ANNEX B OF APPENDIX D
IMPLEMENTING ARRANGEMENT #2 UNDER THE
DOE-RAS MEMORANDUM OF UNDERSTANDING

UNCERTAINTY ASSESSMENT THROUGH INCORPORATION OF MATHEMATICAL GEOLOGY IN DEVELOPMENT OF INVERSE FLOW AND TRANSPORT MODELS

Background

The high costs and risks associated with cleanup of sites, contaminated with radioactive wastes, requires that the uncertainty associated with siting new waste repositories and the cost associated with alternative remediation decisions must fully reflect the uncertainty associated with these decisions. Existing modeling efforts, that address uncertainty, either do not acknowledge the uncertainty in prescribed processes, physical features, initial and boundary conditions, system stresses, field data, and model parameter values (e.g., deterministic models), or they overestimate these uncertainties (e.g., standard stochastic models) by not fully incorporating the constraints imposed by the observational records associated with sites like Hanford, Mayak, Tomsk or Krasnoyarsk. The proposed research incorporates geostatistical methods from the evolving field of mathematical geology with inverse modeling methods that already incorporate historical observational records to better address uncertainty arising from spatial variability.

This joint effort of the Nuclear Safety Institute (IBRAE) of the Russian Academy of Sciences and the US. Department of Energy will initially focus on development of techniques to define:

- model structure associated with the area1 extent/continuity of the fine-grained confining or semi-confining units (e.g., the Hanford unconfined system's mud units), and
- the optimal parameter zones for coarse-grained aquifer units

for use in inverse modeling. This approach will allow use of the observational (hard) and interpretational (soft) data records in a parameterized way that can be incorporated into inverse methods. Subsequent efforts will investigate/develop approaches that combine inverse modeling and mathematical geology techniques to better estimate uncertainty and provide the means to optimize any additional sampling in a way that reduces uncertainties while minimizing cost.

The cooperative effort the first year will involve using the geologic and observational data base for the unconfined aquifer system at the Hanford site (-1330 wells logs) to develop and test methods for:

- structure identification (i.e., area1 extent and continuity of the mud units), and
- to identify plausible parameter zonation schemes for the coarse grained (i.e., aquifer units).

These methods can be further tested and evaluated as part of the ongoing activities at Hanford involving inverse flow and transport modeling of the Hanford Site unconfined aquifer system. Efforts the second year will involve:

- incorporation of the mathematical geological model parameters as part of the inverse modeling at Hanford, and

- feasibility study how the combined inverse and mathematical geology model can be used to: (1) optimize additional sampling to reduce uncertainty at minimal cost and (2) aid decision making by providing quantitative estimates of uncertainty related to spatial variability.

The scientists at IBRAE in the area of mathematical geology will be working with their counterparts at Hanford and the Hanford scientists performing the inverse modeling. This work will build upon and extend technical capabilities at both institutions in the important area of mathematical geology and inverse modeling aimed at full utilization of the observational records to better understand and quantify uncertainty when making cleanup decisions.

Objectives

1. Incorporation of geostatistical methods from the evolving field of mathematical geology, in particular stochastic simulations that allow use of direct and soft data, with inverse modeling methods that incorporate the historical observational record to provide a better approach for addressing the uncertainty arising from spatial variability. Standard geostatistical algorithms (e.g., indicator simulations) as well as artificial neural network algorithms will be used to parameterize spatial information related to model structure (e.g., area1 extent and continuity of hydrogeologic units) and to classify/zone the spatial variability in the hydrogeologic units of the aquifer system under study.
2. Feasibility study how to use this combined inverse modeling and mathematical geology approach to optimize any additional sampling in order to reduce uncertainty and minimize cost.

