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Geostatistical and Stochastic Study of Radio nuclide Transport in the Unsaturated Zone at Yucca Mountain

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**SCIENTIFIC INVESTIGATION PLAN
(SIP)**

Task Title: Geostatistical and Stochastic Study of Radionuclide Transport in the Unsaturated Zone at Yucca Mountain

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REVISION HISTORY

<u>Revision Number</u>	<u>Effective Date</u>	<u>Description and Reason for Change</u>
0	09/28/2004	Initial Issue.
1	05/22/2006	In section 1, Task 4: subhead labeled; and last paragraph added that changes task 4 status to non-quality-affecting with justification. Incorporated DCN 1 into the SIP.

1) Scope and Objectives

The U.S. Nuclear Waste Technical Review Board [Cohon et al. 1998] evaluated the technical and scientific validity of activities undertaken by the Secretary of Energy to characterize Yucca Mountain, Nevada, for its suitability as an underground repository in which to store high-level radioactive waste and spent nuclear fuel. In the report, the Board pinpointed that the study on groundwater flow and radionuclide transport in the saturated and unsaturated zones below Yucca Mountain should, over the next several years, focus on reducing prediction uncertainty. In its 2002, the Board repeated this concern by stating, "... hydrogeologic processes that affect radionuclide transport below the proposed repository in the unsaturated and saturated zones remain poorly understood." However, above the saturated zone, the unsaturated zone (UZ), the area in which the repository would be located, acts as a critical natural barrier by delaying the arrival of radionuclides at the saturated zone and by reducing radionuclide concentrations in groundwater through dispersion and dilution. Before any analysis of saturated zone behavior becomes relevant, quantitative prediction of radionuclide transport in the unsaturated zone becomes critical for performance assessment and design of the repository of the Yucca Mountain Project (YMP).

Scientists at the Lawrence Berkeley National Laboratory (Berkeley Lab) (e.g., Wu et al. 1999, 2001, 2002a, and 2003) have developed several large, site-scale UZ numerical models to characterize groundwater flow and radionuclide transport processes in the unsaturated zone of Yucca Mountain. In constructing these models, they have used a numerical modeling approach, combined with incorporation of field data. The basic conceptual model used in their studies is a layer-wise representation of the unsaturated tuff formation with vertical heterogeneity approximated in the form of three-dimensional (3-D) layers. Flow and transport through fractured media are simulated using a dual-permeability concept. In this concept, a fractured medium is represented by two completely overlapping continua, one representing fracture networks and the other representing porous matrix. The dual-continuum model assumes that both water flow and solute transport can be described by two conservation equations with mass exchange or interaction at fracture-matrix interfaces.

In most UZ flow and transport modeling studies, the TOUGH2 code (Pruess, 1991; Wu et al. 1996) has been applied to simulate groundwater flow from the surface to the water table under various surface recharge rates, representing different climates scenarios (Wu et al. 2002a). In addition, TOUGH2_MP, a massively parallel version of the TOUGH2 code (Wu et al. 200b), has also been developed and used for numerical simulations in the YMP. The proposed study will use both standard TOUGH2 and parallel TOUGH2_MP codes to conduct flow and transport simulations. Both TOUGH2 and TOUGH2_MP are quality approved for use in studies at the Yucca Mountain Repository.

During its development, the flow model is calibrated to match various observed field data, such as water potential, matrix liquid saturation, perched water, temperature, and

isotope and chemical concentration (Wu et al. 2001). Then, solute transport is simulated under steady-state 3-D flow fields, generated by the calibrated flow model. Transport

results are then analyzed in terms of the travel times of radionuclides from the repository to the water table. These calculations set up the basic prediction framework for the study area. However, there are still some important issues that remain to be addressed. In Wu et al.'s studies (2001 and 2002a), the hydraulic conductivity within each layer or rock is assumed to be constant. Historical field measurements, published in peer reviewed journals, show that hydraulic conductivity and other rock properties, even within each rock unit, vary significantly. However, few investigations have been conducted to look at the impact of inner-layer heterogeneity (Zhou et al. 2003). In this study, we propose to take advantage of stochastic methods to enhance the study of solute-transport-prediction uncertainty caused by the spatial variation of hydraulic properties in the unsaturated zone.

