

Hydrogeologic Data Fusion

Industry Programs/Characterization, Monitoring, and Sensor Technology Crosscut Program



Prepared for:

U.S. Department of Energy

Office of Environmental Management Office of Science and Technology

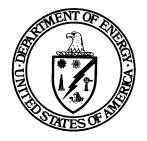
September 1999



Hydrogeologic Data Fusion

OST Reference #2944

Industry Programs/Characterization, Monitoring, and Sensor Technology Crosscut Program



Demonstrated at:
U.S. Department of Energy
Hanford, Pantex, Savannah River Site and Fernald,
Department of Defense, and Commercial Sites



Purpose of this document

Innovative Technology Summary Reports are designed to provide potential users with the information they need to quickly determine if a technology would apply to a particular environmental management problem. They are also designed for readers who may recommend that a technology be considered by prospective users.

Each report describes a technology, system, or process that has been developed and tested with funding from DOE's Office of Science and Technology (OST). A report presents the full range of problems that a technology, system, or process will address and its advantages to the DOE cleanup in terms of system performance, cost and cleanup effectiveness. Most reports include comparisons to baseline technologies as well as other competing technologies. Information about commercial availability and technology readiness for implementation is also included. Innovative Technology Summary Reports are intended to provide summary information. References for more detailed information are provided in an appendix.

Efforts have been made to provide key data describing the performance, cost and regulatory acceptance of the technology. If this information was not available at the time of publication the omission is noted.

All published Innovative Technology Summary Reports are available on the OST Web site at http://OST.em.doe.gov under "Publications."

TABLE OF CONTENTS

1 SUMMARY	page 1
2 TECHNOLOGY DESCRIPTION	page 4
3 PERFORMANCE	page 6
4 TECHNOLOGY APPLICABILITY & ALTERNATIVES	page 11
5 COST	page 12
6 REGULATORY/POLICY ISSUES	page 14
7 LESSONS LEARNED	page 15
APPENDIX	
A References	page 16

SUMMARY

Technology Summary

Problem

The fate and transport of contaminants in the subsurface requires knowledge of the hydrogeologic system. Site characterization typically involves the collection of various data sets needed to create a conceptual model that represents what's known about contaminant migration in the subsurface at a particular site.

How Hydrogeologic Data Fusion Works

Hydrogeologic Data Fusion is a mathematical tool that can be used to combine various types of geophysical, geologic, and hydrologic data from different types of sensors to estimate geologic and hydrogeologic properties. It can be especially useful at hazardous waste sites where the hydrology, geology, or contaminant distribution is significantly complex such that groundwater modeling is required to enable a reasonable and accurate prediction of subsurface conditions.

DATA FUSION MODELING (DFM)

Prediction to Aid Decisions

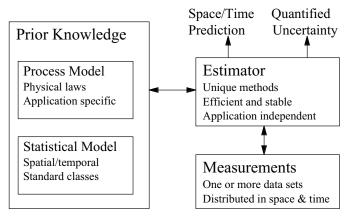


Figure 1: Schematic illustrating the general concepts of Hydrogeologic Data Fusion

Hydrogeologic Data Fusion is a computer code that combines several mathematical techniques to calibrate models of ground-water flow. The mathematical codes associated with Hydrogeologic Data Fusion are used to estimate the input parameters required by the flow models. The codes combine various types of data to improve estimates of the geologic and hydrogeologic parameters. These model input parameters are typically determined using time-consuming trial and error methods that compare model results calculated with a given input parameter set to historical conditions. The groundwater model is run iteratively with refined input parameters until the errors between the simulated and actual conditions are determined to be acceptable. The Hydrogeologic Data Fusion code automates the parameter selection process, which typically results in better estimates for very short periods of time. Reduction of the error value between simulated and actual conditions increases the validity of the model and provides confidence that predictive results will be better accepted by regulatory representatives. Reduction of the time required to obtain acceptable results can substantially reduce cost of a project.

For example, geophysical data collected using electromagnetic and seismic techniques might be combined with lithology determination made from core descriptions to produce a layered model of the subsurface geology. This model can then be used as input to a flow and transport model simulation, that result in an improved prediction of where contaminants are migrating. In Hydrogeologic Data Fusion, the different types of data are not only interpreted together but are mathematically combined; each data type is weighted according to its accuracy.

To perform Hydrogeologic Data Fusion, the following information is required:

- Geologic geophysical, or hydrologic data,
- Models that provide the relationship between the data and the model parameter (the forward models),



A conceptual site model developed by geologists and other scientists familiar with the site.

Hydro-FACT Flow Calibrations and Prediction

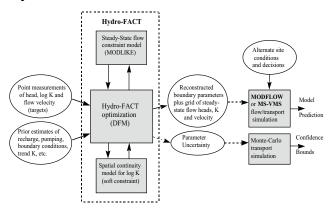


Figure 2: Flow chart for Hydrogeologic Data Fusion Modeling emphasizing the iterative nature of the process.

