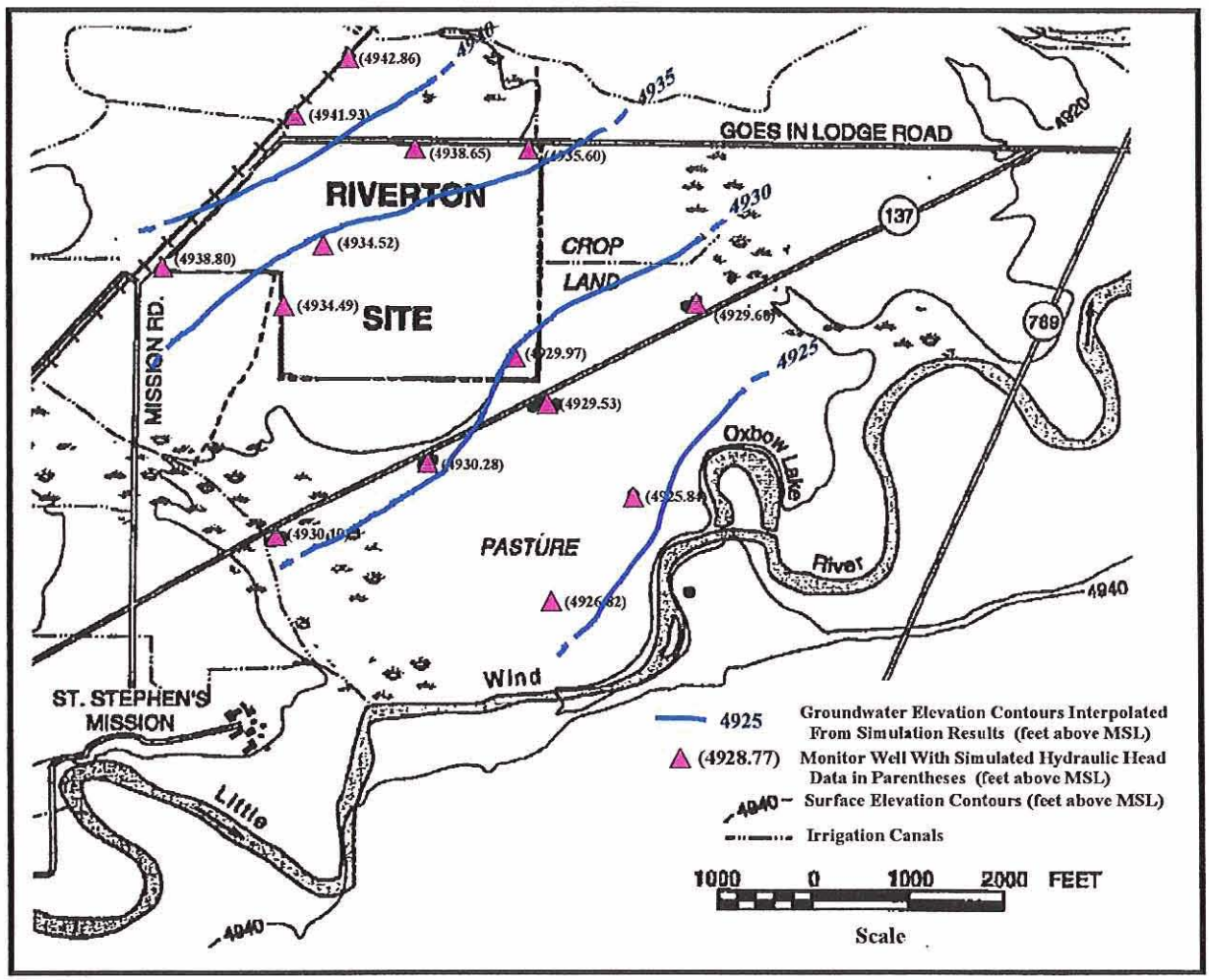



**Figure 8.2 - Groundwater Elevations From Simulation Run With Largest RMSE Compared to Observed Head Data (2.95 feet)**

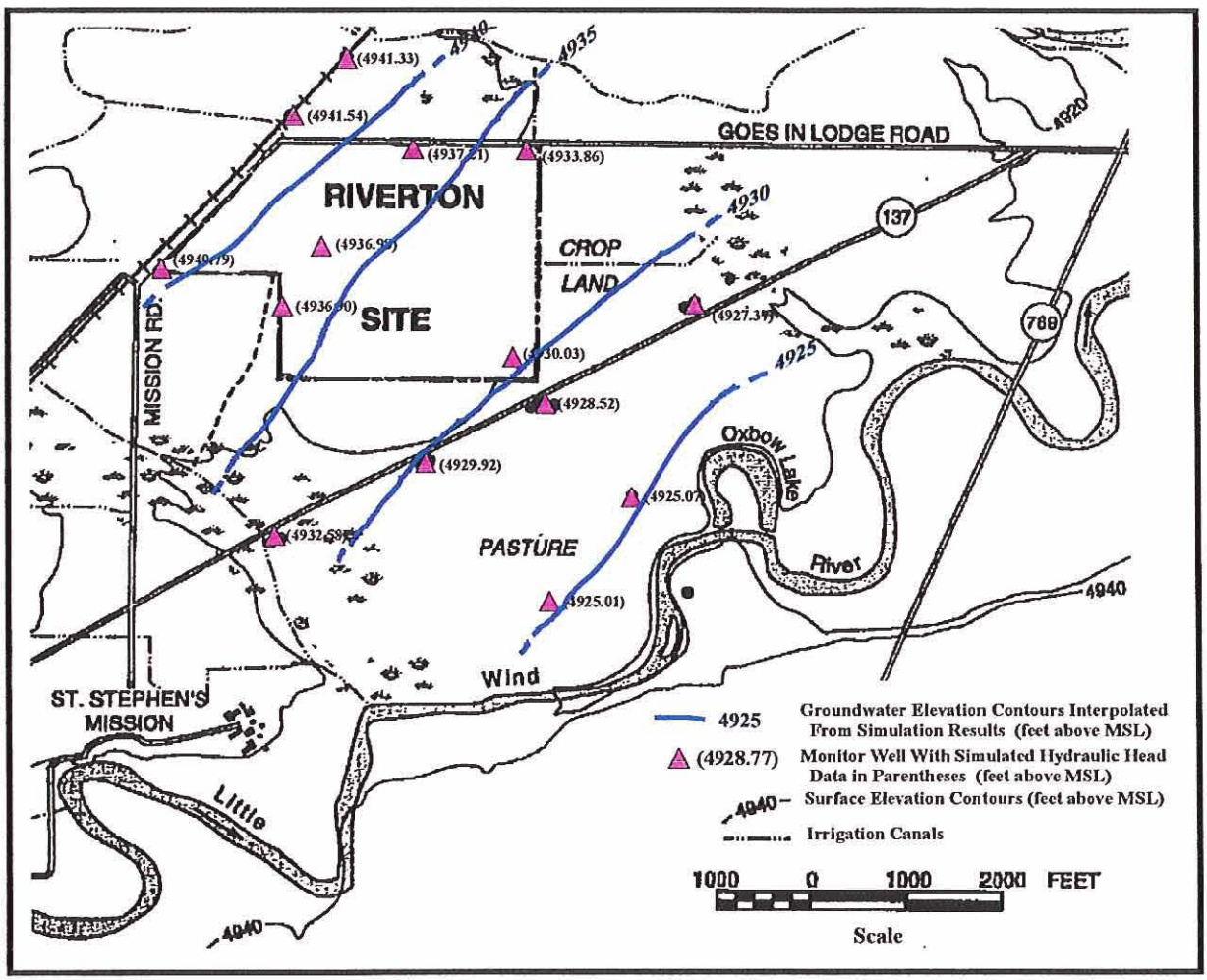



**Figure 8.3 - Groundwater Elevations From Simulation Run With Smallest RMSE Compared to Observed Head Data (1.73 feet)**

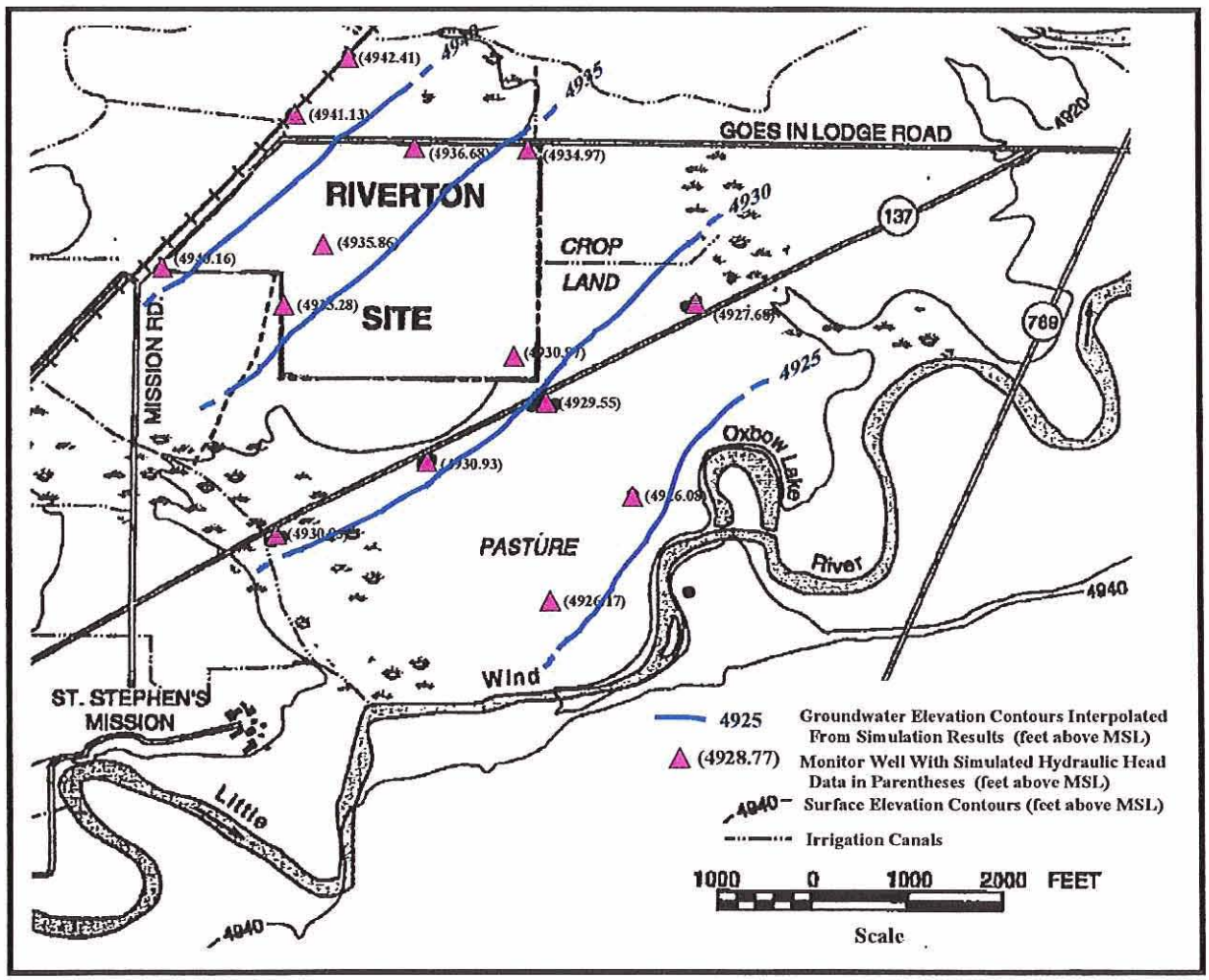



**Figure 8.4 - Groundwater Elevations From Simulation Run With Gradient That Matches Observed Hydraulic Head Gradient (0.0024)**

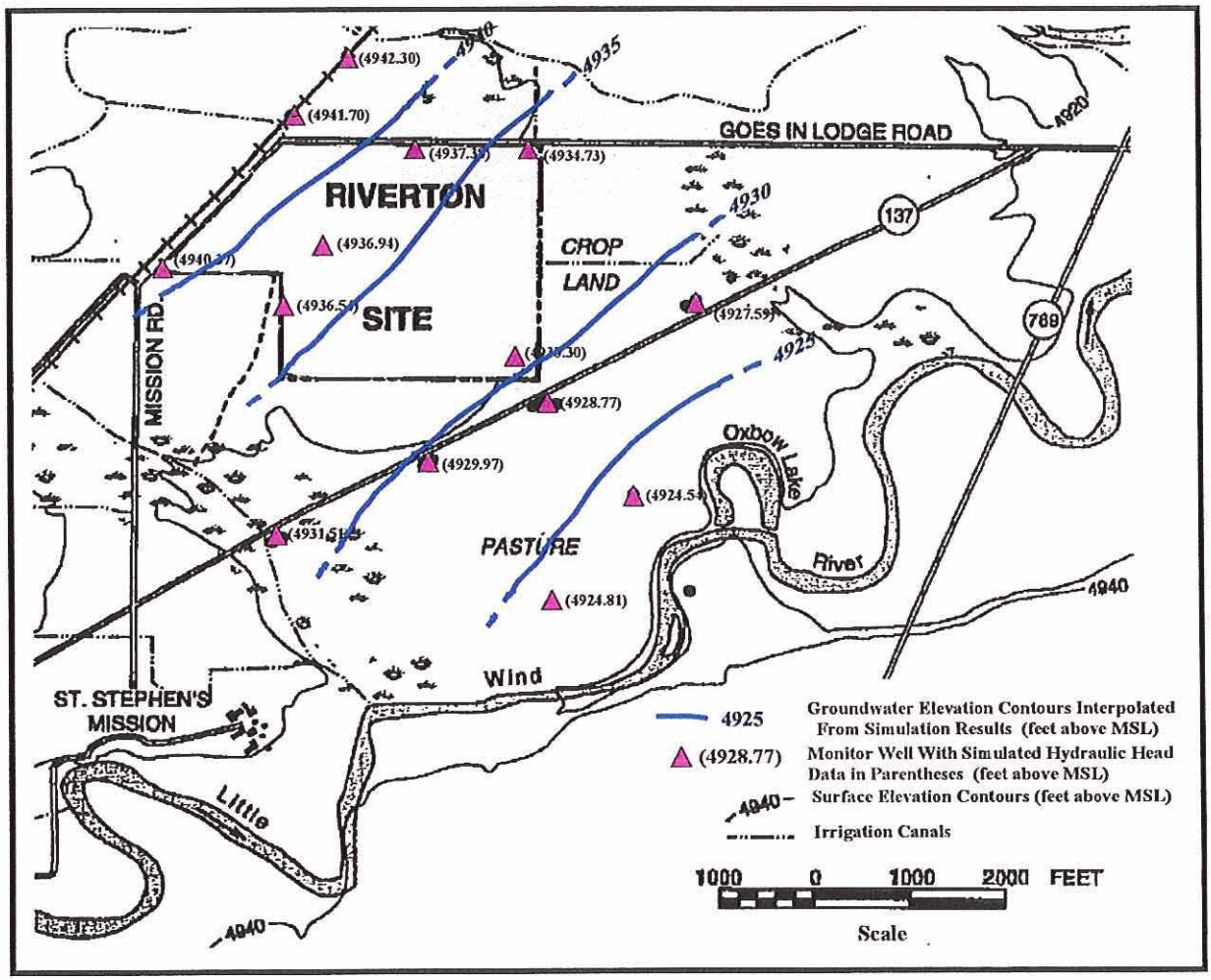



**Figure 8.5 - Groundwater Elevations From Average Head Data Computed From All Monte Carlo Simulations**

## 9. Predictive Simulations

Results of the predictive modeling simulations are quite encouraging with regard to the potential for natural attenuation as the preferred groundwater remedial alternative at the Riverton site. The modeling effort in this study yields a tremendous amount of information, both in the form of graphical and quantitative results. Most of the predictive modeling results are graphically presented for the purpose of showing the likelihood of natural attenuation. As part of this exercise, two types of plots have been selected for inclusion in the report.

The first type of plot contains the mean, or average, concentration distribution from all Monte Carlo runs that have met the conditioning criteria. The transient nature of the plume is visualized by displaying 4 separate time steps for the contaminants of concern: uranium and molybdenum.

The second type of graphic comprises a plot of the spatial distribution of the probability that concentrations are less than a specified threshold, preferably the contaminant's MCL. Such results are very useful in evaluating the likelihood of success of the proposed alternative. A plot indicating a very high probability that the concentrations are less than the MCL within a 100-year time frame is interpreted as a high likelihood of success for natural attenuation.

MCLs are used as the concentration thresholds in the uranium and molybdenum simulations. The MCLs for uranium and molybdenum are 0.044 parts per million (ppm) and 0.1 ppm, respectively.

Figures 9.1 through 9.4 show the mean contaminant plume distributions for uranium through time. Figure 9.1 represents the plume distribution in 1997, the time at which the post-conditioning analysis was performed. Figure 9.2 represents the plume distribution 25 years past 1997 (2022); Figure 9.3 represents 50 years past 1997 (2047); and Figure 9.4 represents 75 years past 1997 (2072). The modeling results at 100 years past 1997 (2097) showed that the uranium is completely flushed from the system by this time.

Figures 9.5 through 9.8 show the results of the spatial distribution of the probability that concentrations are less than the MCL for uranium of 0.044 ppm, during the years 1997, 2022, 2047, and 2072.