Dr. Hu and his colleagues have developed a numerical method of moment (NMM) in the last several years for solute transport in nonstationary, heterogeneous media with complicated initial and boundary conditions [Hu et al. 2003; Wu et al. 2003a and 2003b; Zhang et al. 2000]. Based on the study results, a numerical code, NMM3D1.1, has been developed and added to DOE's QA approved software. NMM3D1.1 and Monte Carlo simulation method were used to study radionuclide transport in the saturated zone of Yucca Mountain (Task 25), with random distributions of hydraulic conductivity in various zones. Those study results give the expected solute flux through a control plane 5,000 m downstream of the contaminant source location, and the upper and lower bounds of prediction errors.

Required Statements:

- This work is subject to NSHE QA Program requirements.
- A study cannot be independent if the conclusions (i.e., confirmation and support) are presumed *ab initio*, therefore the statement, "This SIP presents an independent confirmatory study supporting previously gathered information", is inaccurate and has been altered, per QAP-3.0, Revision 9, Section 4.1 b) 2) Scope and Objectives (page 5 of 20) to, "This SIP presents an independent study utilizing previously gathered information."

This task is a Geostatistical and Stochastic Study of Radionuclide Transport in the Unsaturated Zone at Yucca Mountain.

Objective 1. Estimate the spatially heterogeneous intrinsic permeability and sorption coefficient distributions in the study volume through geostatistical analysis and equiprobable simulation.

Objective 2. Extend the NMM3D method for modeling groundwater flow and solute transport to the UZ. The developed method will be applied to modeling unsaturated groundwater flow from the surface to the water table and solute transport from the repository horizon to the water table. The NMM3D method is mainly used to conduct

sensitivity studies and to investigate the effects of various statistical parameters on flow and transport processes. The study results will help to select the most important parameters for further study through Monte Carlo simulation.

Objective 3. Apply the TOUGH2 code, along with stochastically generated distributions of intrinsic permeability and sorption coefficients, to modeling groundwater flow and radionuclide transport in the two-scale heterogeneous unsaturated zone. The task will focus on evaluating the prediction uncertainty, and specially transport predictions, done by Berkeley Lab.

The following tasks have been formulated to achieve these objectives:

Task 1. Data Collection

To characterize subsurface heterogeneity and to understand its effects on flow and transport processes, substantial amount of field measurement data have been collected from the site. These data include measurements of state variables (e.g., water saturation and water potential) and core-scale rock properties (e.g., porosity, permeability, capillary parameters for rock matrix and sorption coefficient of the rock matrix). Additionally, pneumatic pressure, fracture mapping, and air-permeability data are also available for estimating fracture properties. Qualified data available from the site will be acquired from the TDMS and analyzed to incorporate into the proposed geostatistical model for studying medium heterogeneity and flow model calibration. Unqualified data will not be used in the analysis, but may be used to develop an informational context.

Task 2. Geostatistical Study of Heterogeneity

The purpose of this task is to provide the distributions of intrinsic permeability and sorption coefficients at the study site. The acquired data from Task 1 will be incorporated into the geostatistical study of the distributions of these parameters.

The method used to generate multiple, equiprobable, three-dimensional maps of unsaturated permeability/chemical sorption coefficient consists of three steps: (1) obtain 3-D maps of hydrostratigraphic units, (2) generate an unsaturated permeability/chemical sorption coefficient fields, respectively, for each hydrostratigraphic unit, and (3) build a composite map by superposing the unsaturated permeability/chemical sorption coefficient fields from each unit. Heterogeneity arising from lithologic variability is thereby reproduced in the composite maps. This method has been developed and applied in the study of conservative transport at the Nevada Test Site (NTS) [Shirley et al. 1997] and Yucca Mountain Project (Task 25). The random permeability/sorption fields generated by this approach can then be incorporated with stochastic theory to study chemical transport processes.

Task 3. Monte Carlo Simulation of Groundwater Flow and Solute Transport

Previous UZ flow modeling results from Berkeley Lab will be interpreted to determine the hydraulic boundary conditions of the study site. Since this project focuses on the effects of medium heterogeneity on flow and transport, only one set of boundary

conditions will be adopted here, sensitivity studies on boundary variation will not be conducted in this project. Based on the statistical distribution of unsaturated hydraulic conductivity, the TOUGH2 and/or TOUGH2_MP simulators will be applied to generate the hydraulic head and velocity distribution from the surface to water table in the study area. The generated 3-D flow and chemical sorption coefficient random fields will be used as input data for solute transport calculation. TOUGH2/TOUGH2_MP will be adopted to calculate the transports of various radionuclides from the repository horizon to the water table. From the multiple realizations of the simulations, the means and variances of the transport results will be statistically estimated. The means will be used for predictions, and the resulting variances will be used to analyze prediction uncertainty.

