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Modeling Subsurface Contamination at Fernald

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I. INTRODUCTION

I.1 Background

The Department of Energy's Fernald site is located about 20 miles northwest of Cincinnati. Fernald produced refined uranium metal products from ores between 1953 and 1989. The pure uranium was sent to other DOE sites in South Carolina, Tennessee, Colorado, and Washington in support of the nation's strategic defense programs. Over the years of large-scale uranium production, contamination of the site's soil and groundwater occurred. The contamination is of particular concern because the Fernald site is located over the Great Miami Aquifer, a designated sole-source drinking water aquifer. Contamination of the aquifer with uranium was found beneath the site, and migration of the contamination had occurred well beyond the site's southern boundary. As a result, Fernald was placed on the National Priorities (CERCLA/Superfund) List in 1989. Uranium production at the site ended in 1989, and Fernald's mission has been changed to one of environmental restoration.

Under the CERCLA/Superfund program the Fernald site has been divided into five operable units:

1. Operable Unit 1 (OU1): The Waste Pit Area includes Waste Pits 1 through 6, the Burn Pit, the Clearwell, berms, liners and related soils.
2. Operable Unit 2 (OU2): The Other Waste Units, includes flyash piles, disposal areas in the south field, two lime sludge ponds from the on-site water treatment process, a solid waste landfill and related berms, and soils.
3. Operable Unit 3 (OU3): The Production Area which includes the buildings, utilities, drums, storage tanks, effluent lines, scrap metal, coal pile, and other equipment that comprise the actual production area.
4. Operable Unit 4 (OU4): Silos 1 through 4, includes the K-65 silos 1 and 2 which contain radioactive wastes, silo 3 which contains dried uranium-bearing wastes, and silo 4 which is empty, and related berms, decant system, and soil.
5. Operable Unit 5 (OU5): Environmental Media includes groundwater, surface water, and soil not included in other operable units.

Each of these operable units have a separate schedule for the environmental studies, design, and construction phases. For work done under the EPA's CERCLA/Superfund regulations the work is divided into 4 distinct steps:

- Remedial Investigation (RI)
- Feasibility Study (FS)
- Remedial Design (RD)
- Remedial Action (RA)

The first two steps, RI and FS, are typically done concurrently with the goal being to characterize the site, determine the nature and extent of contamination, assess the risk to the public and environment, and determine the best approach for cleanup.

Each of these phases of the work requires extensive data collection, analysis, modeling and simulation. The initial investigations require that we understand the nature of the contamination and the associated risks. We are currently completing field investigations that will allow us to define the nature and extent of contamination at the site.

II. METHOD

II.1 Subsurface Modeling Efforts To Date

As part of our effort to assess the completeness of our data, develop volumetric estimates of contamination, and produce presentations we have completed eleven related modeling efforts during the period from January 1993 until the present, see Table 1.

Modeling subsurface contamination using geostatistics and kriging offers a number of significant benefits for environmental cleanup. Since remediation schedules are relatively fast paced due to the health risks and public concern, the process of gathering soil and groundwater samples and waiting for laboratory analysis is viewed with much consternation. Coupling GIS technologies for mapping environmental information with computer visualization tools and three dimensional kriging offers one of the best techniques for assessing the completeness of existing data sets, and planning for any additional sampling required.

Likewise, once the models using the existing data have been generated, the same models can be used to assess the effectiveness of new sampling. In turn, the same three dimensional models can be use to quickly compute volumes of contaminants for use in feasibility studies, or produce maps of contamination for environmental reports. We also use the same data, and models, to help determine input parameters for groundwater modeling efforts.

II.2 The Process

The procedure for generating the three dimensional models consists of a five step work process beginning with the data extraction from a relational database, defining the geologic model constraints, analyzing the data statistically, doing the 3D interpolation, and, finally, using computer graphics tools to prepare presentation graphics.