The average molybdenum concentration distribution results are shown in Figures 9.9 through 9.12, with the same sequential time frames as those shown in the uranium results. Figures 9.13 through 9.16 display the distribution of the probability that concentrations are less than the molybdenum MCL of 0.1 ppm. The molybdenum is completely flushed from the aquifer by the 100-year mark (2097).

The results of this analysis suggest that there is a high likelihood of success for natural attenuation processes to be effective as a preferred remedial alternative for Riverton groundwater. The uranium predictive simulations show a zero probability of exceeding the MCL (0.044 ppm) for this contaminant after 100 years of natural attenuation beyond recent conditions. The molybdenum is also completely flushed from the aquifer system within 100 years. A verification monitoring program is essential to determining the probability of success as suggested by the simulations in this study. This is particularly true given that the model runs presented here serve primarily as an aid in decision making.

The GANDT code has the capability of supplying the user with predicted water quality concentrations at each monitor well for each run in a Monte Carlo suite. Accordingly, a distribution of concentrations can be obtained for each well from the probabilistic analyses. Such a distribution serves as a good indicator for concentrations that would be expected during a verification monitoring program. Of greatest importance in evaluating the potential for natural attenuation is the statistical bounds of the predicted concentrations at the verification monitor wells. A plot of average concentrations at each output time, together with the minimum and maximum predicted concentrations, can serve as a guide to the verification monitoring activities. If future monitoring of these wells produces water quality concentrations within these predicted ranges, it is likely the site would be on schedule for flushing within a 100-year time frame. If,

however, the observed concentrations from future monitoring activities are above these predicted ranges, the site may need to undergo additional analyses to evaluate whether it is a viable candidate for natural attenuation.

Key verification monitoring wells located within the area of the contaminant plume include wells 707, 716, 718, and 722. Figures 9.17 through 9.20 show the predicted uranium concentration versus time behavior at each of these wells. The data points represent average concentrations predicted by the simulations, and the error bars delineate the minimum and maximum predicted concentrations. The min-max bounds in each plot provide an estimate of the acceptable range of verification monitoring results that would suggest natural attenuation will lead to site cleanup within 100 years. Also included in these plots is a horizontal line showing the MCL for uranium. Figures 9.21 through 9.24 show comparable transient molybdenum concentrations for each of the key verification monitoring wells.

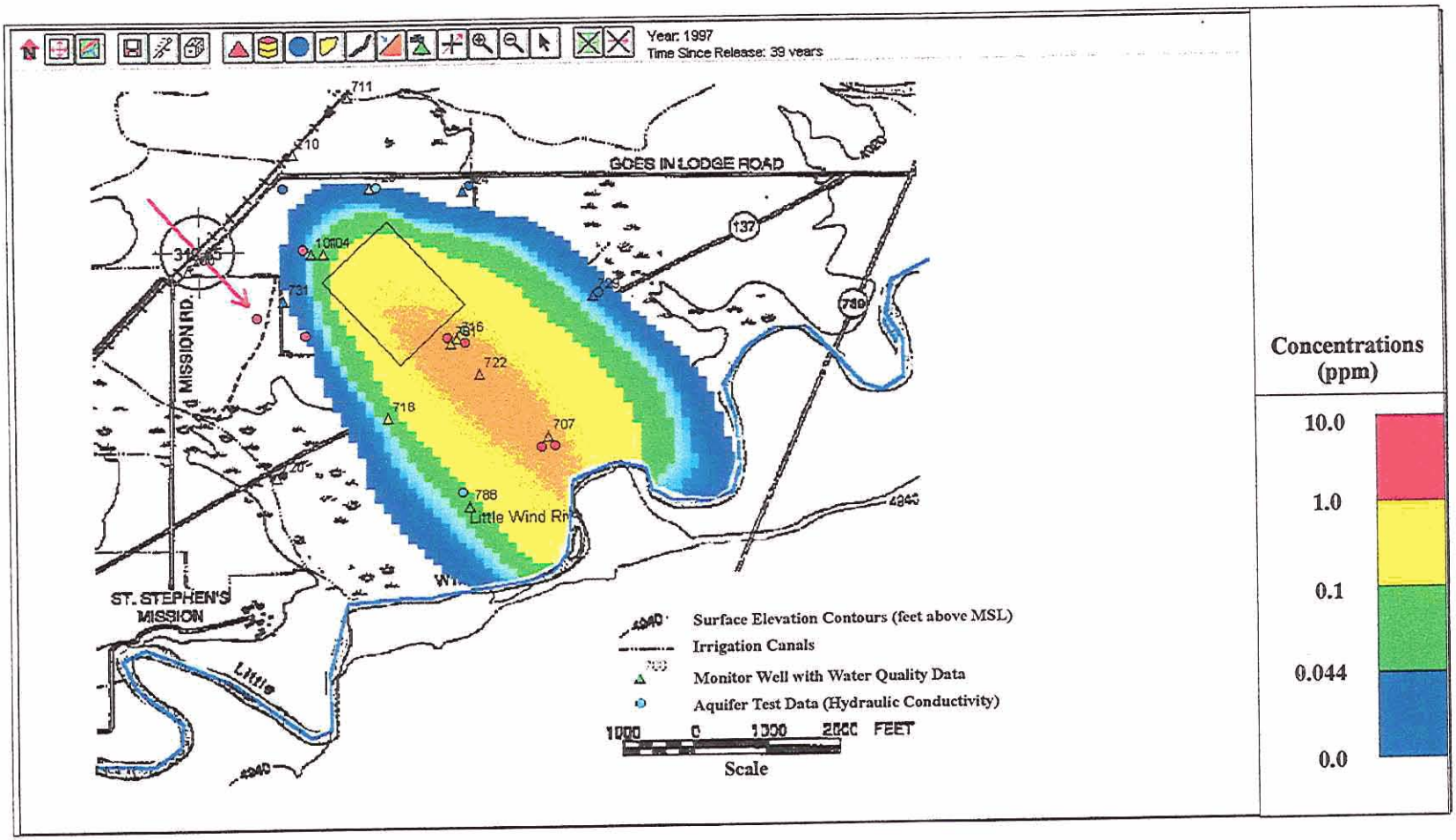



**Figure 9.1 - Mean Concentration Distribution of Uranium From Uncertainty Analysis, at Conditioning Time - 1997**

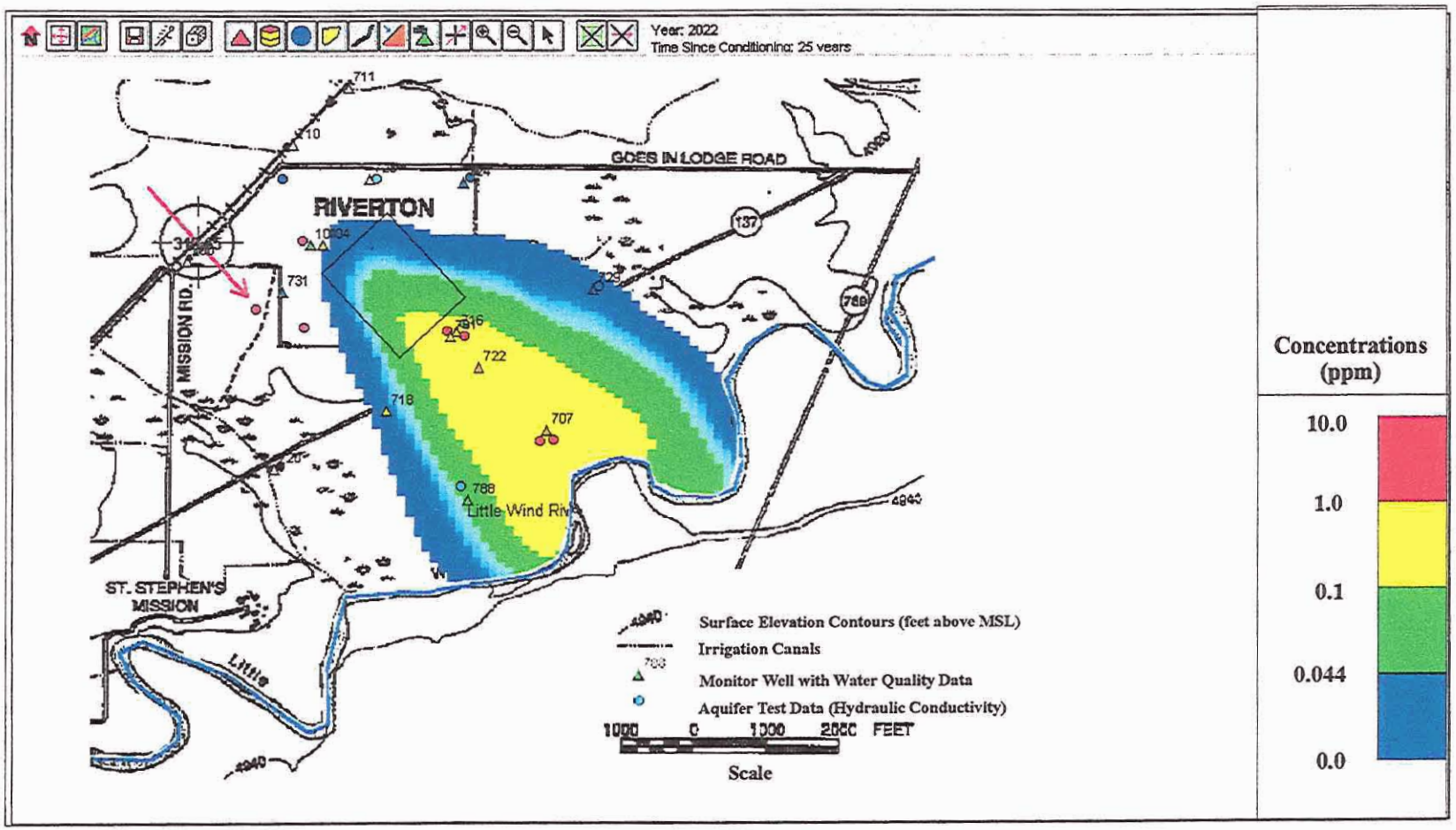



**Figure 9.2 - Mean Concentration Distribution of Uranium From Uncertainty Analysis, 25 Years After Conditioning Time -2022**

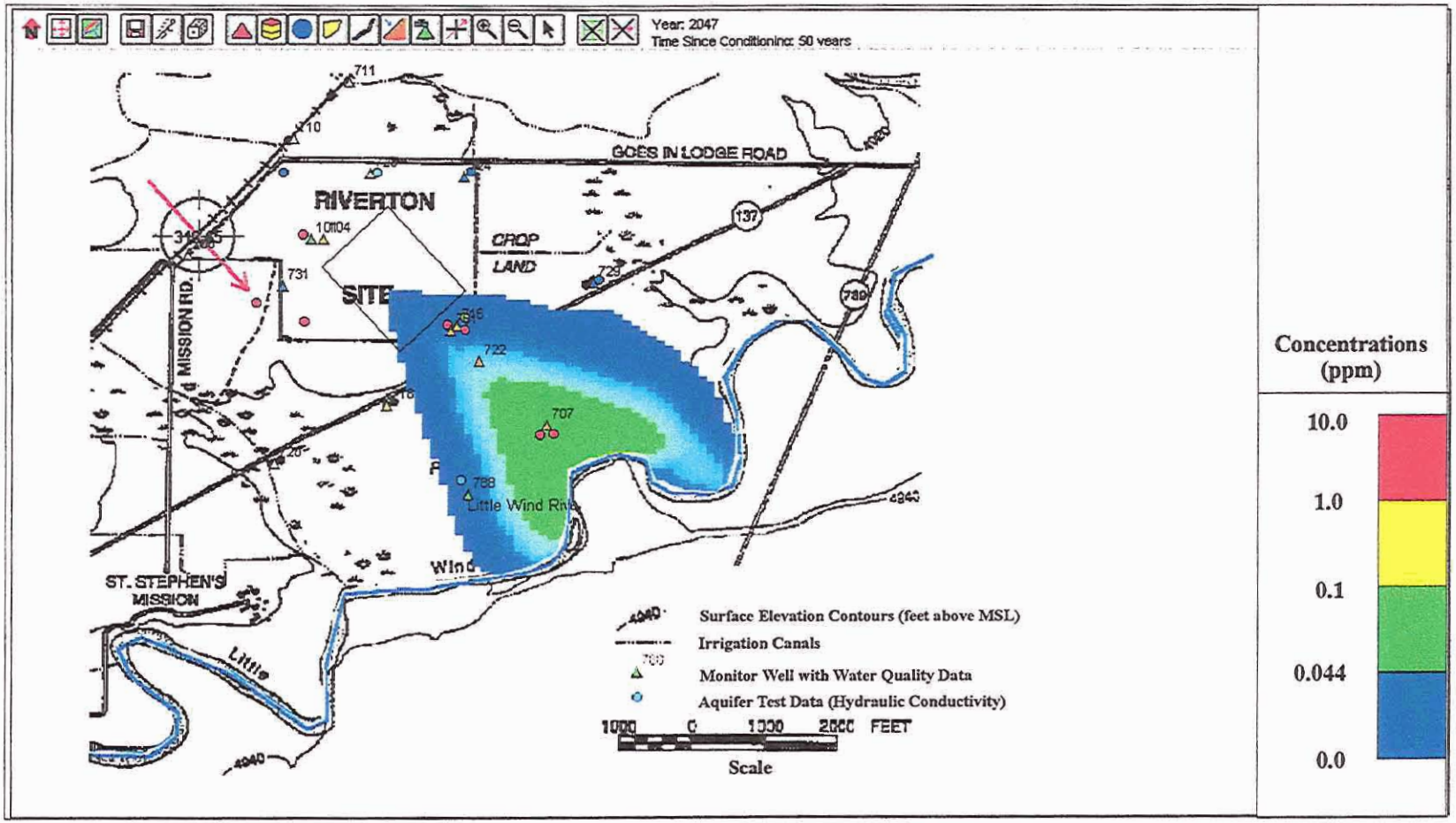



**Figure 9.3 - Mean Concentration Distribution of Uranium From Uncertainty Analysis, 50 Years After Conditioning Time - 2047**

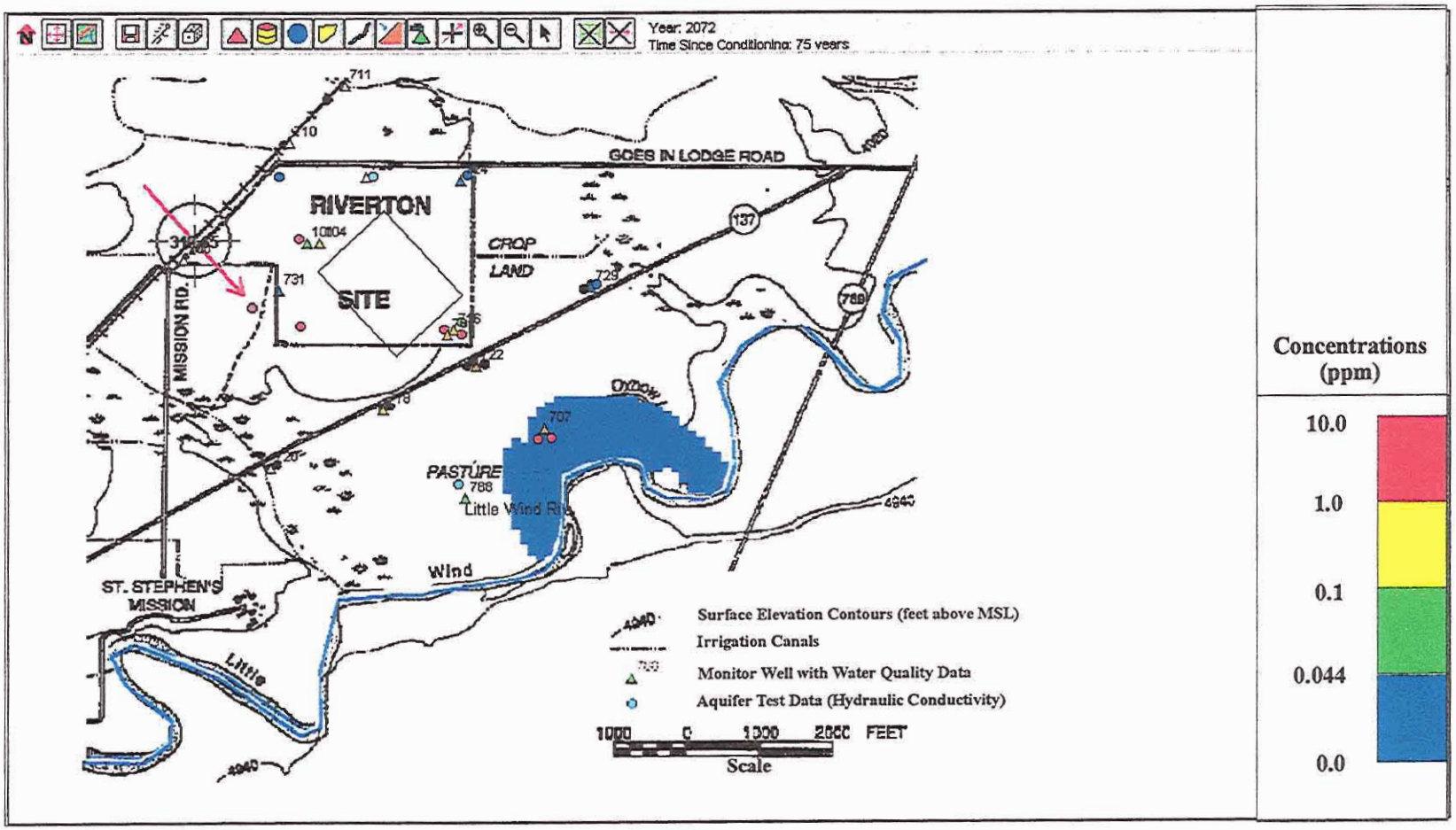



**Figure 9.4 - Mean Concentration Distribution of Uranium From Uncertainty Analysis, 75 Years After Conditioning Time - 2072**