Scope of Work in terms of Milestones and Deliverables

This cooperative effort will use the geologic and observational data base for the unconfined aquifer system at the Hanford Site (based on -1330 wells logs) to develop and test the use of geostatistical methods in conjunction with inverse models. This effort will be integrated with the ongoing site-wide inverse groundwater modeling activity at the Hanford Site that is part of the Groundwater-Vadose Zone Integration Project. Milestones 1 and 2 would be completed the first year of the project and milestones 3 and 4 would be completed during the second year.

PNNL will provide IBRAE researchers with interpreted borehole log data from the Hanford Site, including the interpreted locations of mud units in each borehole, and the borehole location and elevation data. PNNL will provide available data on borehole measurements of hydraulic properties. PNNL will also work with IBRAE scientists to provide them with information on the use of the geostatistical models of the Hanford Site that will be produced, and any requirements/constraints imposed by the groundwater modeling framework that might influence the geostatistical modeling effort.

Milestone 1. This effort involves development of alternative geologic models of aquifer/aquitard structure for incorporation into inverse models through the use of geostatistical methods. This effort will develop and adapt geostatistical conditional stochastic simulation techniques for use in the characterization of uncertainty in hydrogeologic structure (e.g., the area1 extent and continuity of mud units). Results from this effort using the Hanford Site data set will be compared to ongoing

traditional geologic interpretation efforts at the Hanford Site. The geostatistical methods will also be tested using synthetic data sets and by checking the output against the interpretations developed in the ongoing inverse modeling, by Hanford staff, of the Hanford Site groundwater system.

Statistical models to be developed and applied include:

- Sequential-Gaussian simulations
- Sequential-indicator simulations
- Simulated annealing.

Deliverable: Project report that documents the approach for producing alternative models of geologic structure. It will include results of analysis of the synthetic test data cases as well as the results of the application of the methodology to the Hanford data set. Documentation will include text describing the data analysis approach and assumptions, variogram models and other interpretive data analysis. Deliverables will include one hundred 3-dimensional (3-d) simulation grids of the binary mud/aquifer distributions for the Hanford Site generated using sequential-indicator simulation, or other stochastic simulation techniques (e.g., sequential-Gaussian) which might be used based on the exploratory data analysis and variogram modeling.

Deliverable date: 9 months after project start date.

Milestone 2. This effort involves development of stochastic models of heterogeneous, porous aquifer media for use with inverse models. For Milestone 1, the geologic system will be treated as a simple binary system (aquifer/aquitard). In Milestone 2, this system will be extended to include modeling of the spatial variability of the aquifer units. Techniques for the simulation of heterogeneous media (e.g., through the use of geostatistics and conditional stochastic simulation methods) will be adapted/further-developed in order to represent the spatial variability of parameters within the coarse-grained or aquifer units (i.e., to develop parameter zones). Uncertainty in the parameter zones will be accounted for by adapting the approach to develop alternate parameter zonation schemes that can be used directly in inverse models. The approach will initially be tested using synthetic data sets. Then results from the application of this approach to the Hanford Site data set will be compared to ongoing interpretational efforts at the Hanford Site. Finally, the alternate-zonation models for the Hanford Site will be used; by Hanford staff, in their ongoing inverse modeling of the Hanford Site groundwater system.

Deliverables: Project report that documents the approach for producing alternate models of parameter zonation. It will include a discussion of the synthetic test cases as well as a discussion of the application of the methodology to the Hanford data set. Deliverables will include 100 3-d simulation grids of the aquifer units for the Hanford Site generated using sequential-indicator simulation, or other stochastic simulation techniques (e.g., sequential-Gaussian) which might be used based on the exploratory data analysis and variogram modeling. Additionally journal articles discussing the aquifer simulation approach developed in Milestone 2 as well as the model structure identification approach (Milestone 1) will be prepared.

Deliverable date: 12 months after project start.

