11-8-2004

# Groundwater Flow and Thermal Modeling to Support a Preferred Conceptual Model for the Large Hydraulic Gradient North of Yucca Mountain

Phil Oberlander

Greg Pohll
*Desert Research Institute*, greg.pohll@dri.edu

Drew Coleman

Raymond E. Keeler
*Cooperative Agreement Project Director*

Amy J. Smiecinski
*University of Nevada, Las Vegas*, smiecins@unlv.nevada.edu

*University and Community College System of Nevada*

# DOCUMENT CHANGE NOTICE (DCN)

**DCN No.** 1 **to Document No.** SIP-DRI-039, **Revision** 0, **Effective Date:** 15 FEB 05.

**Document Title:** Groundwater Flow and thermal Transport Modeling to Support a Preferred Conceptual Model for the Large Hydraulic Gradient North of Yucca Mountain

**Identify applicable affected page, section, paragraph, attachment, exhibit, table, figure, or other:**

**Replace the following:** Introduction, Scope and Objectives, Approach, Data Collection, Model Formulation, Alternative Conceptualizations, Hydraulic Flow Calibrations, Thermal Transport Modeling, Comparison of Results, and Schedule. The changes provided below accomplish a reduction in scope in response to a budget reduction.

**With:** See attached pages.

**Approved by:**

PI: [redacted] Date: 9 MAR 05
(Signature)

Print name: [redacted]

QA Manager: [redacted] Date: 3-28-05
(Signature)

Print name: [redacted]

QA Manager evaluated acceptability, that it does not violate quality requirements, and for impacts to other procedures; signature above documents this evaluation as successfully completed.

Send electronic version of this DCN to Webmaster.
Attach this DCN as first page of hard copies of document, if any.

**DCN No.** 1 **to Document No.** SIP-DRI-039**, Revision** 0**, Effective Date:** 15FEB05.

**Document Title:** Groundwater Flow and thermal Transport Modeling to Support a Preferred Conceptual Model for the Large Hydraulic Gradient North of Yucca Mountain

## INTRODUCTION

Phil Oberlander is the principal investigator (PI) for the task Groundwater Flow and Thermal Modeling to Support a Preferred Conceptual Model for the Large Hydraulic Gradient North of Yucca Mountain, ORD-FY04-018, under the DOE Cooperative Agreement DE-FC28-04RW12232,. The PI and project staff will evaluate a postulated conceptual hydrogeologic configuration of the large hydraulic gradient (LHG) north of Yucca Mountain. There are multiple conceptual models of the hydrogeology that may cause hydraulic heads similar to the (LHG). There are sufficient uncertainties in the hydrologic interpretation and range in hydraulic properties, such that a certain interpretation of the LHG is not indicated based solely on water level evidence. By combining groundwater temperature information with the water level information, a more rigorous numerical interpretation is formulated of the LHG.

## SCOPE AND OBJECTIVES

The title of this task is Groundwater Flow and Thermal Modeling to Support a Preferred Conceptual Model for the Large Hydraulic Gradient North of Yucca Mountain.

This task will create a two-dimensional, saturated zone, vertical cross-section model of groundwater flow and thermal transport through the LGH. This model is referenced herein as the thermal model. The scope of this study is limited to presenting a postulated hydrogeologic configuration of the LHG. The conceptualization will include the use of postulated hydrogeologic structures and material properties. The thermal model will be spatially limited to the area immediately upgradient and downgradient of the LHG and will not reproduce the many hydrogeologic features of the existing regional and site-scale models. The thermal model will be orientated north to south, approximately along a saturated zone streamline.

The results of the thermal modeling will be compared to temperature data reported for site wells by the U.S. Geological Survey (USGS) and in peer-reviewed journals. Most, if not all, of this reported data is non- qualified. This task will not qualify the reported data and the reported data will be used only as a basis of comparison for the model simulations.

This work is subject to University and Community College System of Nevada (UCCSN) Quality Assurance (QA) Program requirements. This Scientific Investigation Plan presents an independent confirmatory study supporting previously gathered information.

## APPROACH

Modeling the coupled groundwater processes of flow and thermal transport should provide greater insight into the flow dynamics and hydrologic properties of the LHG. Groundwater flow is a major component in distributing the thermal energy migrating upwards from depth and downwards from precipitation. The groundwater temperature distribution therefore reflects groundwater flowpaths, flow rates, and the thermal and hydraulic properties of the surrounding rock. The basis of comparison for the model-predicted groundwater temperature will be non-qualified data reported by USGS and peer reviewed journals.