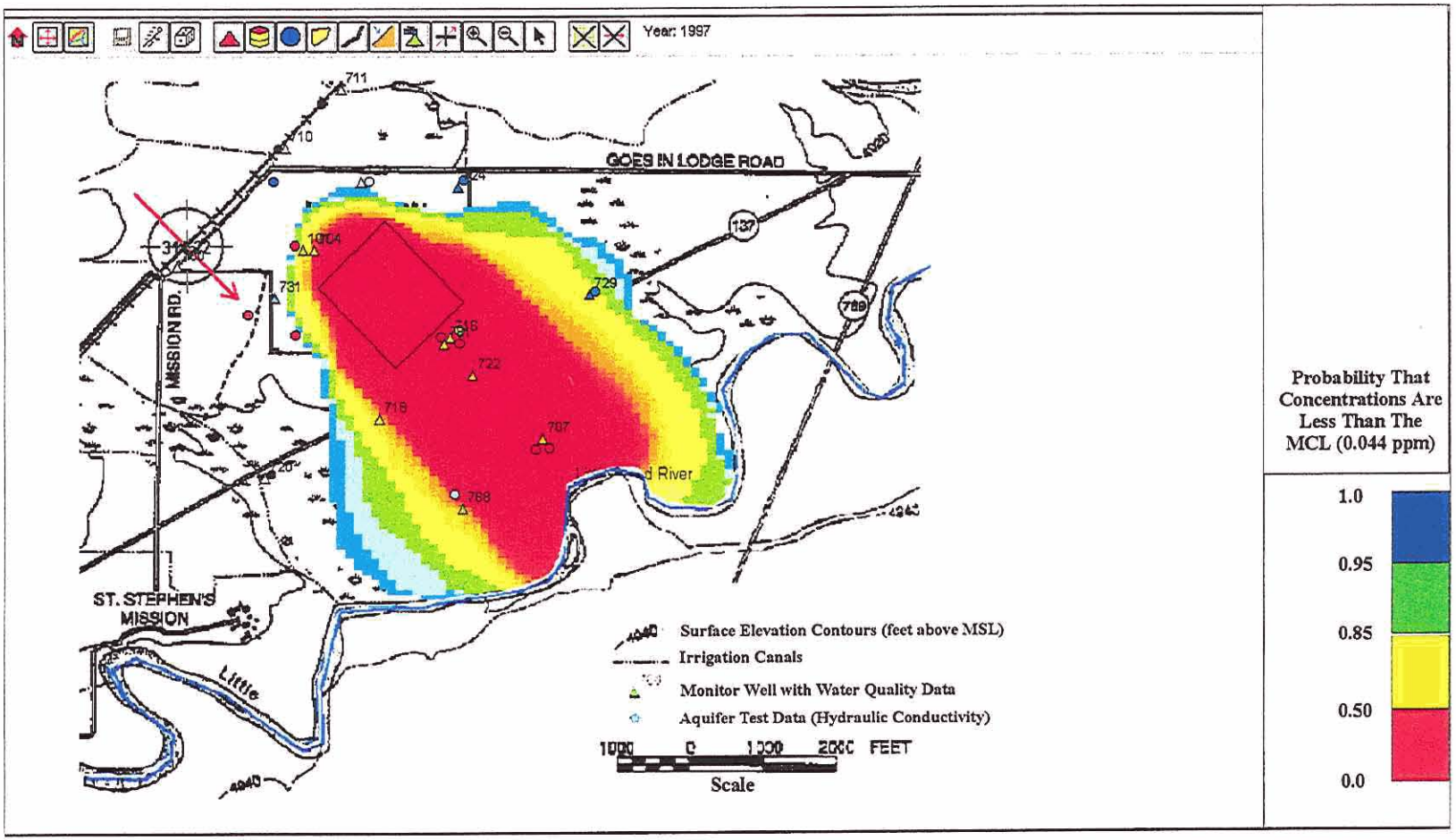



**Figure 9.5 - Probability That Concentrations Are Less Than The Uranium MCL From Uncertainty Analysis, at Conditioning Time - 1997**

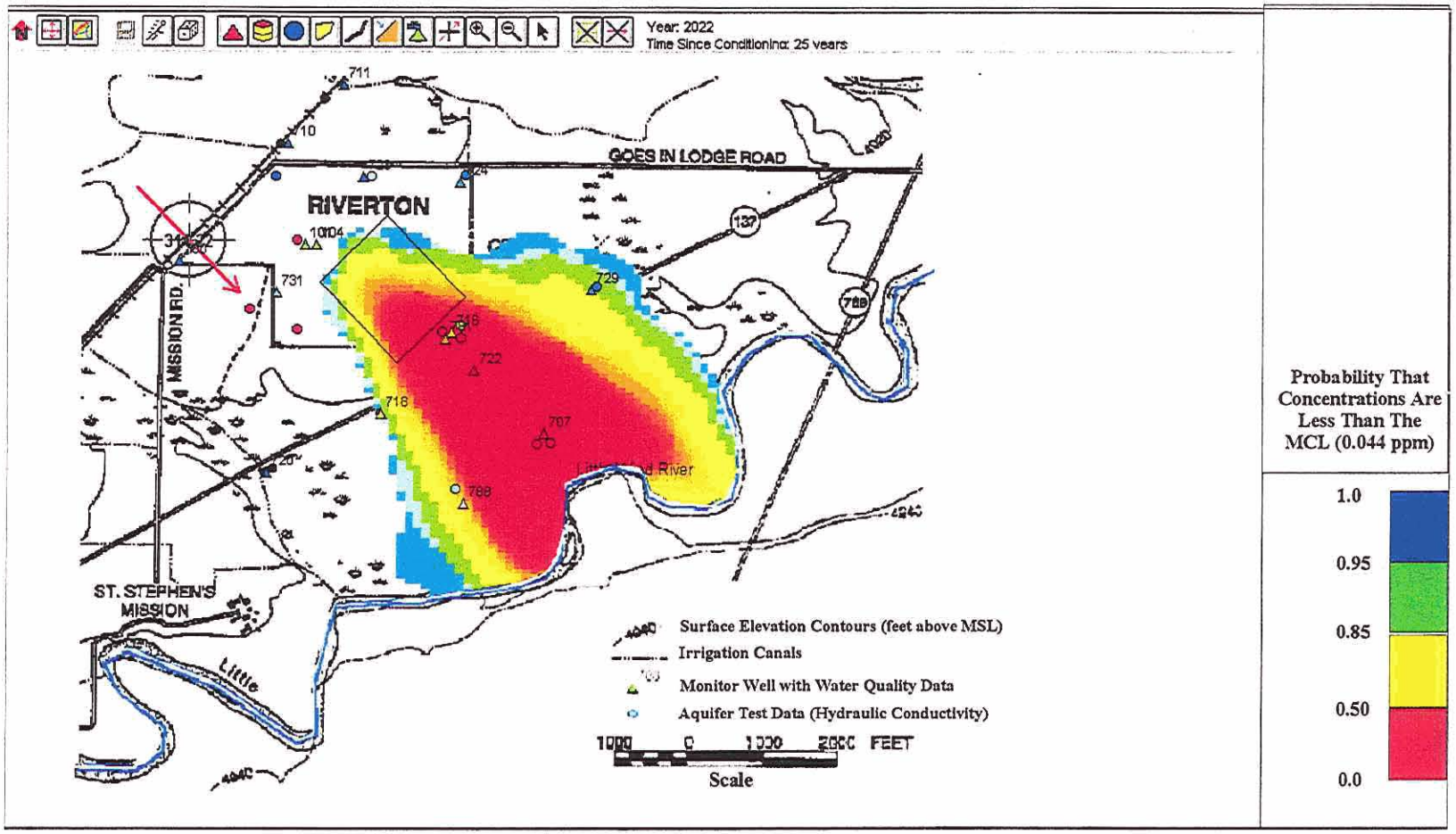



**Figure 9.6 - Probability That Concentrations Are Less Than The Uranium MCL From Uncertainty Analysis, 25 Years After Conditioning Time - 2022**

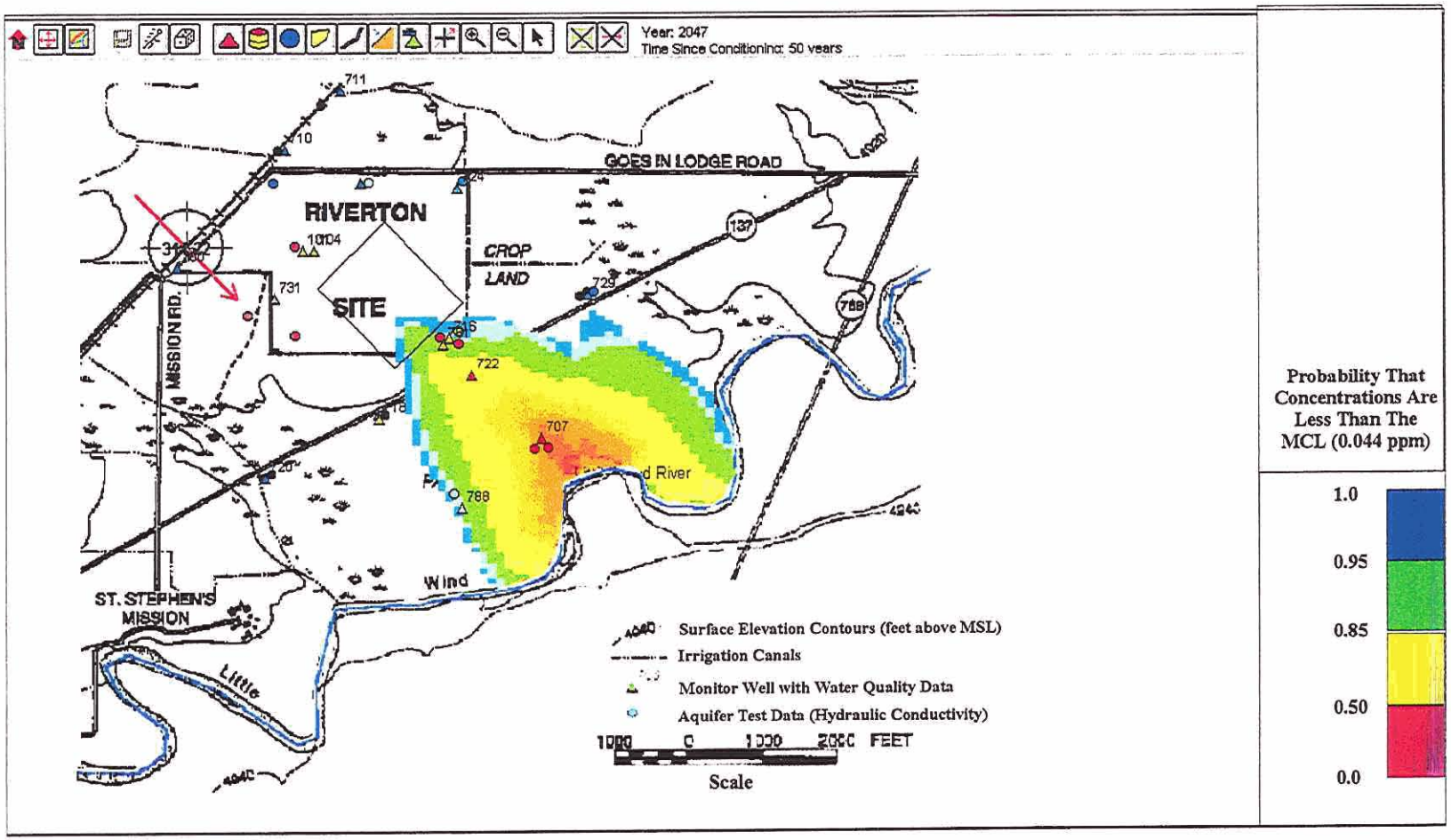
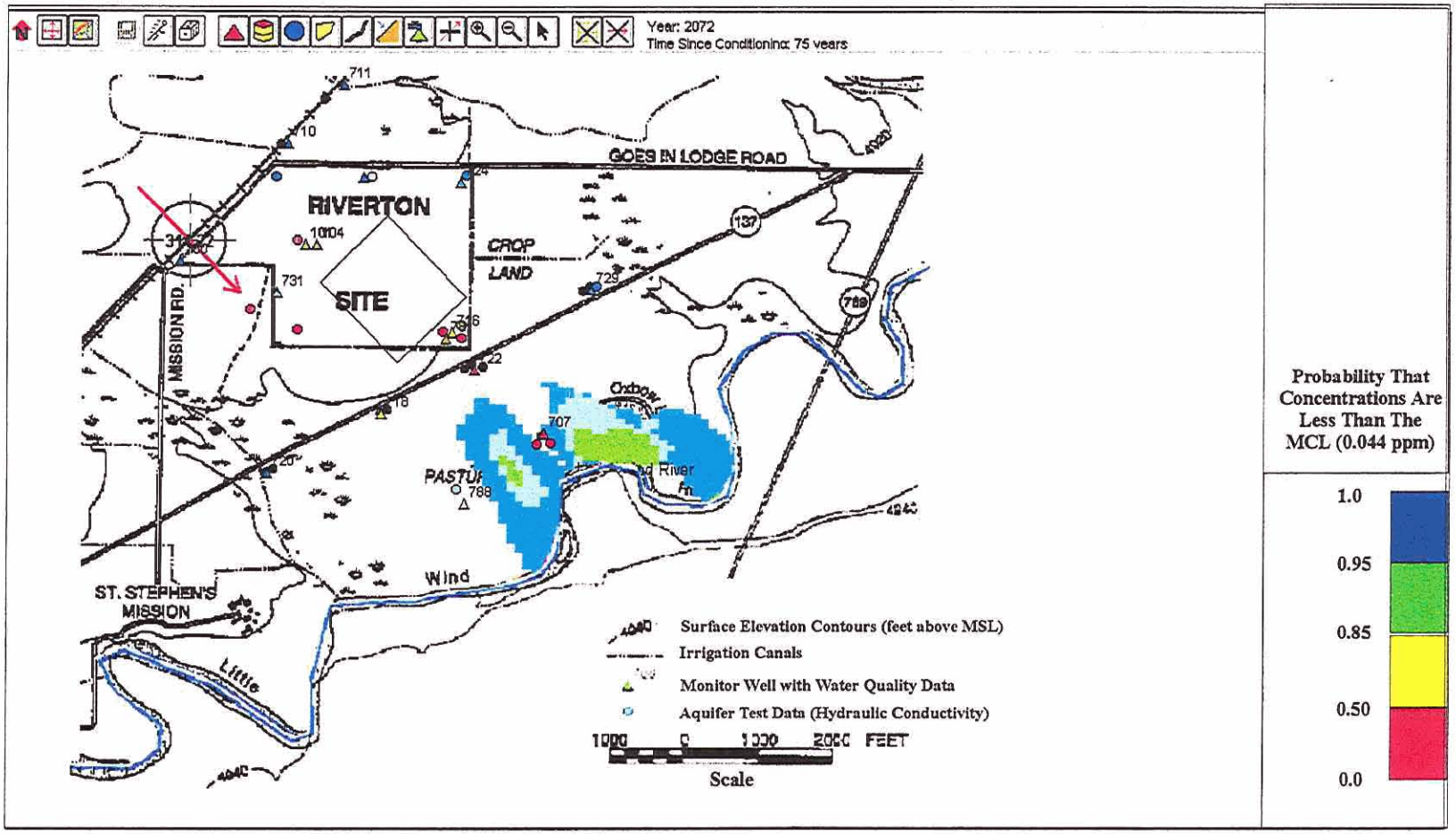



**Figure 9.7 - Probability That Concentrations Are Less Than The Uranium MCL From Uncertainty Analysis, 50 Years After Conditioning Time -2047**




Probability That Concentrations Are Less Than the Uranium MCL From Uncertainty Analysis, 75 Years After Condition Time—2072