Our modeling process starts first with the end user of the data defining what type data he, or she, wants. An environmental data analyst will work with the engineer or scientist to determine the type of data, the date range, validation qualifiers, laboratory analyses, coordinate and depth ranges for the area of interest. Typically we exclude samples rejected during the data validation process, and any samples below the detection limits are set to half

the detection limit.

The analyst will then extract the data by running a query/report against the central sitewide environmental database (SED); these queries are usually written in SQL (Structured Query Language), the industry standard for reporting from relational databases. Once the data is extracted, and checked by the analyst and the end user of the data, the modeling is ready to begin.

One of the most demanding tasks in the whole process is the definition of the geologic constraints and the development of the physical parameters of the model itself. The first tasks in generating the model is determining the area of interest the corresponding spatial extent and maximum depth. A geologist, or other environmental professional, will typically delineate the area of interest to be modeled. The model depth is usually fixed by some geologic boundary such as the top of bedrock or aquifer.

Data from borings in the area of interest are used to define the surfaces representing the various geologic strata, such as bottom of fill and top of bedrock. In our case, we use Intergraph MGLA/MGLM to post geologic contacts from boring data stored in our Sitewide Environmental Database. We use Intergraph's MSM product to perform first pass contouring. Geologists and engineers familiar with the site then review this computer generated surface and provide additional interpretation. The interpreted contours and the posted data are then combined to produce each final geologic strata definition.

Each strata definition is then loaded into MGE Voxel Analyst to constrain the interpolation runs. Likewise, this same geologic information is also input for the groundwater modeling. Finally, the same data gets triple duty in the production of geologic sections and maps for inclusion in our environmental reports.

The heart of our approach to modeling contamination is the use of three dimensional geostatistics. Geostatistics is the branch of mathematics which was originally developed in the early 1970's for use in estimating mineral grades within the deep gold reefs of South Africa. The basis of the theory is to include the spatial nature of the data as well as the core quantitative nature of the same data. The primary tool used to quantify this spatial correlation is the experimental variogram, which is a plot of variance vs. distance, usually qualified according to some directional search criterion.

Once prepared, variograms provide critical input into the actual estimation process, for which we use a technique called kriging. Kriging is a geostatistical interpolation technique, usually a program, which, based on the shape of the experimental variogram model, estimates a parameter of interest at points (or volumes) in space from data realizations made at known locations (e.g. sample analyses at borehole depths). Kriging also gives an estimate of the distribution of the error made at each point (or volume), so that confidence intervals may be derived.

In the 1980's geostatistical techniques and kriging began to be applied to environmental problems, including hydrology, hydrogeology, air dispersion, and environmental sampling design. Most of these studies have employed two dimensional modeling in large part due to the lack of commercially available three dimensional geostatistical software and suitable computing hardware.

II.3 The Computing Tools

The primary computing platform for our subsurface modeling at Fernald is the Intergraph 6480 workstation, with Edge II graphics accelerator. The 6480 runs Intergraph's Kriging Module and Voxel Analyst software. The environmental data normally resides in our central data repository, developed in the Oracle 7.0 relational database, running on a Digital Equipment Corporation VAX 7620. Our Intergraph workstations and servers are connected via a single network. A Novell PC network of 2500 PC's is the primary method of accessing information across the site. Additionally, a network of Intergraph workstations and servers allow users to share drawings and data generated on either type of system.

Figure 1 illustrates the basic dataflow. Environmental data, consisting of sample location, associated field readings, laboratory analysis, water level readings, and boring logs, are first entered into our sitewide environmental database (SED). Our GIS and modeling software run on top of the Intergraph Microstation CAD product, and access the data via SQL queries. Since all of these products use the same graphics front-end we are able to very easily superimpose products developed from different applications. This superpositioning capability extends to facility and site information such as scanned aerial photographs, geologic maps, and engineering drawings. From this synthesis of data products we are able to easily produce hybrid mapping products combining any of the raster, image, vector, analysis, and database data. The Intergraph GeoVoxel software (MGVA) provides the necessary volume calculations for contaminated soil. Reports of environmental data, for use in RI and FS documents, are produced directly from the SED using a variety of Oracle reporting software.