Potential Markets

The primary application of Hydrogeologic Data Fusion is for estimating robust parameters to be used for modeling groundwater flow and contaminant transport. It is applicable to any DOE site or other hazardous waste site where groundwater flow and transport modeling is ongoing. The Hydrogeologic Data Fusion code is especially applicable for use at large, geologically complex sites with significant hazardous waste plumes.

Advantages Over the Baseline

The baseline technology for Hydrogeologic Data Fusion is manual trial and error model calibration of groundwater models. This calibration can be a very time-consuming process where the parameters are varied to produce the best fit to the actual measurements from the field. Relative to the baseline method, the advantages include:

- Automatic estimation of the best fit to the measured parameters,
- A significant reduction in the time to calibrate models,
- · A better match of estimated parameters to measured data and the conceptual model,
- · Quantification of parameter uncertainty,
- · Quantification of parameter correlation,
- · Quantification of uncertainty in contaminant transport.

The use of Hydrogeologic Data Fusion results in a reduction in labor cost to calibrate complex groundwater models.

- A LANL cost study estimates that if Hydrogeologic Data Fusion were applied at three hazardous waste sites at each of the fifteen major DOE facilities, a cost savings of approximately 3.6 million dollars would result.
- Use of Hydrogeologic Data Fusion to produce better quality groundwater modeling might ultimately result in:
 - ♦ A reduction in the number of monitoring wells,
 - ♦ A reduction in the number of treatment wells.
 - Better quality modeling leading to less conservative regulatory decision making (e. g. No Further Action decisions,)
 - ♦ Better documentation of regulatory compliance.

Demonstration Summary

DOE funded the development of a Hydrogeologic Data Fusion Workstation (DFW) in the early 1990s. The work was based on concepts developed for defense and space applications during the last 25 years. Early efforts to apply these concepts to environmental applications focused on integration of geophysical sensors and later evolved into the fusion of hydrogeologic data.

SUMMARY

continued

- The Hydrogeologic Data Fusion product developed under DOE funding is called DFW/VAM3DF and is available for use by government contractors and governmental organizations. It is a fully functional unit that contains the Hydrogeologic Data Fusion model, graphical user interface (GUI), grid builder, database, and interfaces with ARCView, TecPlot™ and Earth Vision™. This platform operates on a workstation and can be applied for hydrological data integration at any site but requires customization before application at any given site.
- HydroFACT, a commercial offering developed by Fusion and Control Technology, Inc., has more limited capabilities. It operates on a PC computer, is fully integrated with either MODFLOW or MS-VMSTM, and provides parameter estimation for groundwater flow calibration.

Demonstration Sites/Key Results

DOE

Hanford/200 West Area: Hydrogeologic Data Fusion Modeling was used to combine geophysical measurements and core data to map the location of a critical geologic layer that controls groundwater flow. Seismic velocity information collected over a wide area allowed for estimation of the location of the critical layer far beyond the location of the core data at a facility where drilling is both expensive and hazardous.

Zone 12 Pantex Weapons Facility: Hydrogeologic Data Fusion Modeling was used to map hydraulic conductivity and estimate flow pathlines in a perched aquifer from which contaminants can potentially migrate to the regional groundwater aquifer. Previous groundwater modeling efforts had not resulted in a robust prediction of contaminant migration.

Savannah River Site/Old Burial Ground and A/M Area: Hydrogeologic Data Fusion Modeling was used for parameter estimation for two very complex groundwater models and the results were compared with the results generated by manual calibration. Hydrogeologic Data Fusion took significantly less time than manual calibration, produced similar results, and quantified the statistical uncertainty.

Fernald: Hydrogeologic Data Fusion Modeling was used to support decision making for site selection of a low-level radioactive waste disposal facility. Hydrogeologic Data Fusion provided critical information to the site-selection process and was used as a clear communication tool for the regulators and the general public.

DoD

Air Force Site/California: Groundwater modeling being done in support of a natural attenuation study had not mathematically converged after six months of manual calibration. HydroFACT was able to compute a calibrated flow model within one day after the MODFLOW input files were generated.

Air Force/Massachusetts: Groundwater models generated with Visual MODFLOW and MODFLOWP at this relatively large site with a significant, ongoing effort at groundwater flow and transport had failed to produce convergence. Hydrogeologic Data Fusion was used for parameter optimization to support calibration efforts. HydroFACT was used to estimate input parameters that resulted in convergence of the model in one week.

Letterkenney Army Depot, Pennsylvania: Hydrogeologic Data Fusion Modeling resulted in a three-dimensional calibrated numerical model that indicated that the hydraulic conductivity was fairly uniform and identified a lobe of slightly lower conductivity under the source area. The estimated hydraulic conductivity field correlated with independent geologic interpretation. Previous modeling efforts had not resulted in a calibrated model and were unsuccessful at delineating a three-dimensional pattern of groundwater flow.