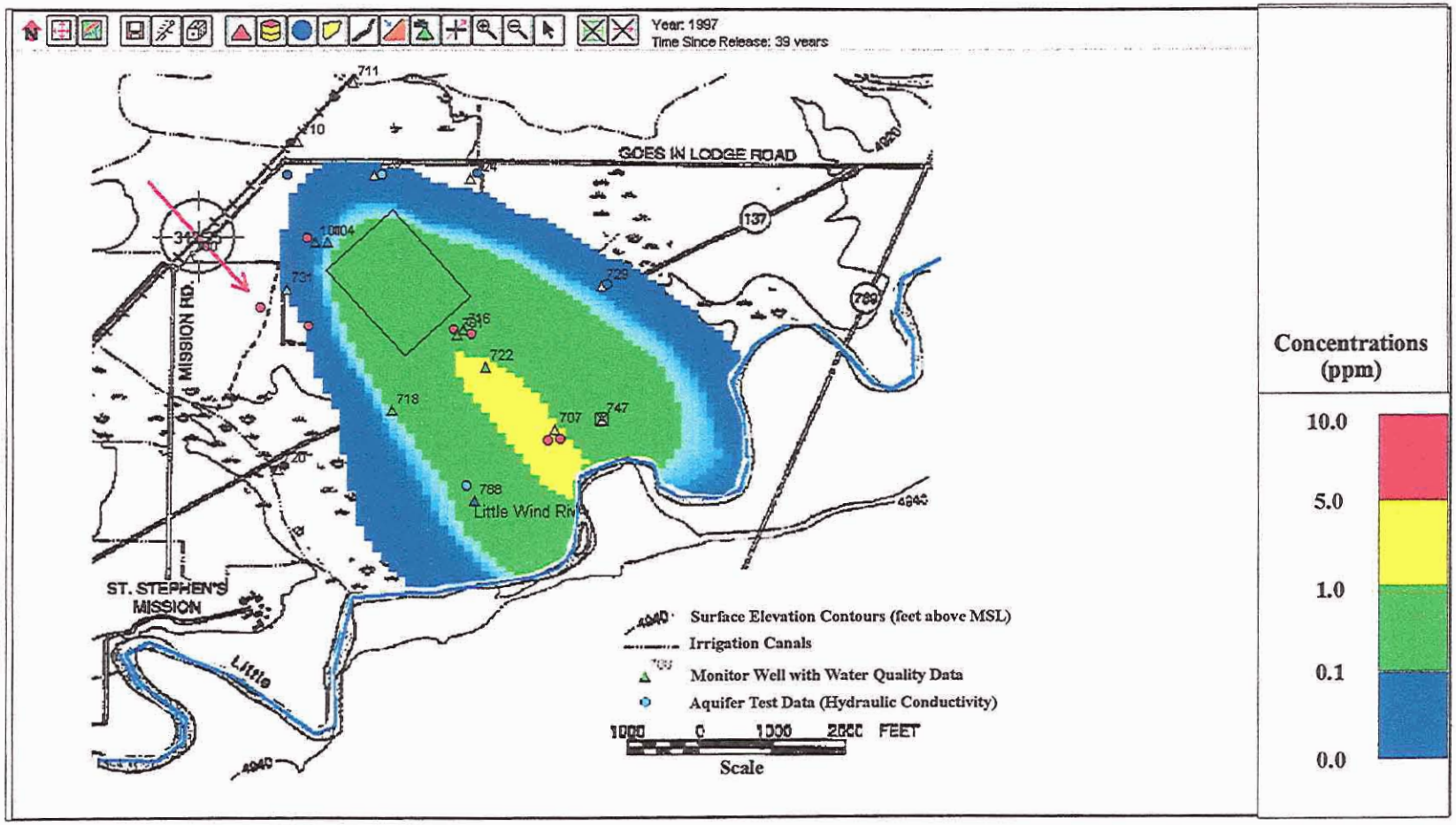



**Figure 9.9 - Mean Concentration Distribution of Molybdenum From Uncertainty Analysis, at Conditioning Time - 1997**

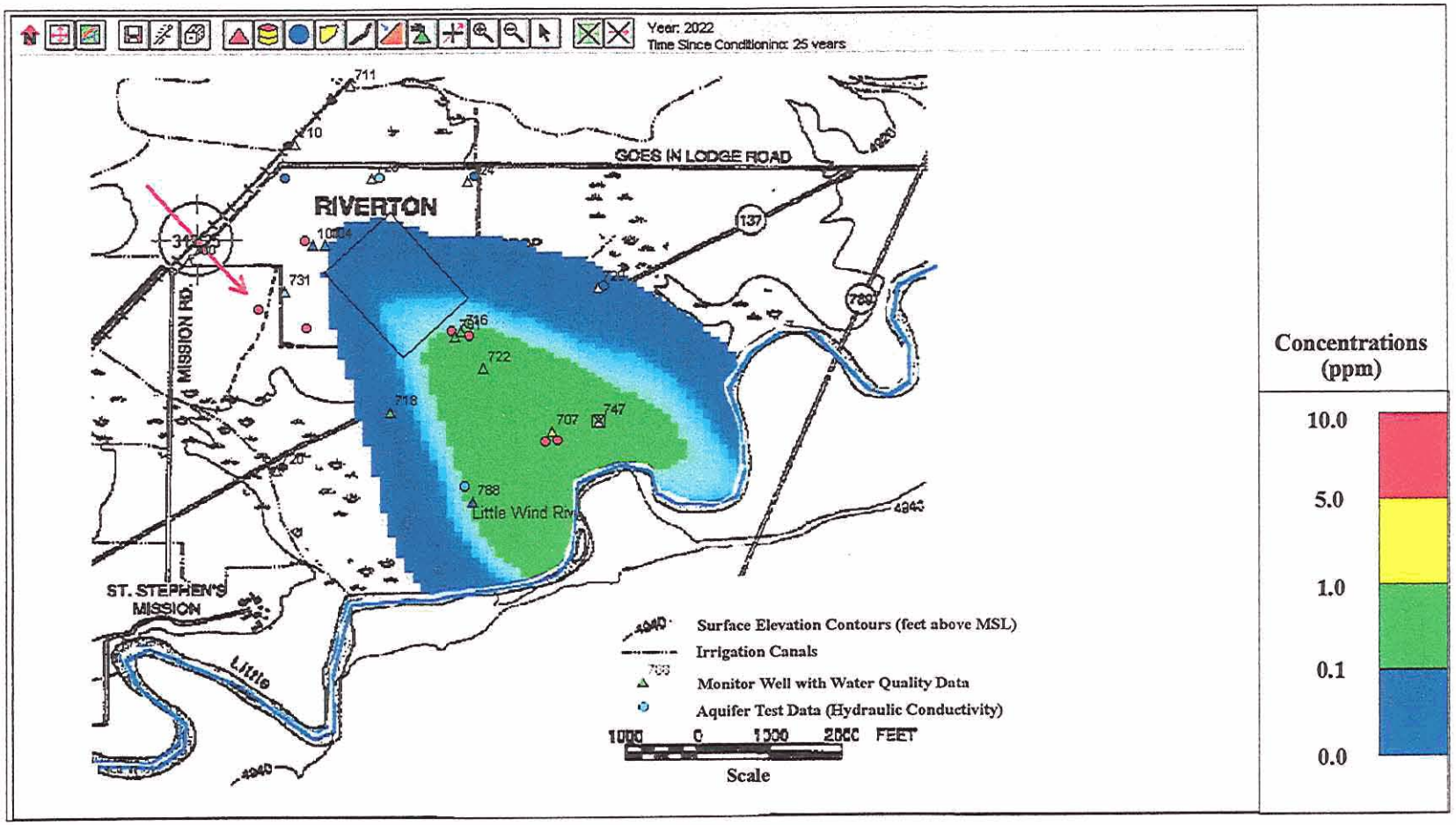



**Figure 9.10 - Mean Concentration Distribution of Molybdenum From Uncertainty Analysis, 25 Years After Conditioning Time - 2022**

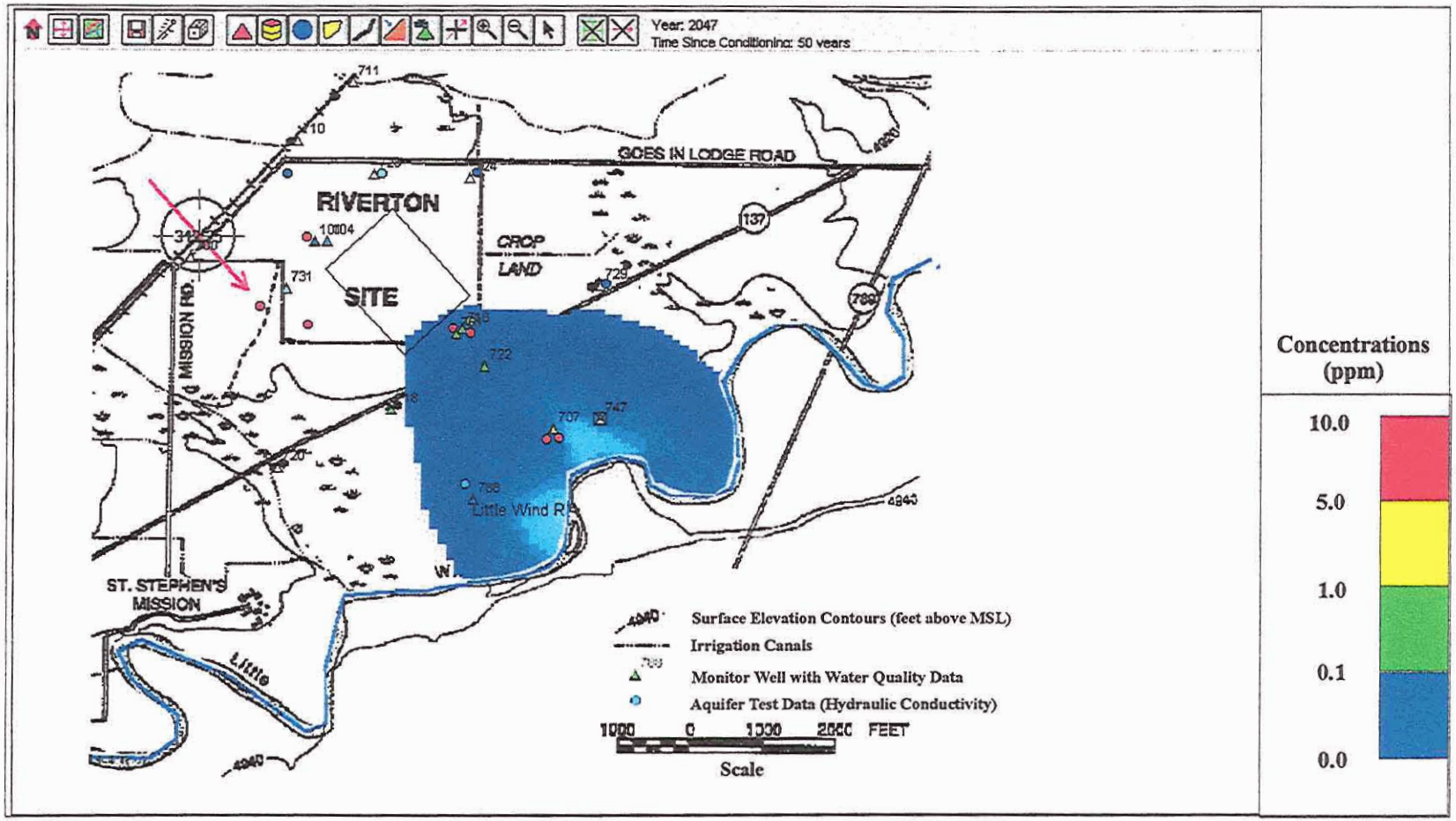



**Figure 9.11 - Mean Concentration Distribution of Molybdenum From Uncertainty Analysis, 50 Years After Conditioning Time - 2047**

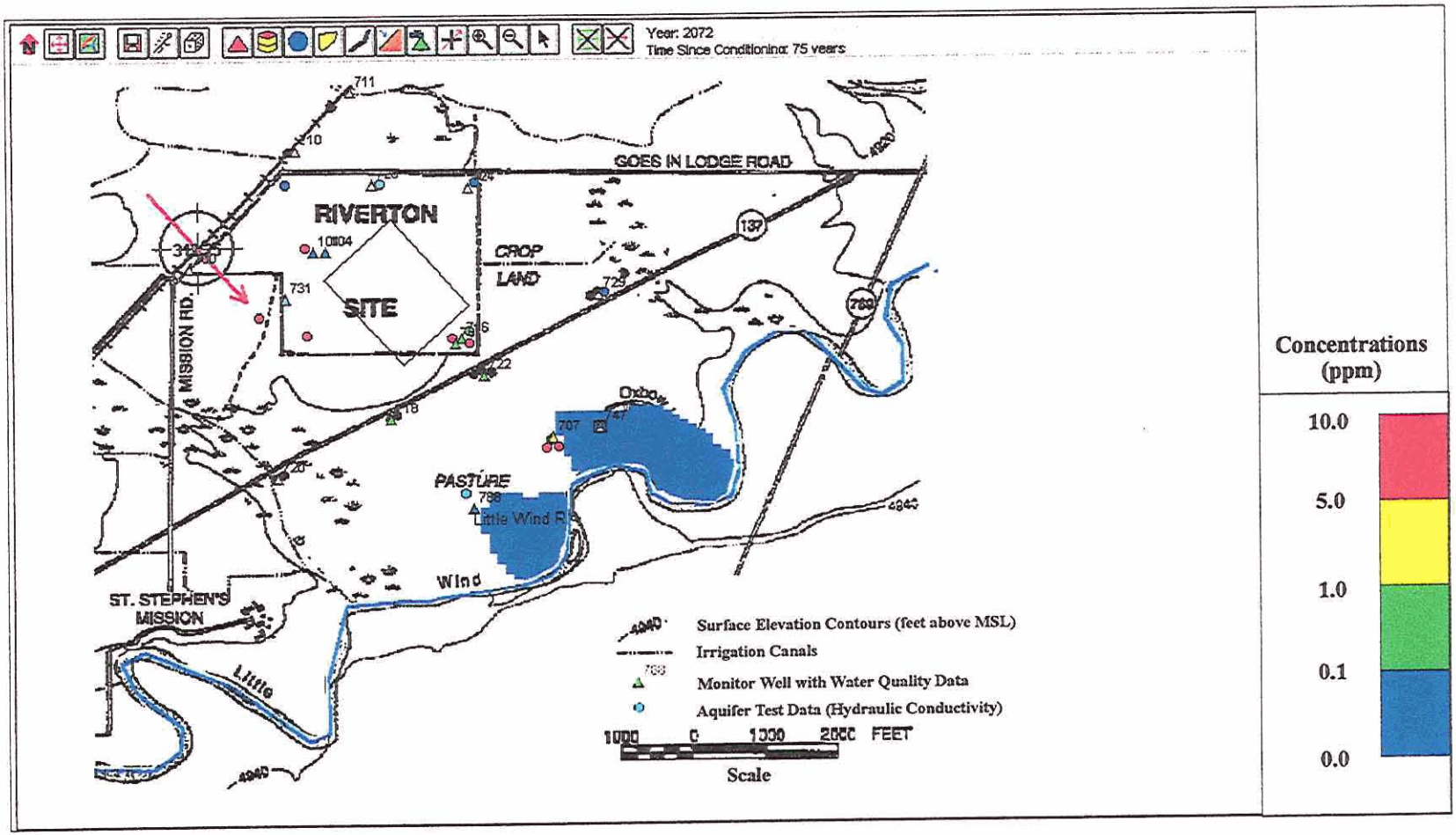



**Figure 9.12 - Mean Concentration Distribution of Molybdenum From Uncertainty Analysis, 75 Years After Conditioning Time - 2072**

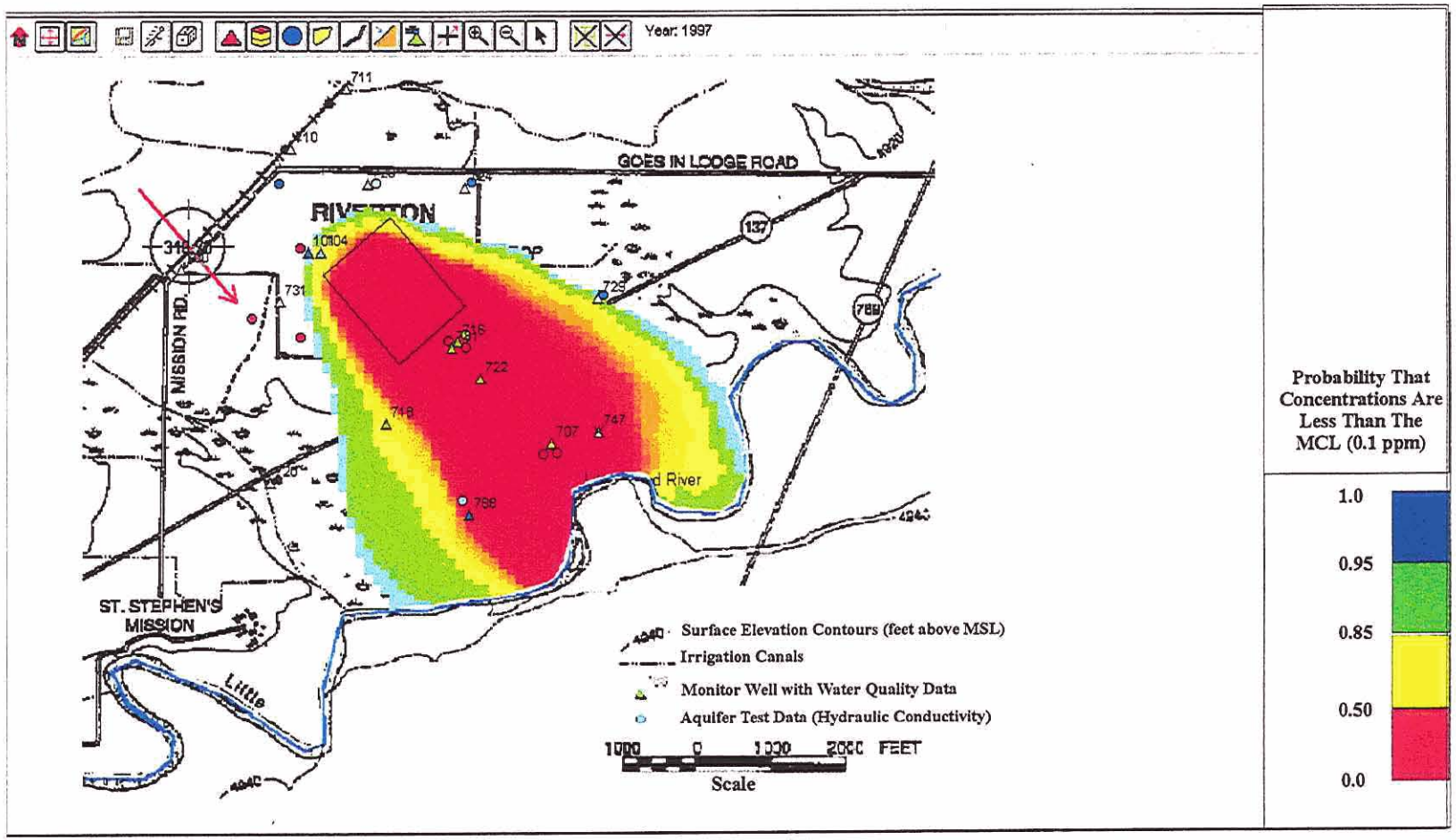



**Figure 9.13 - Probability That Concentrations Are Less Than The Molybdenum MCL From Uncertainty Analysis, at Conditioning Time - 1997**