III. RESULTS

III.1 Using Geostatistics to Locate Sources of Contamination

The kriging techniques utilized at Fernald consist of Simple Kriging, Ordinary Kriging, and Lognormal Kriging. Both point estimates and block type estimates have been utilized. Our three dimensional kriging approach differs from conventional two dimensional approaches in four ways:

1. The estimated values are stored in a single larger matrix with an added index for depth.
2. Vertical variograms of the data are developed; two dimensional kriging usually uses only four horizontal variograms (typically 0, 45, 90, and 135 degrees).
3. The kriging interpolation algorithm accounts for the additional depth (z) component in the weighting calculations. Figure 2 presents a comparison of two dimensional kriging versus three dimensional. The contour map on the left shows the results of two dimensional kriging performed using sub-surface soil samples which lie between 1.5 and 2.5 feet below ground surface. The map on the right shows the results of kriging at 2 feet below ground surface, but based upon all available samples. The maps show that by including input data points which are "near", in a geostatistical sense, the elevation being analysed, more continuity is added and trends in the data appear which would not be seen using two dimensional kriging.
4. Although not a factor at our site, three dimensional kriging can more easily handle dip and strike angles to account for sloping geologic layers.

The three dimensional approach has the following benefits over the traditional two dimensional approach: Can rapidly cut sections without re-kriging. Can rapidly compute

volumes of contaminated material. We believe the three dimensional kriging to be more accurate than a similar two dimensional approach, because we can use all the data instead of a horizontal subset of the data.

III.2 Three Dimensional Visualization

Three dimensional computer graphics tools enable both technical and non-technical audiences to rapidly understand environmental data and our analysis. Whether used to visualize incremental results of sampling programs, or evaluate the impact of using higher cleanup, no better tool exists for helping us understand complex data and concepts. We routinely use computer graphics tools for manipulating the three dimensional models of the contamination, and also for integrating other data such as results from groundwater dispersion simulations, aerial photographs, GIS, and computer aided design (CAD) files.

The Intergraph MGE Voxel Analyst software provides a variety of display tools to allow the environmental professional to better understand the data and the model. Chair diagrams allow use to view the entire block model with a notch cut out of one corner resulting in two vertical sections and a horizontal section between. For more flexibility we can cut sections through the model at any orientation; we often use this to produce sections through the high concentration areas. One of the most useful display functions is the iso-surfaces, a three-dimensional surface representing the outer boundary of a contaminant area that where the concentration is of constant value; this is the three dimensional equivalent to traditional two dimensional contours.

In order to understand the future implications of a contaminated area, we use groundwater dispersion models to predict the flow of contaminant from the identified source. We can import the simulation results into Voxel Analyst to visualize the spread of contamination over time and in the context of other site features. We use CAD drawings and aerial flyover maps to obtain locations of features like buildings and utilities.

III.3 Volume Estimates

One of the reasons for developing geostatistical models of contamination is for volume computations. The three dimensional model allows rapid calculations of volumes for different action levels. The volumetric function was extensively used in the preparation of our Feasibility Study for Operable Units 2 and 5. Volume calculations for the OU2 report focused on Total Uranium volumes.

Volumetrics for OU5 were based on the three-dimensional model of U-Total over the entire site. Cleanup levels varied by cell, depending on vertical proximity to the aquifer. Also, "clean" soil which had to be excavated to get at contaminated soil further down had to be reported. The PRG's (preliminary remediation goal) which defined the cleanup levels changed depending on the risk level and land use objective being proposed. All of these things were made possible by having a model which estimated concentration of Total Uranium for every block in our model.