The TOUGH2 simulation and Monte Carlo method have both been well developed and the results from the Monte Carlo simulation have proven to be reliable. However, a large number of simulations are required for stable results, especially for the variance calculations with several independent random parameters. Therefore, we propose to use the numerical method of moment to conduct the sensitivity study to select the most important parameters, and then use Monte Carlo simulation methods with TOUGH2 runs to investigate the effects of these parameters on flow and transport.

Task 4. Develop and apply a numerical method of moments for a sensitivity study of how various random parameters affect flow and transport (non-quality-affecting task)

Over the past few years, Dr. Hu and his colleagues have applied a stochastic perturbation method to develop a NMM for solute transport in nonstationary media with complicated boundary and initial conditions [Hu et al., 2003; Wu et al., 2003a,b; Zhang et al., 2000]. They have applied this method to study radionuclide transport in the saturated zone of Yucca Mountain (Task 25 of Cooperative Agreement DE-FC28-90NV12081) with random distributions of hydraulic conductivity in various zones. The study results give the expected solute flux through a control plane 5,000 m downstream of the contaminant source location and the upper and lower bounds of prediction error. The modeling results are consistent with those from Monte Carlo simulation. In this project, we will extend the method to flow and solute transport in the unsaturated zone. The developed method is then used to study the effects of property heterogeneity within each rock type in the unsaturated zone on groundwater flow and solute transport. Owing to its calculation efficiency, the method of moment will be used to conduct a sensitivity study and isolate the most important random parameters in certain geologic layers (significantly controlling flow and radionuclide transport) for further study by Monte Carlo simulation. Due to the flexibility of Monte Carlo simulation to various boundary conditions, Monte Carlo simulation will be used to conduct the most complicated study and give the final prediction. The prediction results will be the mean (or expectation) radionuclide transport processes (the arrival times from the repository to the water table), and standard deviations from the mean predictions for various radionuclides.

Due to budget reduction, this task is changed to be non-quality-affecting. The stochastic perturbation method, NMM, will still be extended to flow and solute transport in the

unsaturated zone, but the method will be used to generate data for information only. The information will be used to facilitate Monte Carlo simulation proposed in Task 3 under QA program for final report.

Task 5. Quarterly Reports and Technical Report

We will submit quarterly reports on the progress of the project. The technical report will be submitted to complete the project.

2) Approach

The complex heterogeneity of the natural media and the uncertainty in data for the unsaturated zone below the Yucca Mountain project (YMP) area preclude using traditional deterministic approaches to model solute transport. To overcome the scale dependence of hydraulic parameters, current deterministic numerical methods adopt the concept of macro-parameters (or effective values of parameters), which comes from stochastic theory, to deal with small scale variations of parameters. This adoption, coupled with the flexibility of numerical methods to complex initial and boundary conditions, makes the current numerical modeling approach popular in modeling groundwater flow and chemical transport processes. Small-scale variation of parameters, such as hydraulic conductivity, has significant influence on macro-scale flow and transport processes. Sandia National Laboratory (SNL) has conducted geostatistical studies to investigate parameter variation within a single gridblock (500×500×50 meters). Dispersivity at the grid scale has been obtained. However, geostatistical simulations of the hydraulic conductivity and sorption coefficients at the scale of the site-scale model (30×45×0.9 km) have not been conducted. These geostatistical simulations are the basis for study of dispersion process and for the uncertainty analysis of radionuclide transport prediction in the site-scale.

Large differences exist between the scale of field measurements and the scale of numerical gridblocks and the scale of macrodispersivity being modeled for the YMP. Currently, a very important issue that needs to be resolved is how to scale-up the parameter values to effective macro-scale parameter values, especially the evaluation of macro-dispersivity from micro-scale variation of hydraulic conductivity.