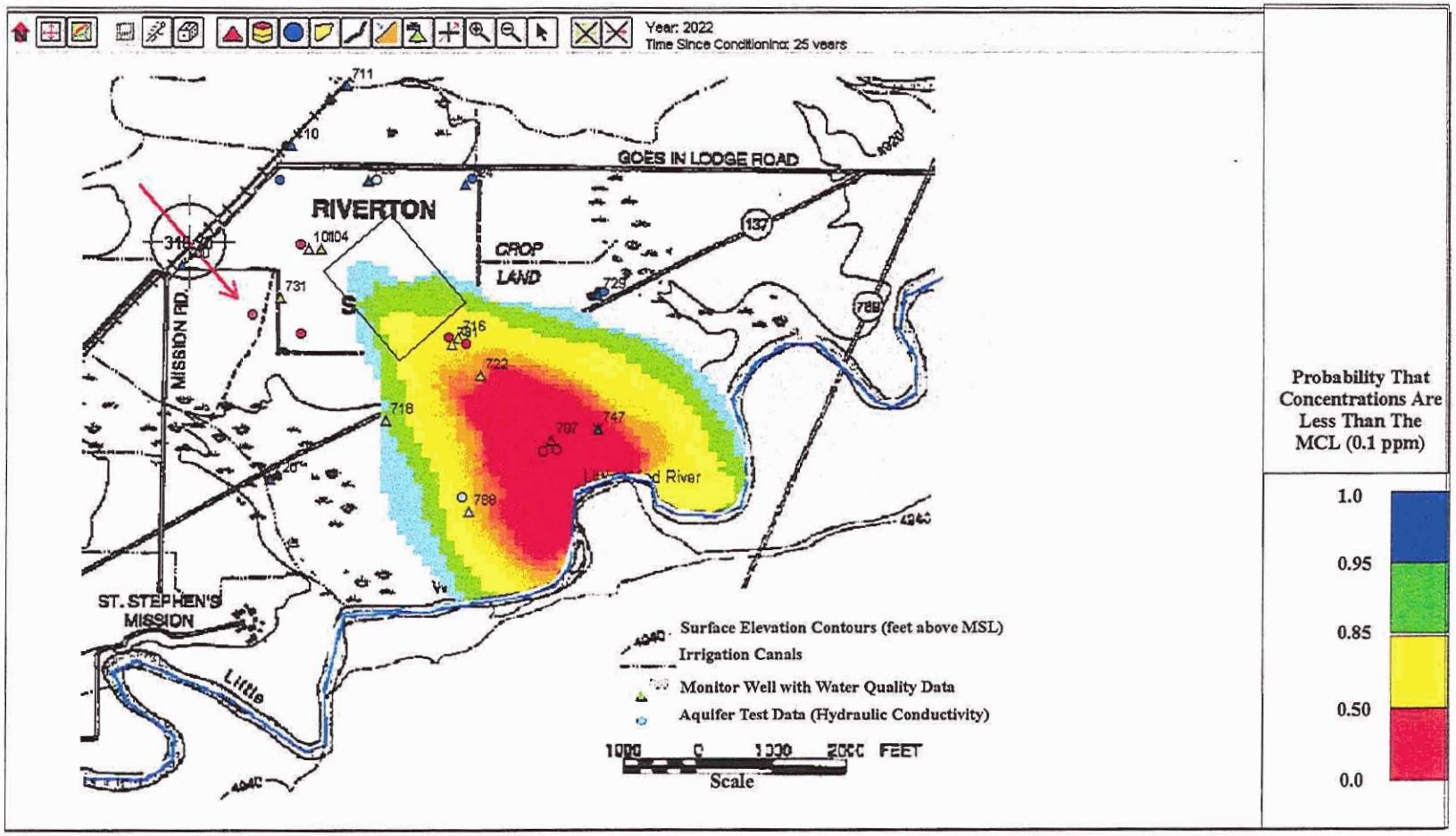



**Figure 9.14 - Probability That Concentrations Are Less Than The Molybdenum MCL From Uncertainty Analysis, 25 Years After Conditioning Time - 2022**

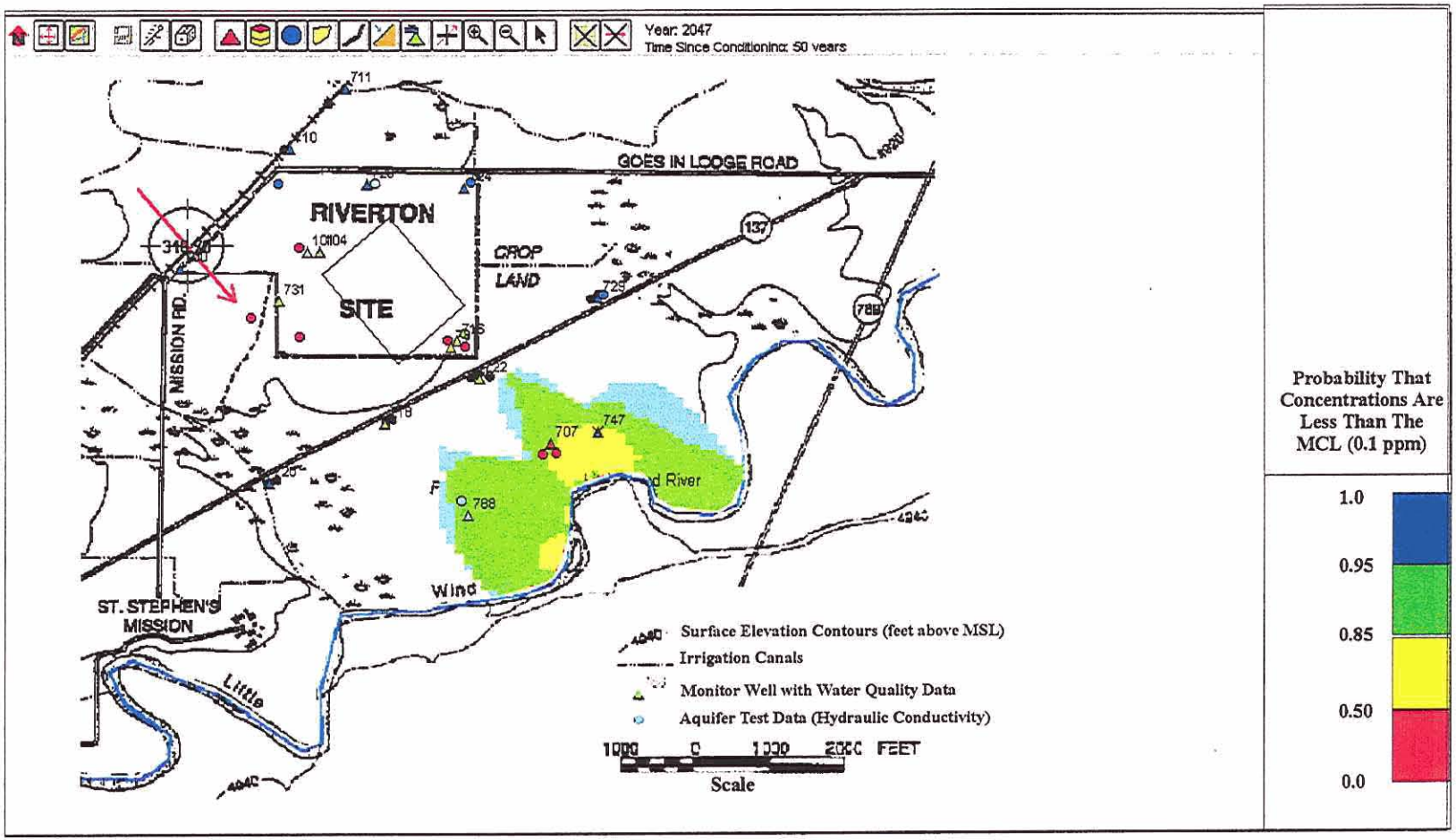



**Figure 9.15 - Probability That Concentrations Are Less Than The Molybdenum MCL From Uncertainty Analysis, 50 Years After Conditioning Time - 2047**

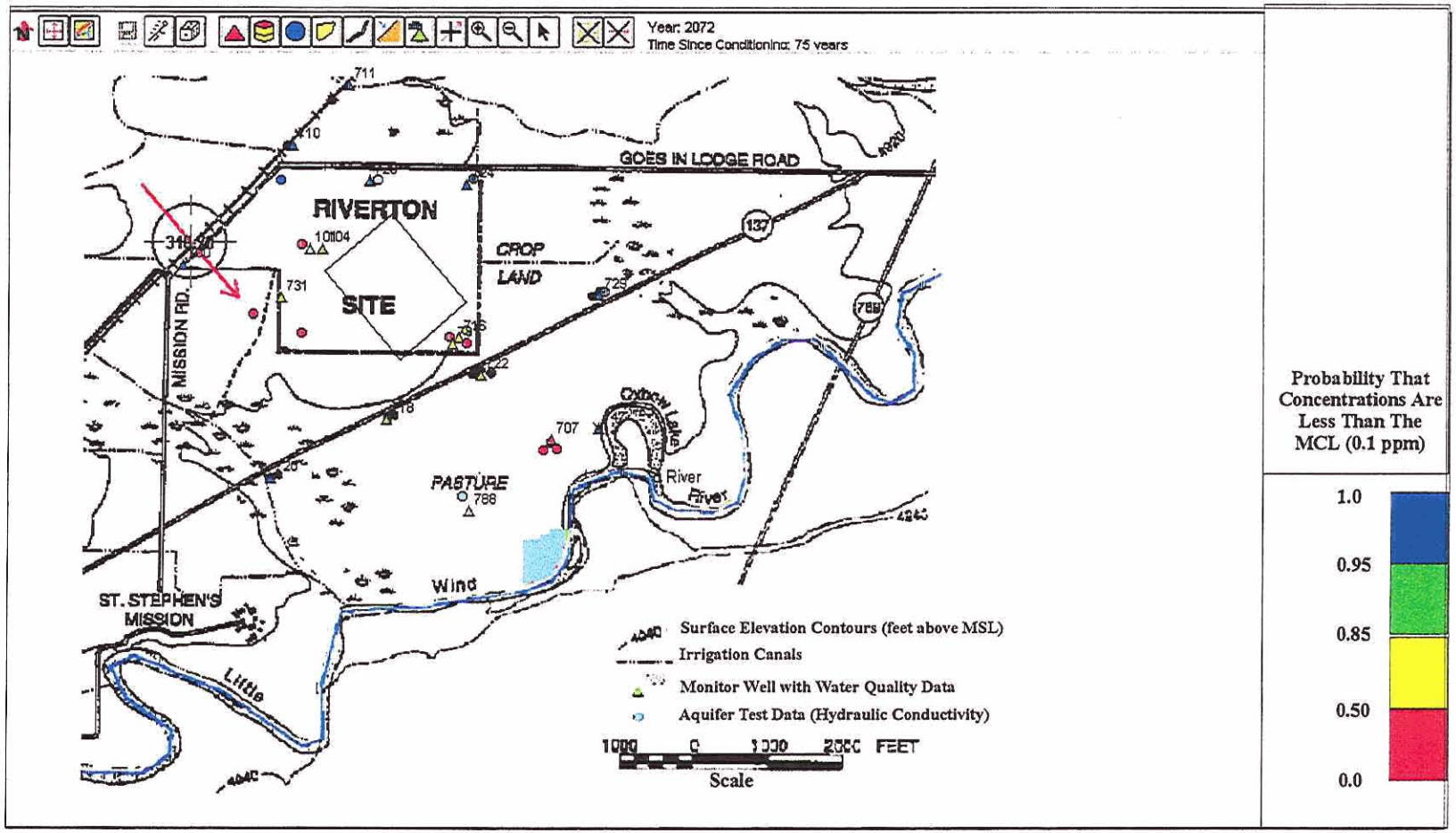



**Figure 9.16 - Probability That Concentrations Are Less Than The Molybdenum MCL From Uncertainty Analysis, 75 Years After Conditioning Time -2072**