III.4 Data Issues

Getting good data is one of the most expensive and time-consuming tasks in an environmental cleanup. At Fernald, prior to our modeling efforts, data had been collected

by many different groups and in different formats. Cleaning up this legacy data, so that it could be used for modeling, proved a time consuming and onerous task. Yet without consistent, validated data the modeling efforts would have been useless.

In our case, we had geologists and other environmental scientists check every record of data against the original laboratory, field, and validation paperwork. In many cases we identified missing information such as missing coordinates on boring locations and incomplete lithologic information.

One of the biggest management concerns in administering a central environmental repository has to be the question of data ownership. While the users of the data have to take responsibility for the data that they use in an individual reporting or modeling effort, there needs to be an entity responsible for the long-term integrity of that data. Data validation is one such area in which central control and decision making is essential in preventing inconsistencies from arising in the data. For instance, different users of the data had differing opinions on whether the laboratory validation qualifiers, like a "U", for undetected, should be used or re-evaluated. Over time the reasoning behind detailed questions like this can be easily lost without some central corporate ownership and commitment to keeping this knowledge accessible.

IV. CONCLUSIONS

A three dimensional geostatistical approach was applied in eleven related modeling efforts at the Fernald Dept. of Energy site. The success of these efforts demonstrates the value of three dimensional modeling for contaminant data analysis and visualization. This effort specifically shows that:

1. Geostatistics are useful in assessing the location of contaminant sources in both soil and groundwater. The three dimensional approach discussed in this paper is essential in understanding and visualizing depth related issues such as excavation, or treatment, cost.
2. Coupling GIS mapping products with three dimensional visualization tools can improve communication between facility owners, regulatory agencies, and the public by making large amounts of complex data more easily understandable by both technical and non-technical audiences. These tools should be used, where feasible, to facilitate open discussions on environmental problems, associated health risks, and appropriate solutions.
3. Three dimensional solid models of contamination provide quick capabilities for estimates of contaminant volumes for different concentration levels, an essential function for analyzing different environmental cleanup alternatives.
4. Special care should be given to maintaining consistent, legally defensible, environmental data repositories at government facilities as this dramatically eases the process of modeling subsurface contamination.

V. RECOMMENDATIONS FOR FURTHER READING

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Table 1: Fernald Modeling Projects

Project Name	Method	No. Cells	Cell Size (ft.)	Constituents of Concern
Data Gap Analysis OU2	Kriging	50x70x20	20x20x2	U-Total
K-65 Silos OU4	Kriging	61x91x6	20x20x5	U-Total, Th-230, Ra-226
Add'l Data for OU2 RI	Kriging	65x45x30 25x20x30 20x20x30	25x25x2.5	U-238
Waste Pits OU1	Kriging	86x88x46	20x20x1	U-Total, Th-Total, Tc-99
Add'l Data for OU2 FS	Kriging	65x45x30 25x20x30 20x20x30	25x25x2.5	U-238, Th-228, Ra-228
Revised OU2 Geology	Load Grid	65x45x30 25x20x30 20x20x30	25x25x2.5	Soil Type
SPA Readings OU5	Inverse Distance	61x39x11	2.5x2.5x2.5	Radiation Readings
Add'l Data for OU4	Kriging	23x35x26	25x25x2.5	Pb-210, Ra-226, Th-228, U-238
Sitewide Geology Model OU5	Direct Assignment	191x201x70	50x50x1	Soil Type
Sitewide FS Volumes OU5	Kriging	56x72x55	125x125x(.5,2,5)	U-Total
Updated Volumes OU5	Kriging	67x74x30	125x125x1	U-Total