The numerical method, coupled with effective parameter values, is effective to predict mean or expectation values of flow and chemical plume distributions. However, it is difficult to apply this numerical method to analyze the uncertainty of prediction, which is associated with the uncertainty of input data of parameters. However, because quantification of prediction uncertainty is as important as the mean value prediction in engineering design, the prediction uncertainty, or possible variation about the expected concentration or solute flux, must be evaluated.

In the present study, we propose to use similar two methods to investigate the effects of inner-layer property heterogeneity within each UZ rock unit on groundwater flow and solute transport processes: (1) For the numerical method of moment, we will extend the

method for the saturated zone to the unsaturated zone; (2) For the Monte Carlo method, the multiple realizations of hydrological parameter distributions generated through Monte Carlo simulation will be used as input data for the TOUGH2 code. Because of its computational efficiency, the method of moment will be used to conduct a sensitivity study and select the most important random parameters for further study by Monte Carlo

simulation. Because of the flexibility of Monte Carlo simulation to various boundary conditions, Monte Carlo simulation will be used to conduct the most complicated study and obtain the final prediction. We may use the TOUGH2 code on multiple workstations and TOUGH2_MP on the DOE's NERSC super computer (located at Berkeley Lab) to resolve the issue regarding intensive computational requirements that may occur with Monte Carlo simulations when using the 3-D site-scale UZ model with 250,000 gridblocks. Together, the two approaches will provide a framework for assessing the uncertainty arising from a variety of mechanisms affecting performance assessment and design of monitoring observation systems. The study results will support DOE's effort for repository license application and is consistent with the U.S. Nuclear Waste Technical Review Board's 2002 recommendation that DOE, "... increase confidence in its performance estimates by, among other things, developing multiple lines of evidence ..." [Cohon, et. al 2002].

Berkeley Lab has developed several 3-D UZ flow and transport models to conduct site-scale modeling investigations of groundwater flow and radionuclide transport in the UZ below the YMP area (e.g. Wu et al. 2003). These site-scale groundwater flow models provide the hydrogeological framework (conceptual model, numerical grids, and boundary and initial conditions to model input parameters) for determining the direction and rate of radionuclide movement from the repository to the water table. The flow calculation has been calibrated against the various field measurements collected from the Yucca Mountain site. A sensitivity study has been conducted to investigate the effect of infiltration rates on flow and transport. Large-scale heterogeneity and geological layering have also been carefully studied. In addition to UZ flow issues, the migration of radionuclides from the UZ repository to the accessible environment depends on transport processes and parameters distinct from the flow model itself. Consequently, a model for radionuclide transport must include the mechanisms of advection, dispersion, matrix diffusion, and sorption. These studies have provided the basic predictive context for future studies of groundwater flow and radionuclide transport in the UZ. However, in these studies, the influence of small-scale heterogeneity and the variation of hydraulic conductivity within each layer on flow and transport were not fully addressed in a 3-D site scale model. In this proposal, we will focus on small-scale, inner-layer heterogeneity and quantify its influence on flow and transport, especially on the associated prediction uncertainty.

The fractured tuffs in the UZ of the YMP area exhibit multiscale heterogeneity in their hydrogeologic properties, with varying statistical characteristics and thus different influences on flow and transport, depending on the process scale. The Yucca Mountain UZ consists of alternating sequences of variably fractured and faulted welded and

nonwelded tuffs, characterized by two scales of heterogeneity: (1) layer-scale heterogeneity and (2) local-scale, inner-layer variation within each layer [e.g., Zhou et al. 2003]. Over the last two decades, extensive scientific investigations have been conducted for the site characterization of Yucca Mountain, including surface mapping, drilling of a large number of deep and shallow boreholes and underground tunnels, measurements and field tests, estimation of hydrogeologic properties, and flow and transport tests. To

characterize the subsurface heterogeneity, the US Geological Survey (USGS) investigators have measured a substantial amount of field data at the site [e.g., Rousseau, 1996; Flint, 1998a and 1998b; Rousseau et al. 1997a and 1997b]. These field data were used for analyses of effective hydrogeologic properties [Bandurraga and Bodvarsson, 1999; Liu et al. 2003a and 2003b] for the 3-D UZ flow model. In those analyses, however, only the average layer-scale (layer-averaged) rock properties were estimated and used for the UZ flow model, and local-scale heterogeneity and lateral variability of layer-scale properties were in general neglected.