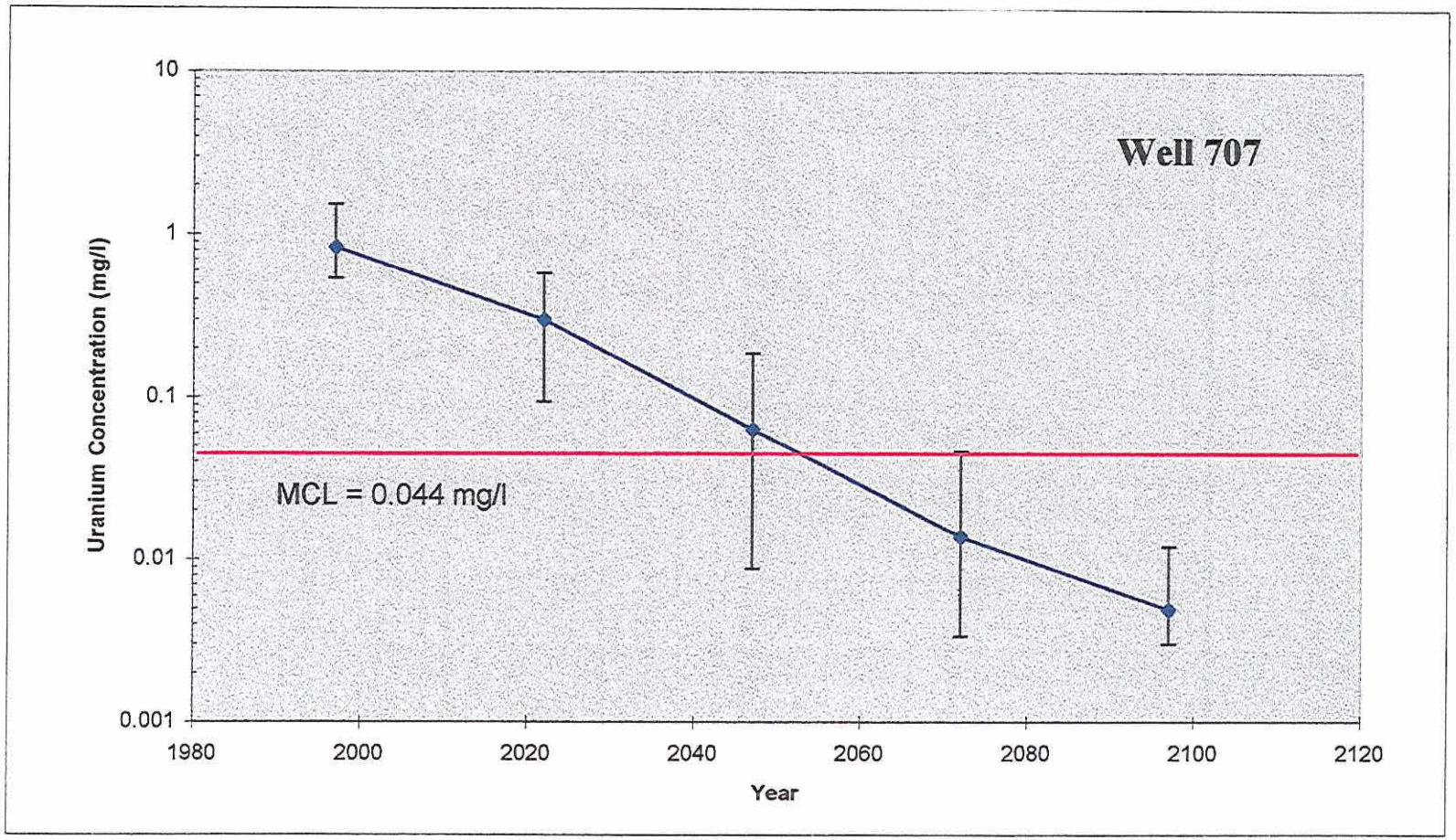



**Figure 9.17 - Uranium Concentration Versus Time for Verification Monitoring in Well 707**

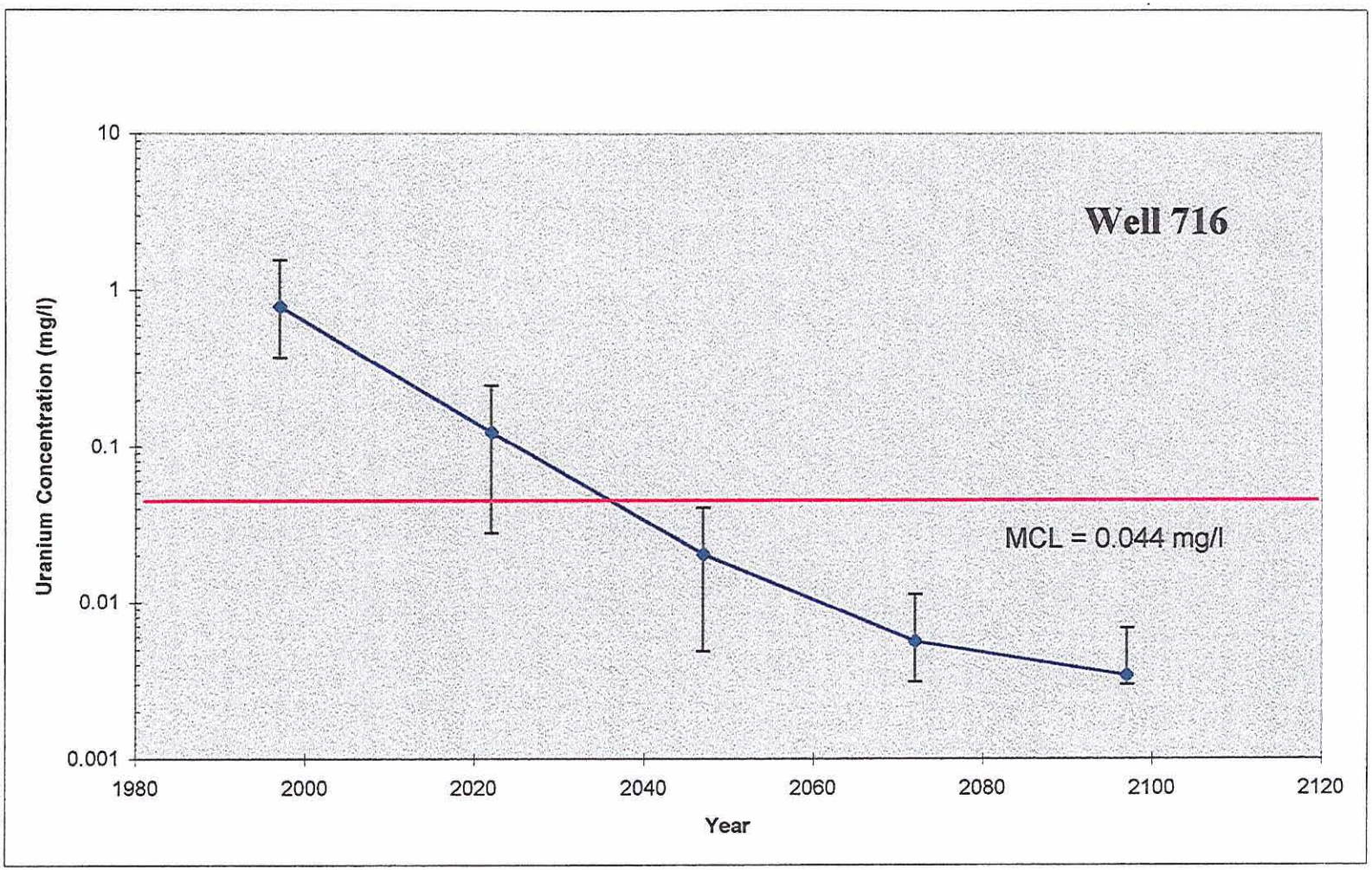



**Figure 9.18 - Uranium Concentration Versus Time for Verification Monitoring in Well 716**

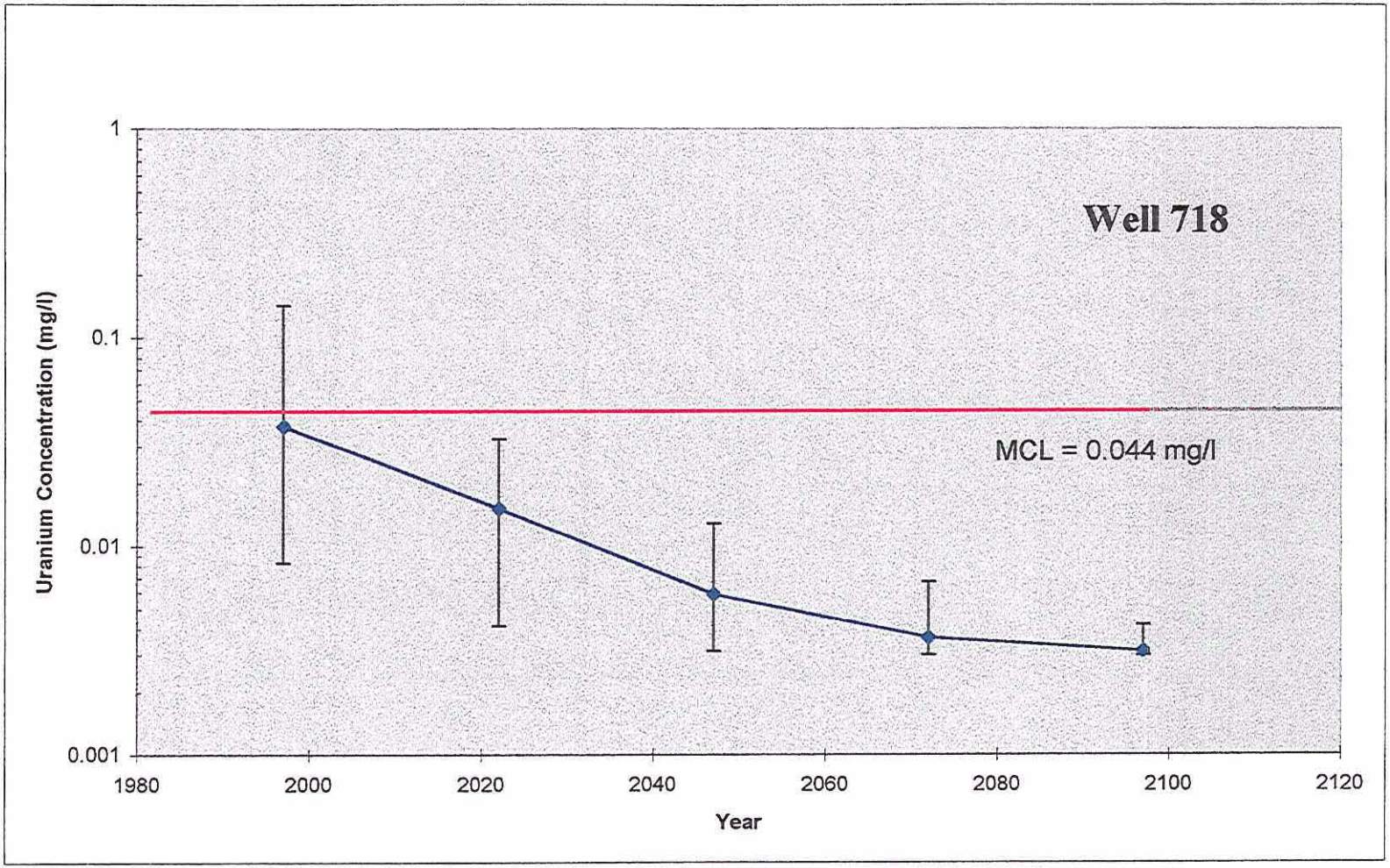



**Figure 9.19 - Uranium Concentration Versus Time for Verification Monitoring in Well 718**

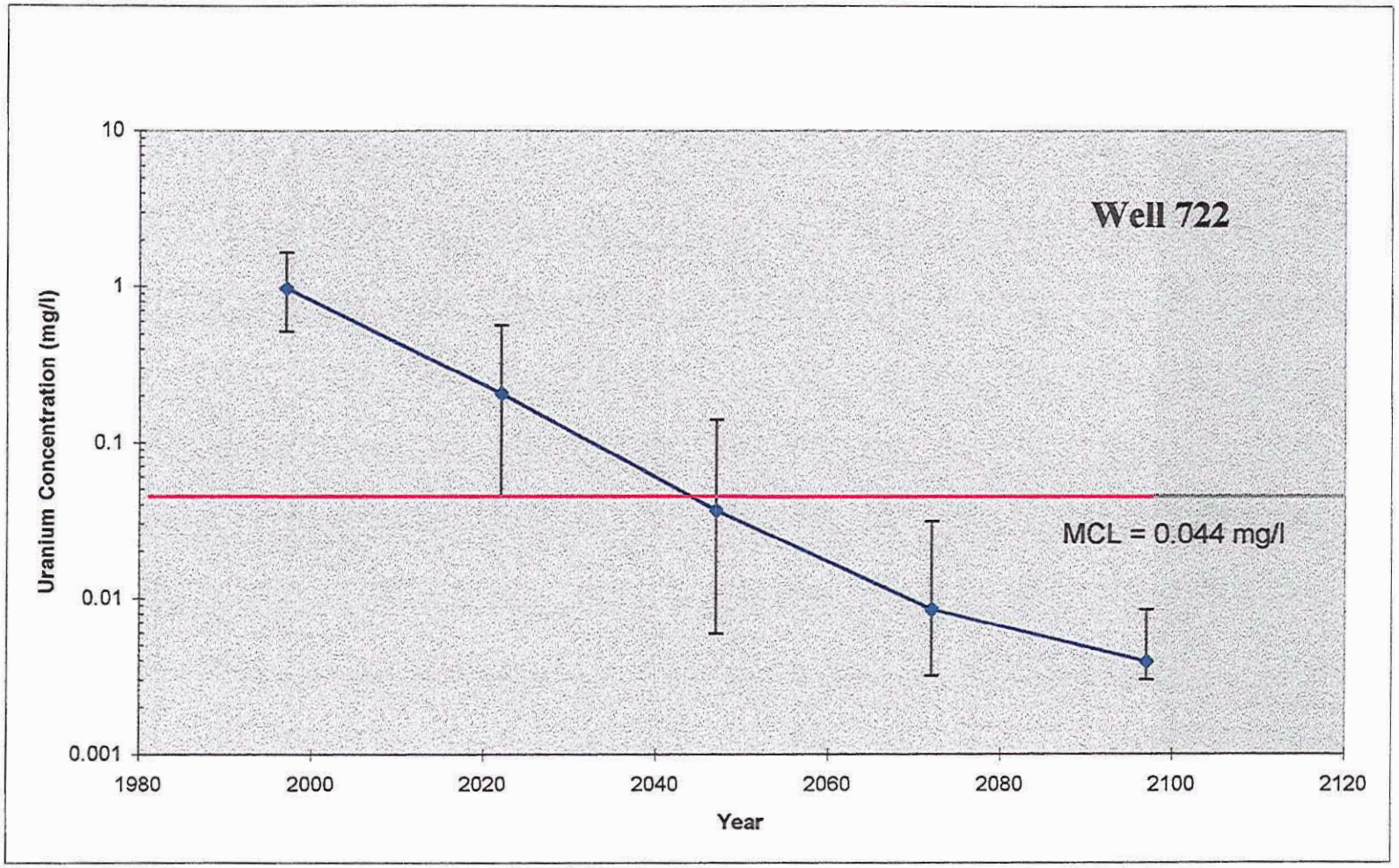



**Figure 9.20 - Uranium Concentration Versus Time for Verification Monitoring in Well 722**

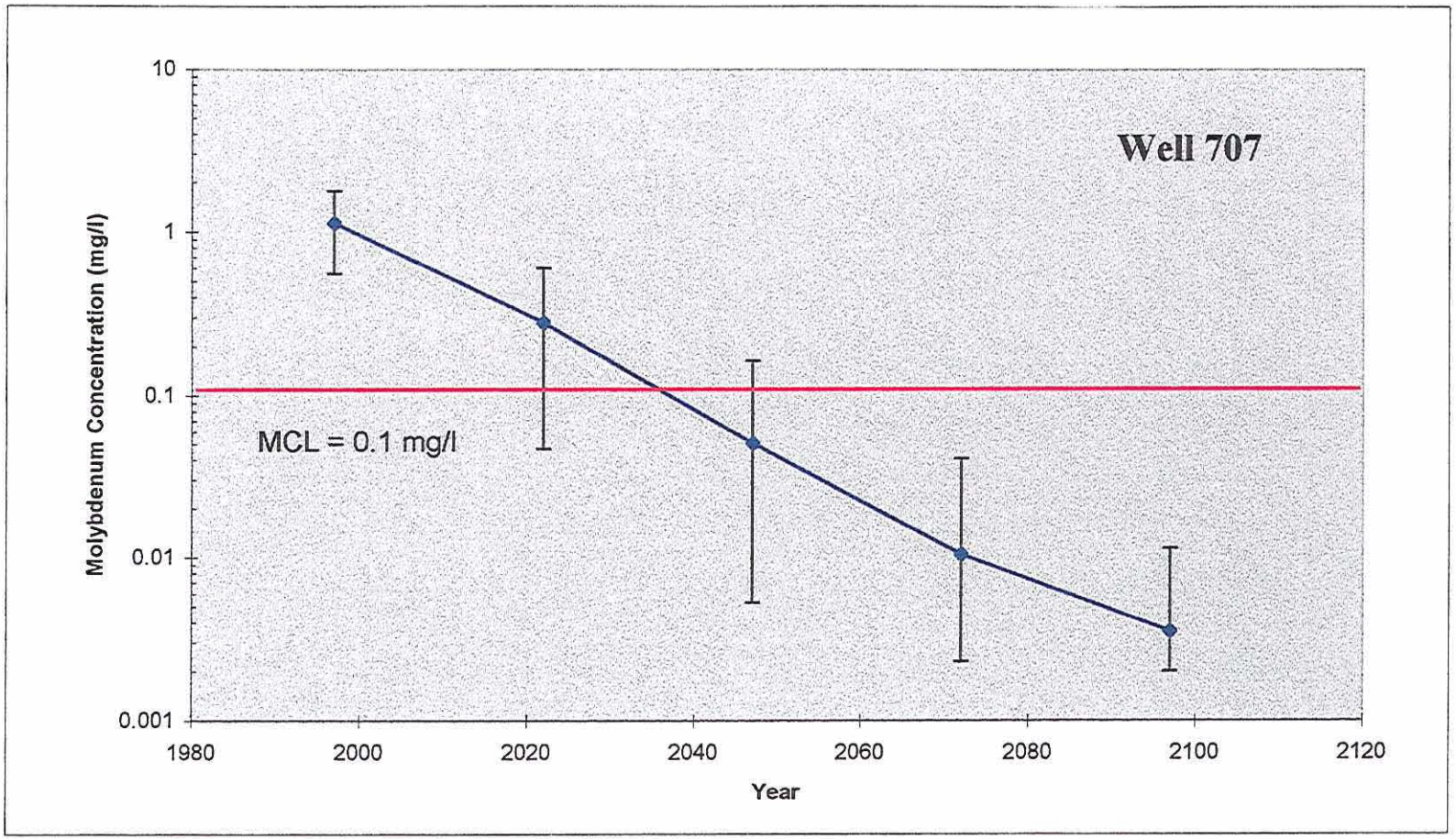



**Figure 9.21 - Molybdenum Concentration Versus Time for Verification Monitoring in Well 707**

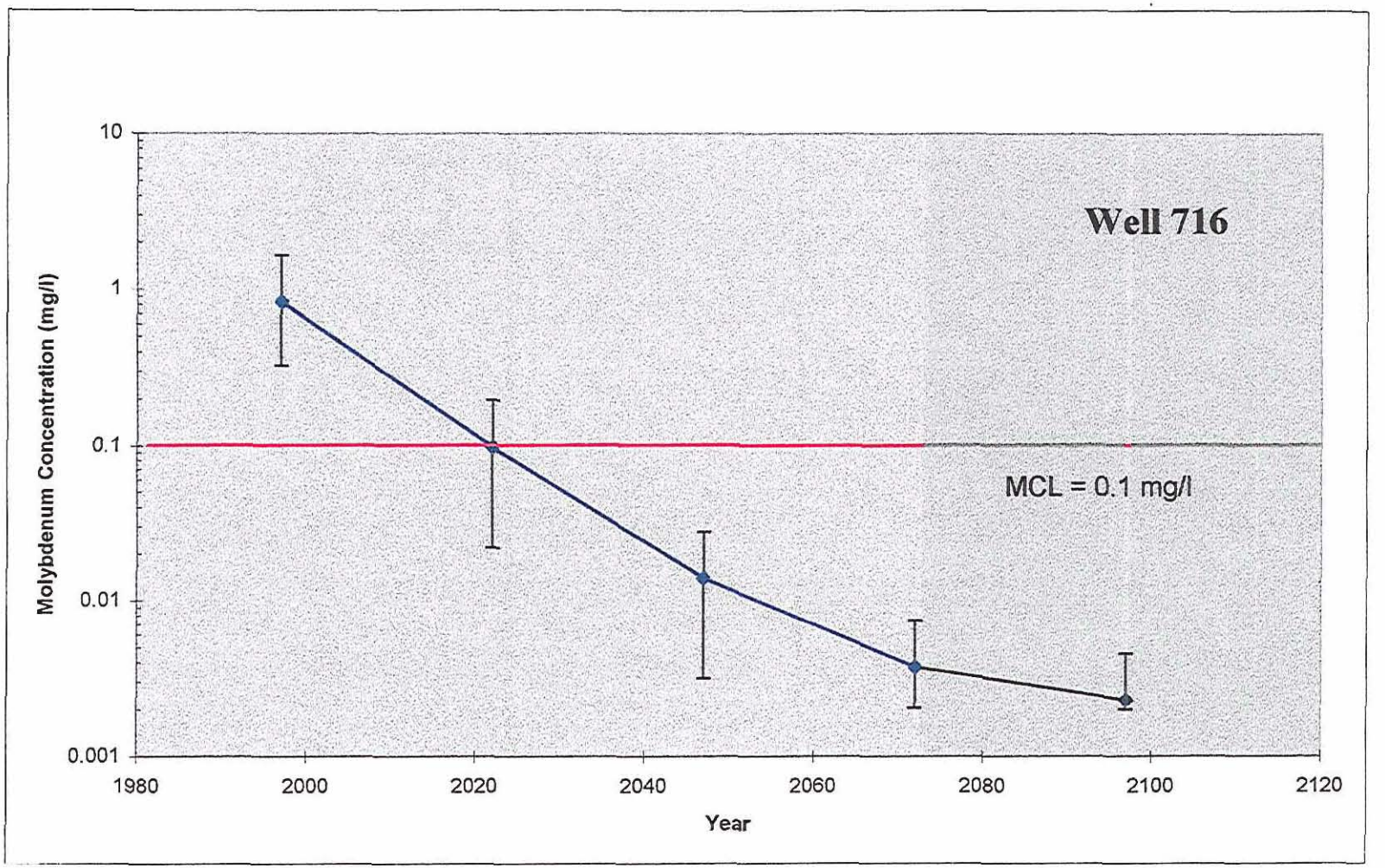



**Figure 9.22 - Molybdenum Concentration Versus Time for Verification Monitoring in Well 716**

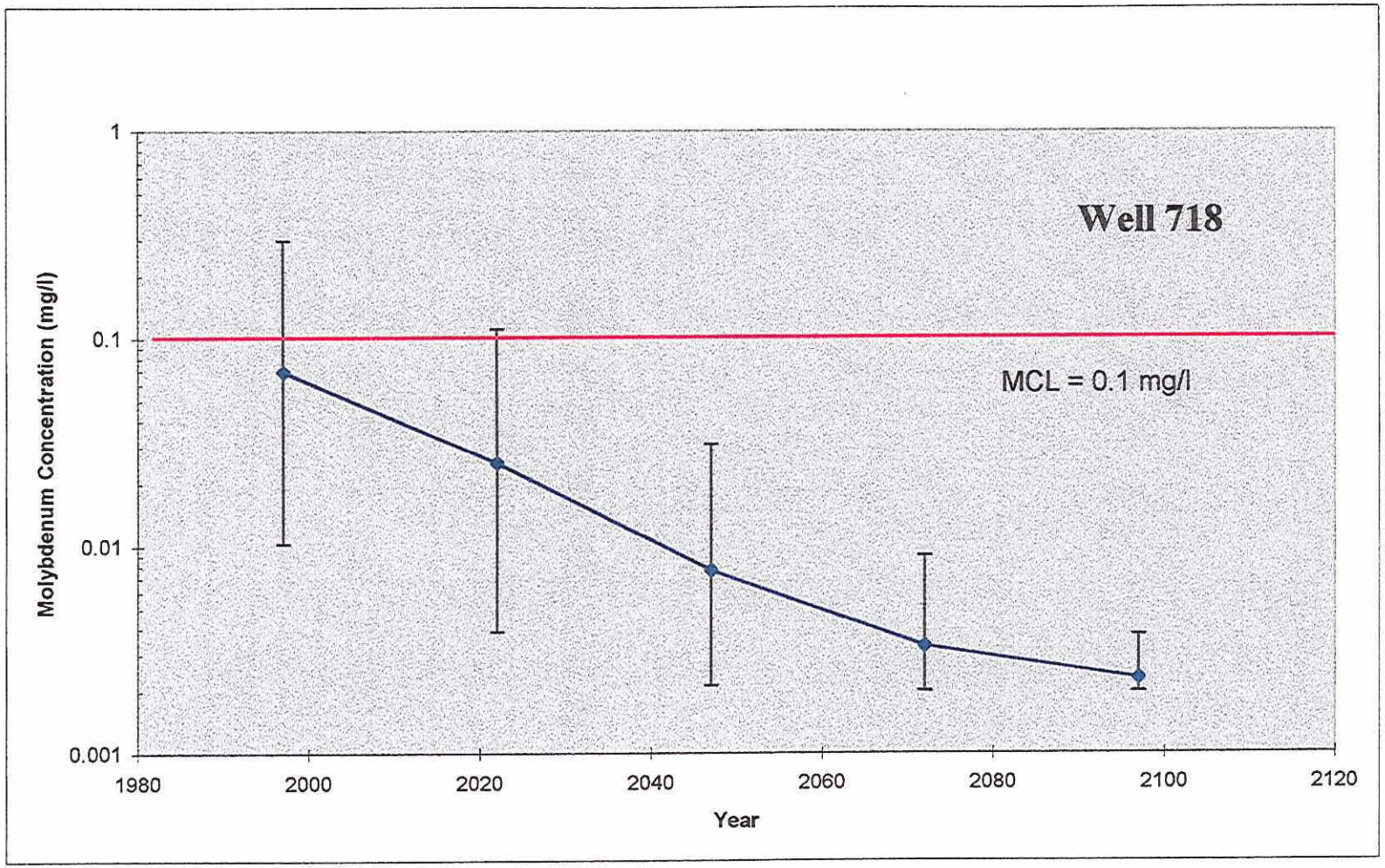



**Figure 9.23 - Molybdenum Concentration Versus Time for Verification Monitoring in Well 718**

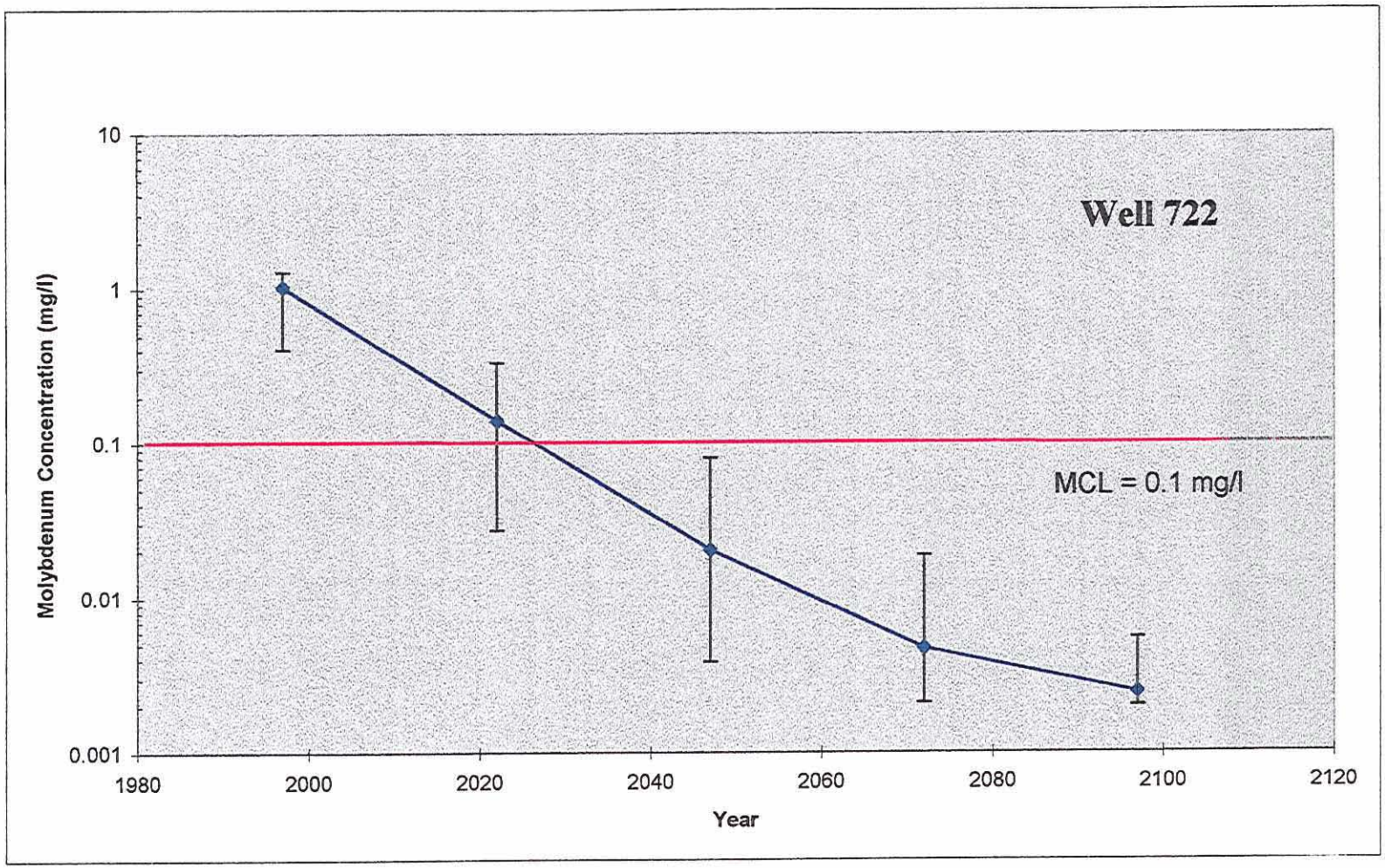



**Figure 9.24 - Molybdenum Concentration Versus Time for Verification Monitoring in Well 722**

## 10. Summary and Conclusions

Probabilistic analyses of groundwater flow and transport at the Riverton site were performed to assess the likelihood of success in implementing a natural attenuation strategy. The GANDT methodology and code set, developed at Sandia National Laboratories (SNL), were used to perform the analyses. Natural attenuation prospects were examined with respect to achieving maximum contaminant levels (MCLs) during a 100-year period, in which controls on site activities are proposed to be maintained.

The results of the probabilistic analyses were quite encouraging. Uranium and molybdenum transport simulations suggest a 100 percent probability of success for natural flushing to meet the MCL's for these contaminants. An important element of a successful natural attenuation strategy is the verification monitoring of groundwater concentrations during future years. This report supplies the predicted concentration ranges for key monitoring wells at the site. If the actual water quality data from these monitor wells is within these predicted ranges then the site should flush within the 100 year period. If observed concentrations are greater than those summarized in this analysis, then the site conditions should be reassessed with regard to the ability of the system to naturally flush. Though the GANDT modeling analysis accounts for uncertainties, it does not necessarily account for all uncertainties through time (e.g., conceptual model uncertainties, climatic changes, etc.). For this reason, and because of regulatory requirements, the site should be monitored routinely, and predictive transport modeling, such as that reported on here, should be revisited and updated if necessary.

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# Appendix A

## Explanation of Monte Carlo Method

Several studies during the last few years (e.g., NRC, 1994; EPA, 1997) have stressed the need for probabilistic modeling assessments, such as those based on Monte Carlo simulation, to address parameter uncertainty and variability explicitly and separately. Variability refers to the observed differences attributable to true heterogeneity or diversity in a parameter (e.g., natural variation in porosity, spatial variation in aquifer hydraulic conductivity), a phenomenon that can be approximated statistically from empirical data. In contrast, uncertainty refers to the lack of knowledge about a parameter, or even about the model that is used to represent a site (EPA, 1997). It stands to reason that an uncertain parameter is not readily measured, and, consequently, is more difficult to justify in the form of a probability density function, or PDF. As a result, any descriptions of the uncertainty in parameters, whether qualitative or quantitative, are likely to be subjective. Regardless of the difficulties that may arise in characterizing variability and uncertainty, there is a consensus among recent studies to insist that all information dealing with these topics for a modeling study should the taken into account, and modelers should not shy away from uncertainty and variability analyses (NRC, 1994; Risk Commission, 1997).