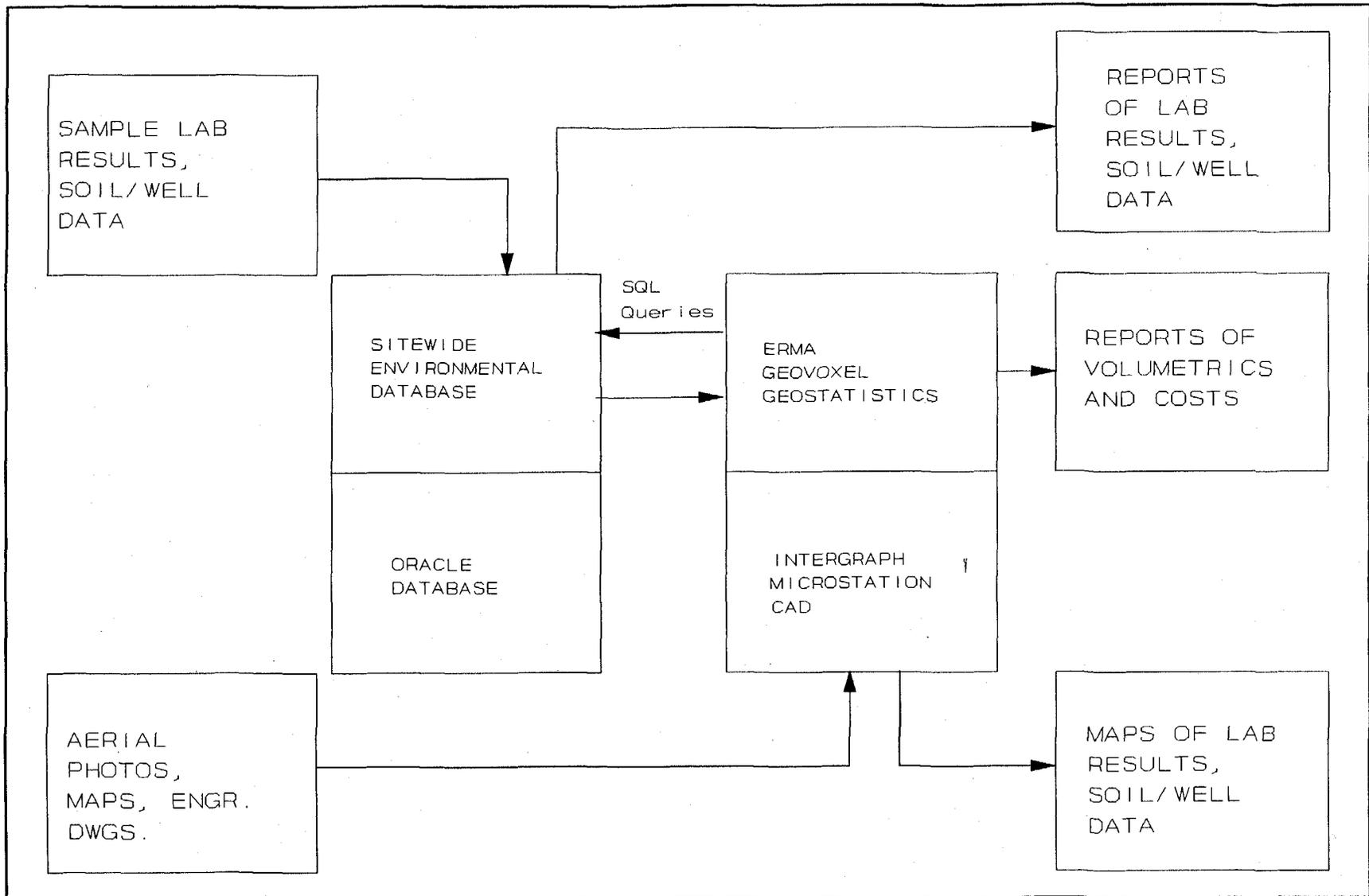


Figure 1 Environmental Mapping and Reporting Dataflow

COMPARISON OF 2-D vs. 3-D KRIGING

2-D Based on Samples at