Contacts

Technical

Dr. David Porter, FACT, Inc., fuserdp@clark.net, 410-451-4043

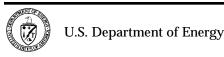
Dr. Peter Huyakorn, HydroGeologic, Inc., psh@hgl.com, 703-478-5186

Management

Charles Nalezny, Office of Science and Technology, Program Manager, Characterization, Monitoring, and Sensor Technology Crosscutting Program, 301-903-1742

Vijay Kothari, vkotha@metc.doe.gov, Federal Energy Technology Center, 304-285-4579

All published Innovative Technology Summary Reports are available at http://em-50.em.doe.gov. The Technology Management System, also available through the EM50 Web Site, provides information about OST programs, technologies, and problems. The OST Reference number for Hydrogeologic Data Fusion is 2944.



TECHNOLOGY DESCRIPTION

Groundwater flow and contaminant transport modeling are important components of environmental management. Models are tools that are essential for understanding the physical processes of groundwater flow and contaminant transport under both natural flow and stressed (pumping) conditions. Models are an integral component of environmental site characterization and assessment, remedial investigation, remedial design, and performance assessment.

Conventional groundwater modeling is based on finite difference or finite-element flow software where the parameters of the model are defined in regions. The parameters to be defined may include hydraulic conductivity, anisotropy, boundary conditions, recharge/drain conductance, source head, pumping flow, etc. In most cases, these parameters are not directly measured but are estimated. In most cases, the measurements available for calibration consist solely of hydraulic head and some measurements of conductivity. Calibration of groundwater models is a very time consuming trial-and-error process where the parameters are varied and then the model is run to produce results that match the head measurements. Calibration continues until the model fits the available data within an acceptable statistical range, or until the analyst runs out of time, money, or patience.

Hydrogeologic Data Fusion is used in conjunction with standard groundwater flow models, such as MODFLOW, to provide a better method for estimating the model parameters. Hydrogeologic Data Fusion is superior to manual calibration because it uses a physical basis for parameter estimation. It also results in the quantification of parameter uncertainty, parameter correlation, and uncertainty in contaminant transport. The Hydrogeologic Data Fusion product developed under DOE funding is called DFW/VAM3DF and is available for use by government contractors and governmental organizations. HydroFACT is a commercial offering with more limited capabilities, which was developed by Fusion and Control Technology, Inc. It operates on a PC, is fully integrated with either MODFLOW or MS-VMSTM, and provides parameter estimation for groundwater flow calibration.

The hydrogeologic algorithms included in HydroFACT and DFW/VAM3DF automatically find the parameter values that produce the best fit to the available measurements. This is done iteratively, producing potential solution within minutes, hours, days, and weeks depending on the platform, size and extent of the problem and quality of data.

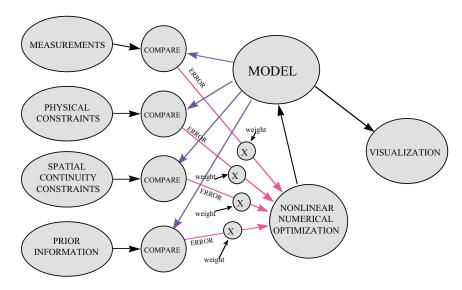


Figure 3: Detailed flow chart for HydroFACT Flow Calibration and Prediction

Parameters estimated with HydroFACT include:

- Hydraulic head,
- Boundary conditions.
- · Conductivity or transmissivity,
- Recharge values,
- · Leakage.



TECHNOLOGY DESCRIPTION

continued

Inputs into HydroFACT can include:

- Direct measurement of hydraulic head, conductivity and flow,
- Prior information on spatial variability of conductivity within hydrostratigraphic units,
- Information on the location of discontinuities,
- Prior information regarding model parameters such as recharge and leakance,
- Relative accuracy of different measurements.

The HydroFACT software system consists of:

- A preprocessor that accepts input grids from MODFLOW and generates HydroFACT input files with default values for all parameter;;
- · Hydrogeologic estimation programs,
- Graphical user interface that facilitates modification of input parameters and run control,
- Utility programs to facilitate analysis.

The system requirements vary significantly depending upon the size of the problem. Operation of the HydroFACT software system requires: Windows95[®] or WindowsNTTM on a PentiumTM or Pentium ProTM personal computer. Problems of 30,000 nodes or more require a 200 MHz Pentium Pro computer with 128 Mbyte of RAM and at least 2 Gbyte of disk space. Smaller applications that involve computation of uncertainty may also require this capability.

The specific features of HydroFACT include:.