The most common method for quantifying uncertainty in a computer modeling system is through the implementation of the Monte Carlo method. In the Monte Carlo method the user specifies a statistical distribution for each uncertain parameter in the mathematical formulation under consideration (e.g., groundwater flow and solute transport equations). Values are selected from the statistical distributions to produce a sufficient number of input combinations to the model to characterize the probability density functions of the parameters. The input combinations are put to the numerical simulator to produce a set of statistical model output results. These results can be displayed in a variety of formats, from simple histograms of model output measures, to cumulative distribution functions, or probability plots of the spatial distribution of model outputs (e.g., average concentration distribution; probability of exceeding a specified concentration threshold, such as the MCL).

To illustrate the concept of the Monte Carlo method, a simple case study can be made of a common activity that most people can relate to that involves uncertainty: commuting. Figure A.1 shows a map of a city in which a person might commute each day from the northwest part of the city where they live to the southeast portion of the city where they work. There are a number of routes that the driver may take to make the commute both to and from work, which are illustrated by the red lines in the figure. The route he/she takes may be dependent on any number of factors and choices at his/her discretion. Factors affecting the time it takes to make the trip may be numerous. Several of these factors might be road construction, traffic congestion due to a large number of drivers on the road, inclement weather, and slow drivers impeding the flow of traffic. Each of these factors may contribute to the time it takes to make the commute, and may also be compounding if two or more affect the commute on a given day. Over the course of a year, for instance, these various factors will affect the commuting time and the driver could assemble statistics on the daily commuting time. Traffic engineers would suggest that mathematical models could be assembled to predict the commuting time, based on statistics associated with factors affecting the commute, as mentioned. Figure A.2 illustrates how this process of accounting for uncertainty in the commuting time might look with graphical constructs. The uncertain parameter distributions are sampled some number of times, run through the mathematical simulator, and a statistical expression of commuting time derived. The result might be that on the best day of the year the driver might make the commute in 20 minutes. On the worst day, when various factors combine to negatively influence the commuting time, the commute might be 2 hours. On average, the driver might have a 45-minute commute. The statistical distribution would illustrate this variability or uncertainty.

By comparison, the fate and transport of contaminants in subsurface media can be modeled to account for uncertainties in the travel time of constituents of concern. Figure A.3 shows a schematic representation of contaminants migrating more or less vertically through unsaturated soils and entering the underlying saturated zone, or aquifer, and eventually discharging to a well

or river. The routes that the contaminants take through the porous media may be varying and dependent on geologic heterogeneities. The factors affecting the flow and transport of the contaminants include hydraulic conductivity, porosity, sorption coefficient, and gradient, amongst others. Each of these factors may have associated uncertainty or variability. Obviously, mathematical models such as those employed in the GANDT code could be used to predict the travel time of the contaminants. Figure A.4 illustrates the relationship between these uncertain parameters and the modeled outcome of contaminant travel time within a Monte Carlo methodology.

A good technical discussion of the Monte Carlo method for quantifying uncertainties is given by Peck et al. (1988), as well as the EPA publication mentioned above (EPA, 1997).