Z=-2.0 ; 3-D Based on All Samples

Contours at 5, 7.5, 10, 20, 50, 100 PPM

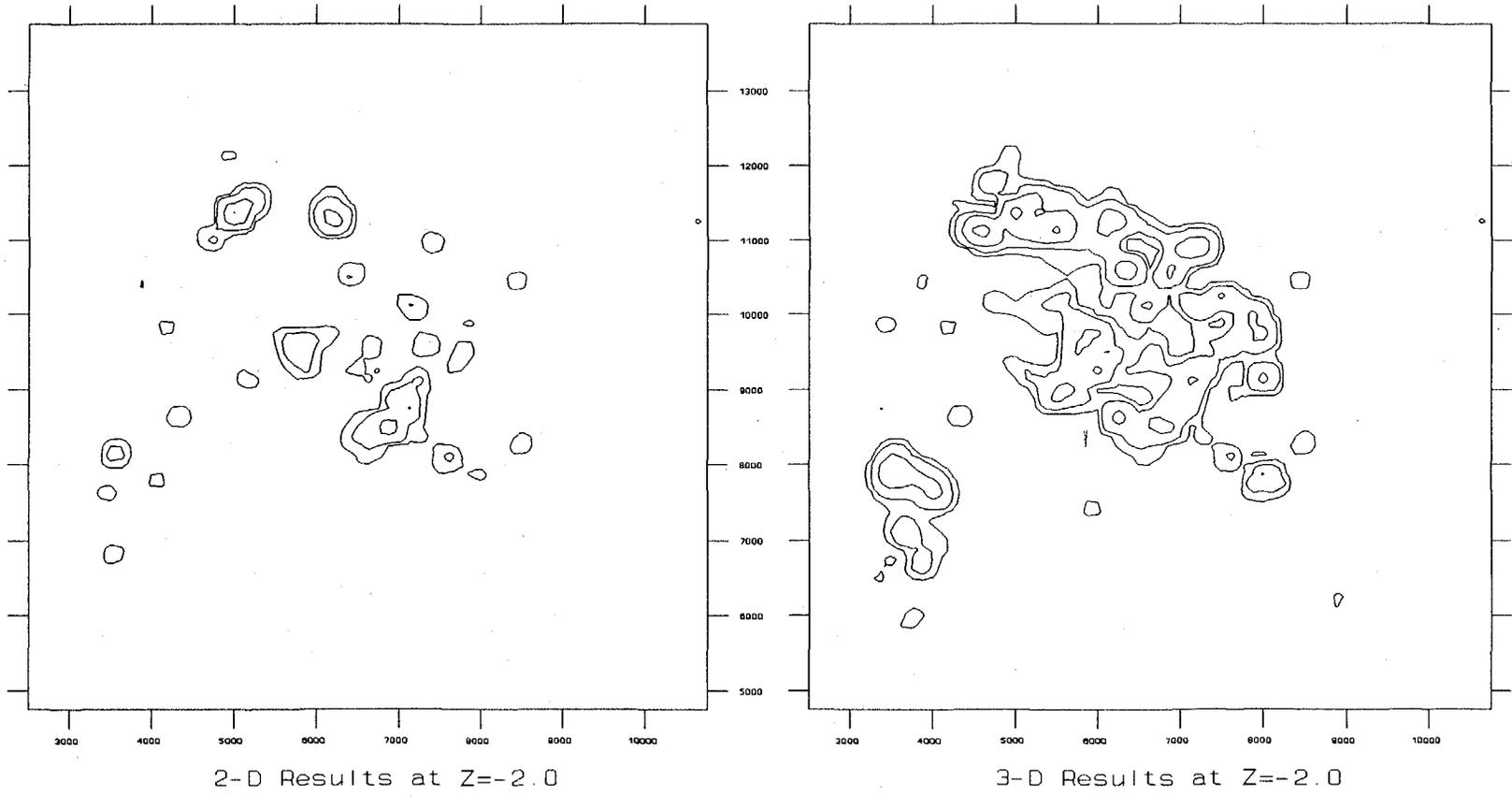


Figure 2: Comparison of 2-D vs. 3-D Kriging