- The capability to model steady-state groundwater flow using quasi-3D or 3D fixed or variably saturated models that are fully compatible with either MODFLOW of MODFLOW-SURFTM (flexible options allow compatibility with other versions; the source code of the flow model is supplied so that the user may modify it),
- The capability to model log horizontal conductivity as the sum of a trend component plus a random component (conductivity
 parameters can be specified independently in different hydrostratigraphic units; separate units allow for modeling of discontinuities or different properties),
- The capability to model log vertical conductivity either directly within zones or using a trend log anisotropy spatial polynomial within each unit,
- The capability to model discontinuities by allowing log horizontal conductivity to be constrained or estimated in zones,
- The capability to allow all model parameters to be specified in zones that can have any form even disjoint (different parameter may have different zone definitions),
- The capability to allow all important model parameters to be estimated separately for each zone with much flexibility in selection of parameters to be estimated,
- The use of Bayesian estimation where the prior uncertainty is specified for all estimated parameters,
- The flexibility options in handling boundary conditions include estimation of boundary parameters,
- The capability to model water-level measurements, log horizontal and vertical conductivity, azimuth, indication and magnitude of the flow velocity (all measurements are represented as interpolation from neighboring nodes so that the measurement considerations do not determine model grid spacing).
- The ability to estimate bias on log horizontal or vertical conductivity measurements,
- · The capability to automatically edit anomalous measurements above a user-defined threshold,
- The use of robust optimization techniques for performing the nonlinear iterations required in the least squares solution,
- The use of robust and efficient sparse linear solvers for computing the Newton-Gauss steps.

The output files from HydroFACT include:

- Files with final estimates of parameters that can be directly input into MODFLOW,
- Files that can be directly read by TecplotTM or EarthVisionTM for viewing the results,
- Files that can be used as a restart files for continuing iterations at a later time.



PERFORMANCE

Demonstrations

The initial geophysical fusion platform was tested at Hanford and Fernald, and later Hydrogeologic Hydrogeologic Data Fusion was demonstrated at Pantex, SRS, and several DoD sites.

DOE/Hanford/200 West Area

Problem or Objectives: In 1995, Hydrogeologic Data Fusion was used in the 200 West Tile field at Hanford to map a thin caliche layer in the vadose zone located at a depth between 30 and 40 feet. This caliche layer is an important hydrostratigraphic layer that retards downward migration of contaminants, including plutonium, to the water table.

Information Used

- Seismic velocity information inferred from surface seismic refraction measurements
- Elevations of the top of the caliche layer determined from cores collected during installation of 25 groundwater wells
- Contaminant measurements in groundwater collected from the wells

Hydrogeologic Data Fusion Results

- Seismic data were used to extrapolate the location of the caliche layer beyond the well data at a facility where drilling is both
 expensive and hazardous.
- Hydrogeologic Data Fusion results quantified the uncertainties on the location of the top of the caliche layer.
- Hydrogeologic Data Fusion results identified a low permeability layer located above the caliche, which was subsequently
 confirmed by directly measuring permeability.

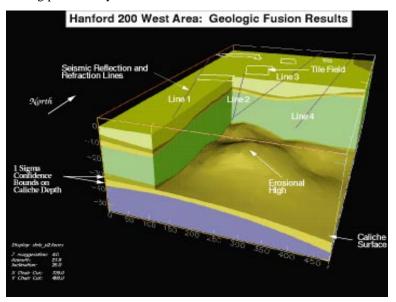


Figure 4: Hydrogeologic Data Fusion results from the 200 West Tile field showing location of seismic lines and modeled location of caliche surface with one sigma confidence boundaries

DOE/Zone 12 Pantex Weapons Facility

Problem or Objectives: Hydrogeologic Data Fusion was used at the Pantex Weapons Facility in Amarillo, Texas in 1995 to predict groundwater flow in the perched aquifer. Previously, groundwater modeling efforts had not resulted in a robust prediction of contaminant migration from the perched aquifer to the regional Ogallala Aquifer. The specific objective was to determine the potential contaminant pathways in a perched aquifer located above a confining unit designated the Fine-Grained Zone (FGZ) in the vadose zone. The extent and surface topography of the FGZ was poorly known. Boundary conditions and leakage through the FGZ were poorly known. Hydrogeologic Data Fusion modeling was used to estimate flow pathlines in the perched aquifer.



Information Used

- Approximately 50 lithologic and geophysical logs
- Hydrologic information including perched water level measurements, slug tests, and recharge information

Hydrogeologic Data Fusion Results

- By jointly processing all available data, Hydrogeologic Data Fusion Modeling was able to map hydraulic conductivity and
 estimate flow pathlines in the perched zone. Information on hydraulic conductivity was provided by both direct conductivity
 measurements and indirect head measurements through the hydrological model.
- The model fit the water-level data with a root mean square (RMS) of 0.6 feet.
- Hydrogeologic Data Fusion quantified the hydrologic uncertainties in terms of the statistical standard deviation.