The existence of local-scale heterogeneity can be seen from the variations of measured state variables and properties within each layer [Flint, 1998b]. By assuming different correlation lengths (1 and 3 m), Bodvarsson et al. [2003] found that local-scale heterogeneity of fracture permeability (only in a TSw geologic unit) has large influence on flow and transport. Zhou et al. [2003] applied a two-dimensional model to study the influence of local-scale heterogeneity on flow and transport. Their study results indicate that local-scale heterogeneity of matrix and fracture properties has a considerable effect on unsaturated flow processes, leading to fast flow paths in fractures and the matrix. These paths shorten the travel times of a conservative tracer from the source (repository) horizon in the UZ to the water table, for small fractions of total released tracer mass. As a result, local-scale heterogeneity also has a noticeable effect on global tracer transport processes, characterized by an average breakthrough curve at the water table, especially at the early arrival times of tracer mass. In this project, we will extend Zhou et al's [2003] study from two-dimensional to three-dimensional modeling. The local heterogeneity in the entire repository domain of the YMP area will be fully studied, and its influences on flow and transport will be thoroughly investigated. In addition, the uncertainty in prediction will be quantified.

In the event that a quality-affecting task is evaluated as non-quality affecting, justification for the evaluation will be provided to the DOE Technical Task Representative and the QA Manager.

A technical report containing the evaluation of transport process will be delivered to the Department of Energy (DOE). In the report, we will give our calculation results for the mean and variance of solute flux through control planes. The results will evaluate prediction uncertainty. The generated random distribution of the hydraulic conductivity and sorption coefficient, as well as the extended NMM3D code, will also be submitted to DOE. Based on the research results, we may submit several papers to academic journals

for publication. The published materials will be reviewed and approved by DOE. Copies of the published articles will also be delivered to DOE.

3) Schedule

Task Name	Completion Date
Write SIP	18-Aug-04
Initial QA Training	21-Jul-04
Ongoing QA Training and Compliance	31-May-07
Data Collection	31-May-06
Geostatistical Analysis of Hydraulic Conductivity and Sorption Coefficients	29-Dec-06
Monte Carlo Simulation of Groundwater Flow and Solute Transport	29-Dec-06
Develop and Apply Numerical Method of Moment in Sensitivity Study of Flow and Transport Affecting Random Parameters	29-Dec-06
Computations Complete	29-Dec-06
Technical Report Preparation	31-May-07

4) Interface Controls

Other than source data, there are no technical inputs that originate outside of the task. The personnel involved in this task are listed below:

Internal Interfaces

Ming Ye, Ph.D.

Graduate Student (To be selected)

External Interfaces

If subcontracts are approved, the following external interfaces will be used.

Subcontract (Consultant): Yu-Shu Wu, Ph.D., Earth Sciences Division, Lawrence Berkeley National Lab

Subcontract (Consultant): Xiaolong (Bill) Hu, Ph.D., Florida State University

Yucca Mountain Cooperative Agreement Technical Contact: Raymond Keeler

DOE Technical Task Representative: Eric Smistad

Information will be transferred to and from Drs. Hu and Wu by two methods, either through electronic transfer (i.e., ftp transfer of zipped files) or direct physical transfer of media, such as CDROM. Transfers by either method will be recorded in the scientific notebook. Because of DRI firewall procedures, zip files will be renamed to a different file extension.

5) Standards

There are no applicable published industry standards or criteria.

6) Implementing Procedures

It is not anticipated that any implementing procedures will need to be written for this task, as no measurements or observations are going to be made, only existing qualified data will be used.

7) Samples

No samples or test materials are to be used, collected or created, thus no procedures are being developed to handle samples.

8) Equipment and Instrumentation

No field or laboratory test equipment or instrumentation will be used in the study, thus no procedures are being developed to control access or maintain calibration.