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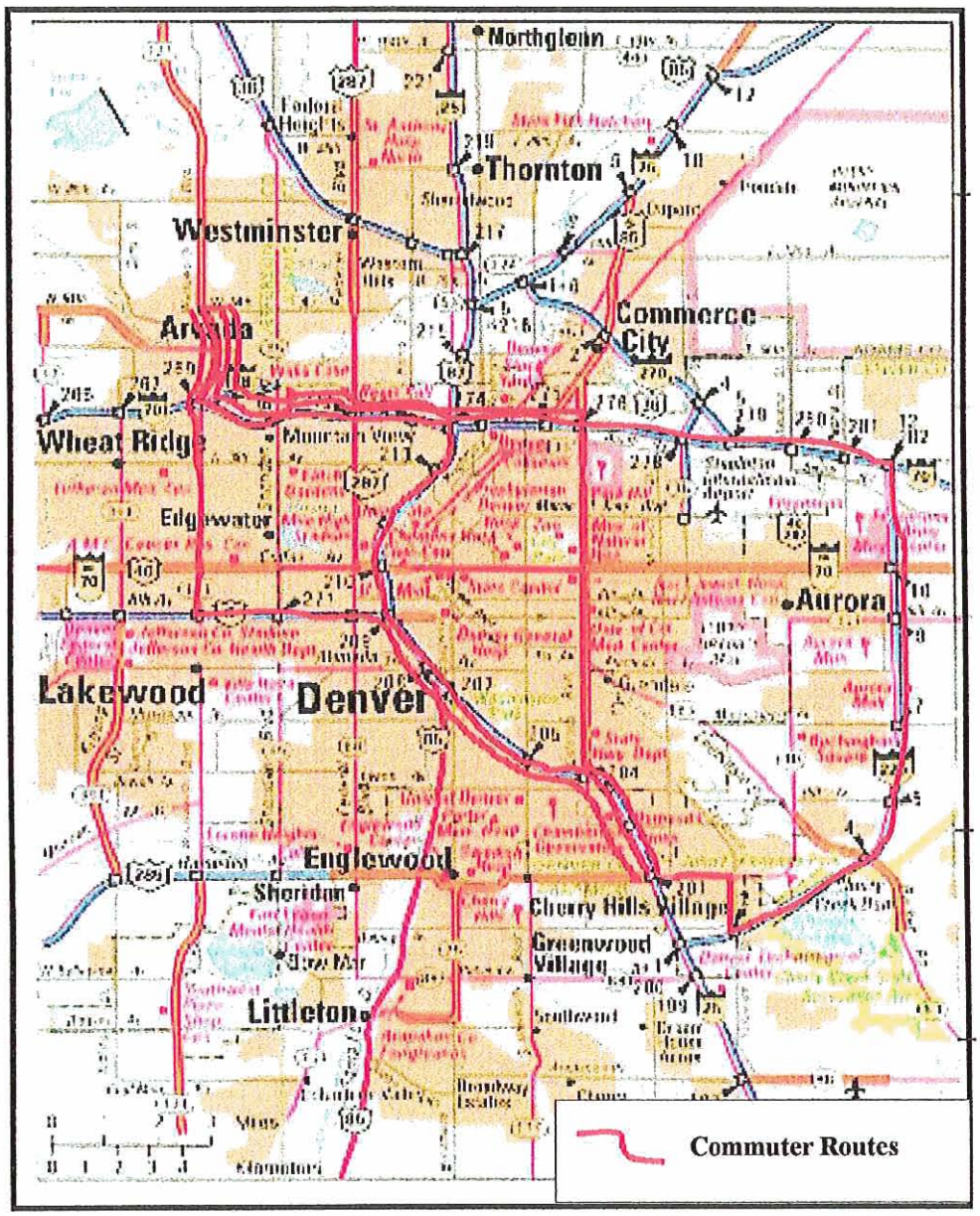


**Figure A.1 - Various Commuter Routes Between the Northwest And Southeast Areas of the City**

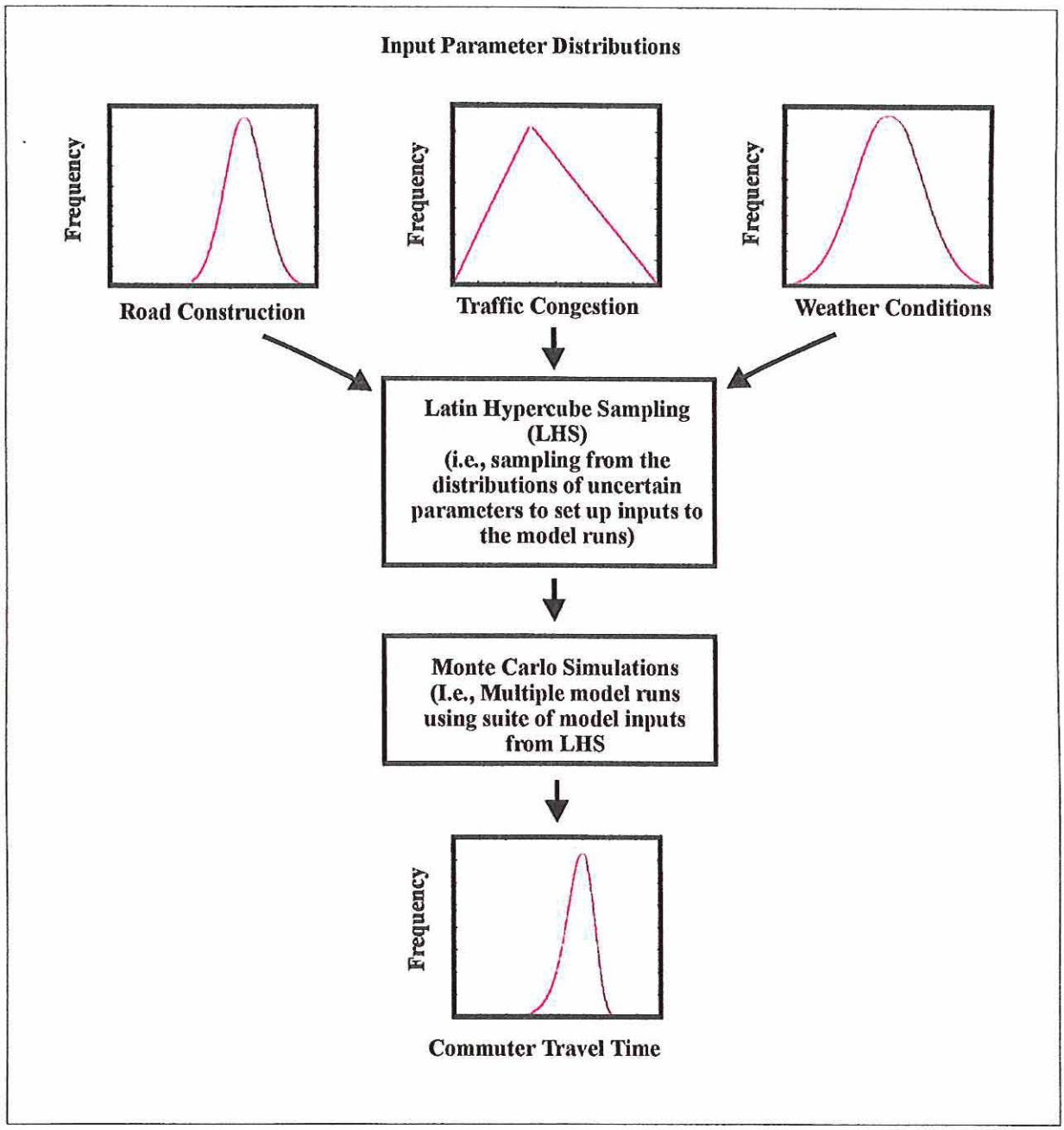


**Figure A.2 - Conceptual Depiction of the Monte Carlo Simulation Process for Propagating Parameter Uncertainty into Model Output Uncertainty**

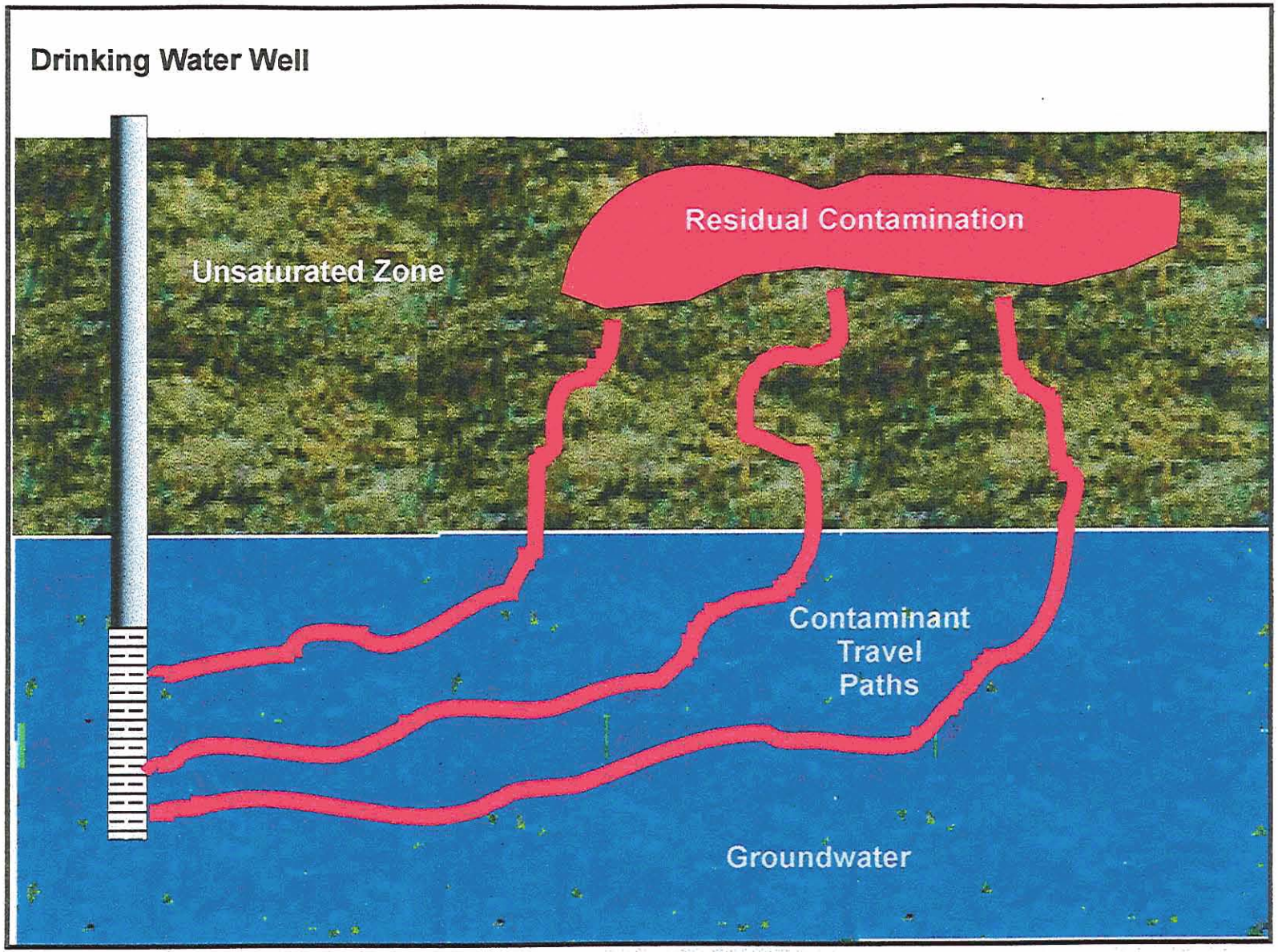


**Figure A.3 - Contaminant Travel Paths Through Subsurface Soils and Groundwater**

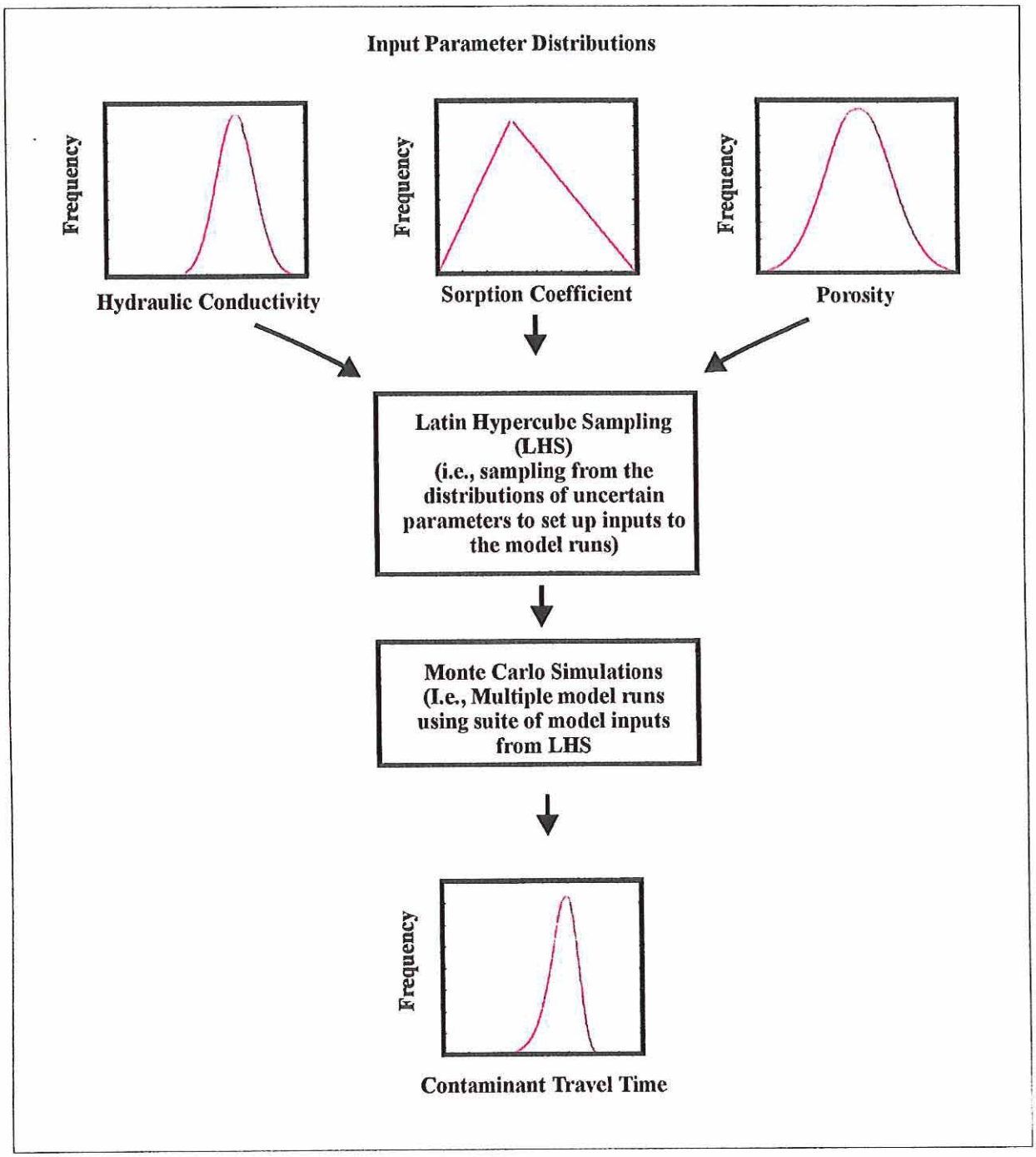


**Figure A.4 - Conceptual Depiction of the Monte Carlo Simulation Process for Propagating Parameter Uncertainty into Model Output Uncertainty**

# Appendix B

## Groundwater Elevation Data

## Water Level Elevations from the SEE.UMTRA Database for the Riverton, WY Site

| Well Location | Average Water Level Elevation* | Minimum Water Level Elevation* | Maximum Water Level Elevation* | Standard Deviation of Water Level Elevation |
|---|---|---|---|---|
| 100 | 4938.35 | 4937.91 | 4939.56 | 0.59 |
| 101 | 4937.05 | 4935.91 | 4938.45 | 0.89 |
| 102 | 4937.10 | 4935.42 | 4937.93 | 1.07 |
| 103 | 4936.83 | 4935.83 | 4938.11 | 0.99 |
| 104 | 4938.44 | 4935.80 | 4937.53 | 0.58 |
| 105 | 4939.97 | 4935.93 | 4938.34 | 1.07 |
| 106 | 4935.35 | 4933.43 | 4937.32 | 1.01 |
| 107 | 4935.28 | 4933.98 | 4937.02 | 1.31 |
| 108 | 4935.25 | 4933.17 | 4942.05 | 2.36 |
| 109 | 4934.96 | 4933.63 | 4935.76 | 1.39 |
| 110 | 4935.68 | 4933.80 | 4937.39 | 1.38 |
| 111 | 4937.05 | 4936.29 | 4938.15 | 0.78 |
| 112 | 4938.36 | 4937.90 | 4939.48 | 0.58 |
| 113 | 4936.76 | 4935.60 | 4938.50 | 1.25 |
| 701 | 4926.82 | 4925.89 | 4928.70 | 1.23 |
| 702 | 4928.46 | 4925.17 | 4928.78 | 1.42 |
| 703 | 4929.09 | 4928.85 | 4930.53 | 1.32 |
| 704 | 4929.09 | 4928.13 | 4930.30 | 0.80 |
| 705 | 4925.71 | 4921.80 | 4928.59 | 1.56 |
| 706 | 4925.06 | 4923.32 | 4928.97 | 1.31 |
| 707 | 4926.71 | 4925.43 | 4928.00 | 0.94 |
| 708 | 4925.18 | 4922.14 | 4927.45 | 1.79 |
| 710 | 4941.41 | 4940.87 | 4942.58 | 0.54 |
| 711 | 4939.53 | 4938.10 | 4940.90 | 0.66 |
| 712 | 4937.33 | 4936.68 | 4938.70 | 0.55 |
| 713 | 4937.00 | 4936.00 | 4938.62 | 0.97 |
| 714 | 4936.52 | 4935.29 | 4937.00 | 0.90 |
| 715 | 4935.78 | 4934.80 | 4937.31 | 0.99 |
| 716 | 4931.00 | 4930.32 | 4931.78 | 0.53 |
| 717 | 4930.95 | 4930.29 | 4931.75 | 0.56 |
| 718 | 4930.74 | 4930.08 | 4931.33 | 0.51 |
| 719 | 4931.09 | 4930.49 | 4931.88 | 0.49 |
| 720 | 4935.19 | 4934.56 | 4935.71 | 0.48 |
| 721 | 4933.68 | 4932.91 | 4934.13 | 0.48 |
| 722 | 4928.92 | 4928.21 | 4929.62 | 0.56 |
| 723 | 4928.93 | 4928.22 | 4929.66 | 0.60 |
| 724 | 4933.35 | 4932.41 | 4934.87 | 1.08 |
| 725 | 4932.94 | 4932.32 | 4934.18 | 0.24 |
| 726 | 4935.79 | 4934.90 | 4937.17 | 0.97 |
| 727 | 4941.22 | 4940.17 | 4942.73 | 1.30 |
| 728 | 4938.33 | 4937.32 | 4938.81 | 1.22 |
| 729 | 4926.74 | 4925.02 | 4929.73 | 2.50 |
| 730 | 4926.20 | 4924.87 | 4928.47 | 1.98 |
| 733 | 4938.96 | 4937.19 | 4940.72 | 2.50 |

* - feet above mean sea level