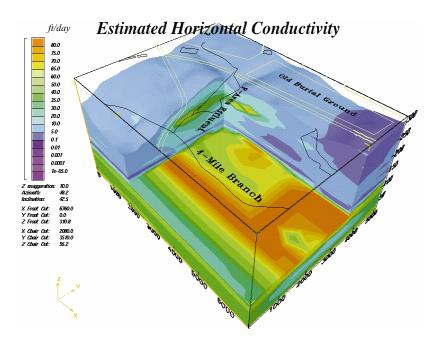


Figure 5: Map showing location of estimated flow pathlines in the perched water zone

DOE/Savannah River Site/Old Burial Ground

Problem or Objective: A calibrated groundwater flow and transport model had previously been developed to determine potential pathways for migration of TCE, PCE, and tritium in interlayered clay and sand layers to where they cropped out in stream drainages. The groundwater model is very complex and has an extremely heterogeneous conductivity field that includes discontinuous layers. The model had previously been calibrated using manual methods. Hydrogeologic Data Fusion was used for parameter estimation; the results were then compared with the results of the manually calibrated model.

Information Used

- Measured head data from 237 observation wells were used as calibration targets.
- The fraction of mud-sized sediments measured from core material was used to estimate horizontal conductivity (Kh) and vertical conductivity (Kv) using an empirical function.
- Elevations of key geologic intervals determined from core data were used to define the elevation of 21 nodal layers.
- The recharge drain boundary condition was applied to the top nodal layer and a no-flow boundary was applied to the bottom nodal layer.

Hydrogeologic Data Fusion Results

Hydrogeologic Data Fusion was used for parameter estimation and VAM3DF was used for flow and transport modeling.

- The results were consistent with those generated by manual calibration.
 - ♦ The models have similar pathlines, recharge rates, and trends in hydraulic conductivity.
 - The conductivity field is different. The field generated with Hydrogeologic Data Fusion Modeling is smoother due to the spatial correlation parameters that were used.
 - ♦ The use of the Hydrogeologic Data Fusion Modeling reduced the RMS from 3 feet to 1.3 feet.



- Hydrogeologic Data Fusion Modeling took significantly less time than manual calibration.
- Hydrogeologic Data Fusion Modeling quantified the statistical uncertainty in the tritium breakthrough curves not provided by manual calibration.

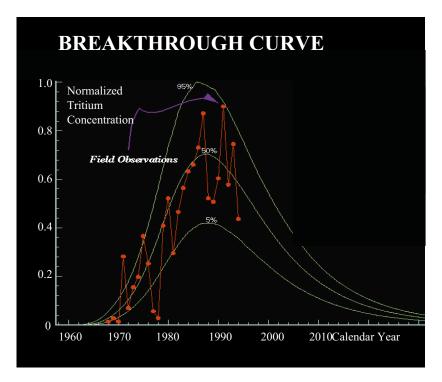


Figure 6: Calculated and measured tritium breakthrough curves for the Old Burial Ground model at SRS.

DOE/Savannah River Site/A/M Area

Problem or Objectives: A calibrated groundwater flow and transport model had previously been developed at SRS for flow and transport of TCE and PCE in layered Coastal Plain sediments. Hydrogeologic Data Fusion Modeling was used to optimize the existing model that had been calibrated using manual techniques.

Information Used

· Head data from monitoring wells were used as calibration targets.

Hydrogeologic Data Fusion Results

- The results were consistent with those generated by manual calibration.
- Pathlines, pathline uncertainty, capture zones, and contaminant concentrations were computed.
- Hydrogeologic Data Fusion Modeling fit the measured water level data to within 1.0 foot.
- Hydrogeologic Data Fusion took significantly less time than manual calibration.

DoD/Air Force Site/California

Problem or Objectives: Groundwater modeling was being done in support of a remedial demonstration using natural attenuation in sediments overlying volcanic rock. Groundwater modeling was required for regulatory permitting and demonstration of compliance. The existing groundwater model did not converge after six months of manual calibration. The HydroFACT model was used for input parameter estimation.

Information Used

- There are no natural boundaries in the model so general head boundary conditions were used and HydroFact was used to
 estimate the source/sink head.
- Thirty-eight (38) water level and 17 pump test measurements were available.



Hydrogeologic Data Fusion Results

- · HydroFACT was able to compute a calibrated flow within one day after the MODFLOW input files were generated.
- The RMS fit to the water level was 0.3 feet.
- The rapid calibration of the predictive model with quantified uncertainty can be used to demonstrate regulatory compliance.