Milestone 3. Feasibility study on the spatial information classification/zonation algorithms based on artificial neural network algorithms. This effort would examine the possibility of application of artificial neural network (ANN) algorithms for use in development of both (1) alternative geologic models (as discussed in Milestone 1) and in (2) the development of parameter zones (as discussed in Milestone 2) that would be used in inverse modeling of geohydrologic systems. Models to be developed and applied include:

- Multilayer perceptrons
- Probabilistic Neural Networks for classification and General Regression Neural Networks and their basic developments at IBRAE
- Self-organizing maps

The ANN approaches would be initially developed and tested using synthetic data sets (when appropriate) as discussed under Milestones 1 and 2. The promising ANN approaches would then be tested using the Hanford data set and the resulting aquifer structure/parameter zonation models compared to the results developed under Milestones 1 and 2. Finally, the most promising approaches for representing Hanford Site structure and zonation will be tested, by Hanford staff, in their ongoing inverse modeling of the Hanford Site groundwater system.

Deliverables: Report on feasibility study of the approach based on artificial neural network algorithms to produce alternate models of structure and parameter zonation. Additionally a journal article/presentation discussing the important aspects of this effort will be prepared.

Deliverable date: 18 months after project start.

Milestone 4. Feasibility study on the development and testing of approaches for incorporation of mathematical geology, esp. geostatistical and ANN model parameters, directly into the hydrologic inverse modeling. The goal of this milestone is to investigate methods for using the combined mathematical geology and inverse models to:

- optimize additional sampling to reduce uncertainty at minimal cost, and
- provide quantitative estimates of uncertainty related to spatial variability.

The initial development and testing would use synthetic data sets (when appropriate) and the promising approaches would then be tested using Hanford data and the inverse model of the Hanford Site groundwater system.

Deliverable: Report on feasibility study that documents the effort. It will include a discussion of the synthetic test cases and a discussion of the application of this methodology to the Hanford data set.

Deliverable date: 23 months after project start

Principal Investigators:
Dr. Christopher Murray, Pacific Northwest National Laboratory
Prof. Mikhail Kanevski, Nuclear Safety Institute of the Russian Academy of Sciences (IBRAE RAN)

Reports:
All reports shall be prepared and submitted by the 1 5th of each relevant month to:

Dr. Christopher Murray
Pacific Northwest National Laboratories
3 110 Port of Benton Blvd.
Richland, WA 99352
EMAIL: chris.murray@pnl.gov

A copy of each report should be submitted by fax to:

Mr. Skip Chamberlain, Program Manager
U.S. Department of Energy, Office of Science and Technology, EM-53
199 10 Germantown Rd.
Germantown, MD 20874, USA
FAX: 202-488-3 158

PROPOSED PERIOD OF PERFORMANCE AND PAYMENT SCHEDULE

This project will be conducted over 24 months. The beginning of the contract is October 1, 2000. The completion of the project is September 30, 2002. The total project cost is $ 200,000 USD. The payments will be made through standard DOE-EM procedures according to the following schedule:

Schedule	Payment	Deliverable
December 2000	$25,000	Progress Report
March 2001	$25,000	Progress Report
June 2001	$25,000	Report outlined in Milestone 1
September 2001	$25,000	Report outlined in Milestone 2
December 2001	$25,000	Progress Report
March 2002	$25,000	Report outlined in Milestone 3
June 2002	$25,000	Progress Report
September 2002	$25,000	Report outlined in Milestone 4

The payments will be made upon receipt of the specified deliverables. The final payment will be paid upon acceptance of the Final Report by DOE.

The responsibility of the parties for the violation of the terms of the Contract shall be determined by the Joint Coordinating Committee for Science and Technology.

LEGAL ADDRESS

Russian Academy of Sciences, Nuclear Safety Institute
52, B. Tulskaya
113191 Moscow, Russia

Tel: +(7-095) 952-242 1
Fax: +(7-095) 958-0040

BANKING INFORMATION: **XXXXXXXXXXXX**

Signed: 5/31/00

Mr. S Chamberlain, PE
Program Manager
U.S. Department of Energy

/L. Borshov/

Prof. Mikhail Kanevski
Principal Investigator
IBRAE

31.05.2000