9) Software and Models

QAP-3.2, "Software Management" will be implemented for the software to be used in this study. Qualified software will be obtained through the NSHE QA staff when needed. One numerical code for chemical transport prediction will be developed in this task. The software development and implementation will be conducted in accordance with QAP-3.2, "Software Management." A module to provide runtime documentation may be developed and qualified to assist in meeting QA requirements. The commercial software packages that may be used in this study include:

- Microsoft Word: preparing documents and reports
- Microsoft Power Point: preparing presentations
- Microsoft Excel: tabulation, figure drafting and analysis of data*
- Tecplot, version 10.0: Graphic display of quantitative data
- Intel Visual Fortran, version 8.0: compilation of FORTRAN source code
- Surfer, version 8.0: Graphic display of model surfaces
- GSLIB, 2nd Edition: Geostatistical library written in Fortran 77
- MathCad, version 8.0: analysis of data*
- TOUGH2, version 1.6 and TOUGH2-MP, Version 1.0 from the YMP qualified software database

*any developed macro will require qualification as a routine in accordance with QAP-3.2

It is expected that bounding surfaces will be obtained from the Conceptual and Numerical Models for UZ Flow and Transport (MDL-NBS-HS-000005 Rev00) or more detailed model promulgated from this effort. Use of these models will be done in accordance with QAP-3.3

10) Procurements and Subcontracts

A subcontract may possibly be executed with Dr. Xiaolong (Bill) Hu to provide for continuity through the life of the project. Dr. Hu (possible subcontractor) has recently

accepted a position at the Florida State University. The subcontract would be to provide for his continuing involvement in the project, so it will entail coverage for 6 months of his time and 4 trips from Tallahassee, FL to Las Vegas, NV for consultation. No quality affecting work will be performed under this subcontract; it is to provide consultation and theoretical development.

A subcontract may be executed with Dr. Yu-Shu Wu of the Earth Sciences Division, Lawrence Berkeley National Lab. The subcontract will be to provide for Monte Carlo simulation using the qualified unsaturated zone model and TOUGH-2 or TOUGH-MP. This will entail coverage for 3.6 months of Dr. Wu's time, computer support costs and 2 trips from Berkley, CA to Las Vegas, NV for consultation. Quality affecting work will be performed under this subcontract; the LBL Yucca Mountain QA procedures will be followed.

11) Hold Points

QA acceptance of the Unsaturated extension of the currently QA accepted NNM3D code.

12) Quality Control

The NNM3D code, as a part of the QA acceptance process, will address computational accuracy, precision and error. The study will explicitly investigate the nature of parameter uncertainty in flow and transport in the unsaturated zone and this will be discussed at length in the technical report.

Access to electronic data will be controlled by limiting access to that data. A directory on the DRI computer network will be established and access limited to personnel working on this project. This network is backed up on a regular basis; the backups are stored in secure off-site storage. Access lists will be recorded in the scientific notebook.

13) Data Recording, Reduction and Reporting

The output of such programs as GSLIB routines, NNM3D, and TOUGH-2 will be written to hard disks on the DRI networks. All reduced data will be obtained from either the NSHE Technical Data Archive (TDA) or the BSC-maintained Technical Data Management System (TDMS). Data that are used, reduced, or produced in this work will be submitted to the Technical Data Archive (TDA) and/or the BSC-maintained Technical Data Management System (TDMS) in accordance with QAP-3.6, "Submittal of Data to the Technical Data Management System." QA records produced as a result of the NSHE

QAP's will be controlled in accordance with QAP-17.0, "Quality Assurance Records". Quarterly report deliverables will be submitted to the cooperative agreement administrator in accordance with the Cooperative Agreement. QA records may include reports, other documents produced, hard copies of data used if available, and copies of literature cited. Any data obtained from the TDA or TDMS will be stored in a access restricted directory with scheduled backups and off-site storage, and entries made into the scientific notebook at the time of acquisition.

It is not anticipated that any non-qualified data will be used in this study, however if it does become necessary to use unqualified data, QAP-3.7, "Qualification of Unqualified Data", will be followed.

14) Reviews and Verifications

Technical reviews and QA reviews will be conducted; the SIP technical and QA reviews are expected to be initiated by August 30, 2004; The scientific notebook technical and QA reviews are planned to start by March 1, 2006 and the Technical report technical and QA reviews are planned to start April 20, 2006.

15) Records and Submittals

The scientific notebook, the generated data (in the form of read only media such as DVD's or CDROM's) and the technical report will be the QA records produced and transmitted by this study. QAP-17.0, "Quality Assurance Records", will be used for the protection and transmittal of QA records. Data will be transmitted as QA records. Documents produced and submitted to DOE will be produced in accordance with QAP-3.4, "Technical Reports".

16) References

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