DoD/Air Force/Massachusetts

Problem or Objectives: This is a relatively large site with a significant ongoing effort to understand groundwater flow and transport in sand, silt, and clay overlying bedrock. The stratigraphic framework is very complex and is updated often as new geologic information is available. The current groundwater model uses a complex, 25-layer model. Groundwater models generated with Visual MODFLOW and MODFLOWP failed to produce convergence; Hydrogeologic Data Fusion was used for parameter optimization to support calibration efforts.

Information Used

- · Groundwater head measurements
- Travel times for contaminant plume
- Lithologic data
- Salt water interfaces and stream flow boundary conditions for 80% of the side boundary with fixed head boundary conditions for the remaining 20%

Hydrogeologic Data Fusion Results

- HydroFACT was used to estimate input parameters that resulted in convergence of the model.
- The model fit all 337 available water level measurements with a RMS residual of 0.7 feet and also fit the conductivity data.
- The use of velocity angle measurements allowed pathlines to match observed plume distributions.
- This project was an example where Hydrogeologic Data Fusion was used to optimize conventional methods. A manually
 calibrated model required two months to develop and had an RMS error of 2.3 feet.

DOE/Fernald/Ohio

Problem or Objectives: Hydrogeologic Data Fusion was used to support decision making for site selection of a low-level radioactive waste disposal facility. The objective was to map the thickness of clay layers and the distribution of sand bodies that could provide preferential contaminant pathways in the clay.

Information Used

The model of the confining zone was updated in real time with lithologic information generated with a cone penetrometer truck (CPT) during site characterization.

Hydrogeologic Data Fusion Results

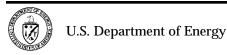
- Three-dimensional maps of clay layers and sandy zones were used to determine location where the clays were the thickest and sand bodies were not present to provide contaminant pathways.
- The visual maps were an important aid to the decision making process for selecting the site location for the waste facility.
- Early identification of inconsistencies between boring and CPT data focused the field effort and enabled more robust characterization.
- The maps produced provided a clear communication tool for the regulators and the general public.

DoD/Letterkenney Army Depot/Pennsylvania

Problem or Objectives: Previous efforts at modeling groundwater flow in highly weathered and fractured bedrock had not resulted in a calibrated model or delineation of the three-dimensional pattern of groundwater flow. As a result, a large-scale dye-tracing program was undertaken in 1996.

Information Used

- Lithologic data and geologic data compiled from site Remedial Investigation/Feasibility Study (RI/FS) reports, geologic logs, geophysical logs, the USAEC IRDMIS data base, geologic maps, hydrogeologic maps and watershed maps
- Water level data from 21 wells; pump test results from 15 wells
- No flow boundary conditions on the bottom and three sides; one side was modeled as head-dependent flux



continued

Hydrogeologic Data Fusion Results

- Hydrogeologic Data Fusion Modeling resulted in a three-dimensional calibrated numerical model.
- Hydrogeologic Data Fusion Modeling indicated that the hydraulic conductivity was fairly uniform and identified a lobe of slightly lower conductivity under the source area.
- The estimated hydraulic conductivity field correlated with independent geologic interpretation.
- The velocity distribution based on fusion-estimated hydraulic conductivity and hydraulic head distributions was used to compute pathlines starting at potential and confirmed contaminant sources. The model identified pathlines that had the potential for off-site flow.
- The model fit the water level data with an RMS error of 2.8 feet
- Conductivity estimates, pathline results and calculated uncertainties provided critical information for future site characterization and remediation strategies.

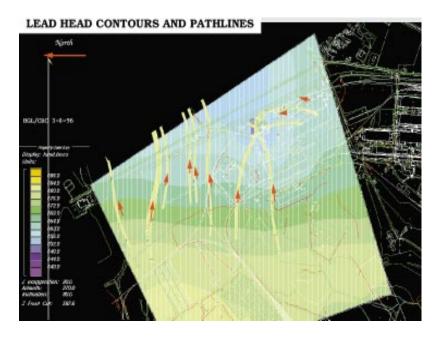


Figure 7: Map showing estimated flow pathlines and head contours.

TECHNOLOGY APPLICABILITY AND ALTERNATIVE TECHNOLOGIES

Technology Applicability

The primary application of Hydrogeologic Data Fusion is for robust parameter estimation for groundwater flow and transport modeling. It is applicable to any DOE site where groundwater flow and transport modeling is ongoing and is especially applicable to large, geologically complex sites.

Competing Technologies •

Manual calibration is the baseline technology for Hydrogeologic Data Fusion Modeling. Conventional groundwater modeling is based on finite difference or finite element flow software where the parameters of the model are defined in regions. Typically, the only data available for calibration is measured hydraulic head and hydraulic conductivity. Several classes of models have been developed to assist with parameter estimation.

Direct deterministic inverse models such as MODFLOWP, MODINV, and PEST use inverse modeling for parameter estimation. These models have limitations resulting from non-uniqueness, convergence difficulties, and inability to quantify uncertainties.

Geostatistical inverse modeling such as INVERT-3 resolves some of the problems associated with inverse models. These models are not distributed commercially and have significant computational demands.

Hydrogeologic Data Fusion provides a better method for estimating parameters based on measured data and prior knowledge. In contrast to the other competing technologies, Hydrogeologic Data Fusion uses a physical basis for parameter estimation. Relative to baseline method, the advantages include automatic estimation of the best fit to the measured parameters, significant reduction in the time to calibrate models; better match of estimated parameters to measured data and conceptual model. It also results in quantification of parameter uncertainty, parameter correlation, and uncertainty in contaminant transport.

Patents/Commercialization/Sponsors

A Hydrogeologic Data Fusion system called DFW/VAM3DF was developed under DOE funding and is available for use by government contractors and governmental organizations. It is a fully functional unit that contains the Hydrogeologic Data Fusion model, graphical user interface (GUI), grid builder, database, and interfaces with ARCView, TecPlot and Earth Vision. This platform operates on a workstation and is generalized to apply to any site for hydrological data integration but requires customization before application at any given site.

HydroFACT is a commercial offering developed by Fusion and Control Technology, Inc.; it has more limited capabilities, operates on a PC, is fully integrated with either MODFLOW or MS-VMS™, and provides parameter estimation for groundwater flow calibration. It is currently being marketed and user support is available.

COST

Information in this section is summarized from a report prepared by Los Alamos National Laboratory (LANL) (Van Eeckhout, 1997). LANL was tasked to perform the cost analysis as an independent team for the DOE Office of Science and Technology. They determined that the cost impact of Hydrogeologic Data Fusion varies on a site by site basis but the benefits of this particular Hydrogeologic Data Fusion methodology over manual trial-and-error modeling derive mainly from the ability to rapidly combine diverse sources of information to quantify and reduce uncertainty. For a very complex site, savings might be on the order of manmonths of time (or allowing convergence to occur where none might occur manually), whereas for a simpler site the savings might be on the order of man-weeks. For groundwater modelers skilled in manual trial-and-error methods, the training time to perform the work using Hydro-FACT might be on the order of several weeks. Both the traditional and Hydrogeologic Data Fusion methodology require the use of computer technologies.

The most easily quantified direct savings from Hydrogeologic Data Fusion result from reduced labor costs for groundwater model calibration and optimization. Other potential sources of direct savings include possible reduction in the number of monitoring wells and/or a reduction in treatment wells due to the improved quality of modeling results. Indirect savings may result from better demonstration of regulatory compliance, better match to measured data and prior knowledge, and a more quantifiable parameter uncertainty. Because the savings are so site-dependent, the cost savings will be determined using several of the specific case histories discussed in Section 3.

Site 1: Two Areas at the DOE Savannah River Site

Characteristics of Area:

- Complex groundwater model with an extremely heterogeneous conductivity field
- Large number of wells
- · Boundary conditions poorly defined

Computation results:

- Hydrogeologic Data Fusion RMS fit to data was 1 ft and 1.3 ft at the two sites; manual trial-and-error fit was 3 ft at one of the sites.
- Site personnel estimated 75% less effort than manual calibration.

Estimated cost savings per area:

- If it took 4 months to perform the calibration manually, the Hydrogeologic Data Fusion could do it in 1: 3 months savings at \$20,000 per month (using \$240,000 as the cost per man-year) = \$60,000. However, the code cost \$5,000 and it took one month to train, so the net savings = \$35,000 per Type 1 stand-alone area (yielding more accurate results plus quantified uncertainty).
- Applied to additional sites, the code cost and training time would not be relevant and savings would thus be greater.

Site 2: A DoD Massachusetts Site

Characteristics of Area:

- Ongoing, complex flow and transport modeling
- Hundreds of water level measurements
- Variable boundary conditions and numerous ponds

Computation results:

- Hydrogeologic Data Fusion RMS fit to data was .7 ft; manual fit was 2.3 ft.
- Hydro-FACT solved the problem within a week; manual method took 2 months.

Estimated cost savings per area:

- If it took 8 weeks to perform the calibration manually, and Hydrogeologic Data Fusion could do it in 1: 7 weeks savings at \$5,000 per week = \$35,000.
- However, the code cost \$5,000 and it took 4 weeks to train, so the net savings = \$10,000 per Type 2 stand-alone area (yielding more accurate results plus quantified uncertainty).
- Applied to additional sites, the code cost and training time would not be relevant.



Site 3: A DoD California Site

Characteristics of Areas:

- Site characterized by sand/gravel and claystone overlying volcanic rock
- 38 water level and 17 pump test measurements available
- No natural boundaries so Hydro-FACT estimated source/sink heads

Computation results:

- Hydrogeologic Data Fusion RMS fit to data was .3 ft; manual fit unknown.
- Hydro-FACT solved the problem within one day after data files created.

Estimated cost savings for this area:

- If it took 5 weeks to perform the calibration manually, and Hydrogeologic Data Fusion could do it in 1 (including data file creation): 4 weeks savings at \$5,000 per week = \$20,000.
- However, the code cost \$5,000 and it took 4 weeks to train, so the net savings = **-\$5,000 per Type 3 stand-alone area** (yielding more accurate results with quantified uncertainty).
- Applied to additional sites, the code cost and training time would not be relevant, allowing the savings to be positive.

Now let us make some further assumptions:

- 1. Let us take the 15 major sites often times listed for DOE Weapons Complex Facilities: LANL, Sandia National Laboratory, Lawrence Livermore National Laboratory, Hanford, Savannah River Site, Fernald, Idaho National Engineering Environmental Laboratory, Paducah, Portsmouth, Rocky Flats, Oak Ridge, Mound, Pinellas, Kansas City, and Pantex;
- 2. Each location has two areas like sites 1 and 2 above and four areas like site 3;
- 3. Then the total projected savings across the DOE complex would be:

15 x [2 x (Type 1 area costs) + 2 x (Type 2 area costs) + 4 x (Type 3 area costs)]
- 15 x [site software cost + site training cost]=
15 x [2 x (\$60,000) + 2 x (\$35,000) + 4 x (\$20,000)] - 15 x [\$5,000 + \$20,000] =

DOE COMPLEX SAVINGS: \$3.68 million.

REGULATORY/POLICY ISSUES

Regulatory Considerations —

- Hydrogeologic Data Fusion is a computer tool designed to expedite and optimize standard computer modeling activities and as such is not directly regulated by environmental legislation.
- The three-dimensional visualization of the sites may facilitate regulatory acceptance of the final model.

Safety, Risks, Benefits and Community Reaction

- Because Hydrogeologic Data Fusion is a computer tool, it does not directly impact worker and community safety. There is
 an indirect impact due to the improved interpretation and presentation of results that may result in the minimization of the
 number of samples collected and analyzed.
- There is no potential environmental impact or potential exposures that result from the use of Hydrogeologic Data Fusion.
- Hydrogeologic Data Fusion has an indirect positive influence on community and regulatory reactions due to the better quality
 of the modeling effort.
- Community perception has been positive because Hydrogeologic Data Fusion results in integrated three-dimensional visual reconstructions that are accessible to non-technical and technical reviewers alike.

LESSONS LEARNED

Implementation Considerations •

- When considering the implementation of Hydrogeologic Data Fusion, the relative advantages relative to manual calibration should be considered. The comparison should be made in terms of data interpretation and model calibration needs. If few data are available, then Hydrogeologic Data Fusion can be used to help to determine what new data are needed and to optimize the data acquisition. If a large amount of data are available, then Hydrogeologic Data Fusion can provide better answers faster and with quantified uncertainty.
- Experience has shown that scientists and engineers who are currently using manual trial and error calibration methods can be
 become proficient with Hydrogeologic Data Fusion in a few weeks time. Hydrogeologic Data Fusion is so much faster than
 manual calibration when applied to large data sets that it does not take long to regain lost productivity due to training time
 through higher productivity.
- HydroFACT can be used to solve most MODFLOW steady flow problems.
- DFW/VAM3DF is a flexible and robust tool that either solves or can be customized to solve the remaining hydrogeologic Hydrogeologic Data Fusion problems.
- The speed and organization of Hydrogeologic Data Fusion relative to manual methods makes it practical for real-time monitoring and optimization of characterization and remediation activities.
- The quantification of uncertainty by Hydrogeologic Data Fusion makes engineering designs with quantified safety margins possible.
- The quantification of uncertainty can be used to guide data acquisition by determining what additional data are necessary to
 produce a sufficiently accurate result.

Technology Limitation/Need for Future Development

- Geostatistical parameters such as correlation distance and standard deviation are obtained from conventional methods. Better results would be obtained by determining geostatistical parameters as part of the fusion process itself. A statistical maximum likelihood method has been formalized. Work is ongoing to improve computational efficiency and to implement and test the method.
- Data types are limited and the relations of some of the data types to needs are unclear. However there is ongoing work in
 the environmental community to develop new data types and to establish data relations and data surrogates for what needs to
 be reconstructed. As these new data and relations are developed, Hydrogeologic Data Fusion can take immediate advantage
 of them.

Technology Selection Considerations

- If a site has substantial hydrogeologic data integration and model calibration needs, then Hydrogeologic Data Fusion can be helpful.
- Model productivity is improved relative to manual methods in terms of speed and accuracy.



APPENDIX A

REFERENCES

Van Eeckhout, Edward, 1997, Use of Hydrogeologic Data Fusion to Optimize Contaminant Transport Predictions, Los Alamos National Laboratory Report LA-UR-98-845.