**DCN No.** 1 **to Document No.** SIP-DRI-039, **Revision** 0, **Effective Date:** 15FEB05.

**Document Title:** Groundwater Flow and thermal Transport Modeling to Support a Preferred Conceptual Model for the Large Hydraulic Gradient North of Yucca Mountain

This task will use a two-dimensional, reduced form, of the saturated zone base case model reported on 9 April 2003 and documented as LA0304TM831231.002. That model was produced with the FEHM groundwater code and is in the project baseline as FEHM V2.20, STN/CSCI 10086-2.20-00.

Persons conducting this project will have 3 to 5 years experience in groundwater modeling.

The sequence of work is described below.

### *Data Collection*

The current interpretations of stratigraphy, hydrologic properties, thermal properties, and the most recent site-scale and regional-scale modeling will be evaluated for formulating the thermal models. The hydrogeologic property data will be obtained from the Yucca Mountain Project, Technical Data Management System (TDMS). Comparison and collaborative data will be obtained from journal articles and U.S. Geological Survey reports. Data will be managed according to QAP-3.1 Control of Electronic Data.

### *Model Formulation*

Hydrologic parameters will be derived from the site-scale and regional-scale models. Spatial discretization may be finer than regional-scale models for computational purposes. Hydraulic and thermal properties will be generalized within hydrostratigraphic layers. The model will use a single porosity and permeability within each model element. The model will not include any postulated repository affects and only ambient groundwater temperatures will be considered. The thermal model of the LHG will approximate to the current saturated zone regional interpretation.

The thermal model will be steady state for both groundwater flow and thermal transport. The top of the model will be a prescribed hydraulic flux and temperature at the water table. The model will extend to the depth of the Paleozoic carbonate aquifer or deepest thermal log. The bottom of the model will be simulated as a prescribed hydraulic head and a spatially variable thermal flux. The upgradient and downgradient boundaries will be prescribed hydraulic fluxes or hydraulic heads based on the requirements for numerical stability. Both the hydraulic heads and groundwater temperatures will vary with depth. Hydraulic head at the water table surface and any hydraulic heads at depth will be the calibration parameters. The spatial thermal distribution between the upgradient and downgradient boundaries will be the evaluation parameters.

Thermal rock properties will be extracted from the project database. Because there is less thermal data at distance from the potential repository location, generalized information will be used in the thermal model. The methodology of Rautman (1995) may be used to assign thermal conductivity unless data that are more explicit are available.

The groundwater modeling code FEHM will be used for the simulations. This software was baselined 28 Jan 2003, as FEHM V2.20, STN/CSCI 10086-2.20-00.

Software will be managed according to QAP-3.2 Software Management.

### *Alternative Conceptualizations*

This section omitted.

### *Hydraulic Flow Calibrations*

A groundwater flow model of each conceptualization will be calibrated to hydraulic heads. The PEST code may be used for the calibration as needed. The PEST code is within the project's software baseline as PEST V 5.5, (STN)/CSCI Number 10289-5.5-00. The hydraulic parameters will be allowed to vary over a wide range to represent alternative conditions. Modeling will be performed according to QAP-3.3 Models.

### *Thermal Transport Modeling*

Adding thermal properties and heat transport to the calibrated groundwater flow models will simulate the spatial distribution of temperature. Temperature at water table and upgradient boundaries will be prescribed based on observed conditions. The resulting spatial distribution of simulated temperatures within the body of the model will be the basis of comparison. Statistical measure of the fit of the simulated temperatures to the observed temperature data will also be provided. Microsoft Excel spreadsheet functions will be used for the statistical analysis. Modeling will be performed according to QAP-3.3 Models.

### *Comparison of Results*

This section omitted.

## SCHEDULE

| Deliverables for Task ORD-FY04-018 | Completion Date |
|---|---|
| Quarterly Reports | Ongoing |
| Complete model analysis | 1-July-05 |
| Submit the final data to the TDA | 30-Oct-05 |
| Submit the final report | 30-Nov-05 |

## SOFTWARE AND MODELS

Programs such as Excel, PowerPoint, and Word are used to create reports, presentations and documents. Model simulations will be performed according to QAP-3.3. The groundwater modeling code FEHM will be used for the simulations. This software was baselined 28 Jan 2003, as FEHM V2.20, STN/CSCI 10086-2.20-00. Parameter estimation may use the PEST code to estimate hydraulic conductivity. The PEST code is within the project's software baseline as PEST V 5.5, (STN)/CSCI Number 10289-5.5-00. The model



will be managed according to QAP-3.3. The model simulations performed will be numeric representation of a hydrogeologic conceptualization and cannot be quantitatively validated.

## QUALITY CONTROL

Error associated with data reduction performed by task personnel will be minimized by verifying the accuracy of the reduced data to the raw data and that the reduction processes are accurate. Data verification will be performed by someone other than the originator. These reviews will be documented in the scientific notebooks for this task and in conjunction with the technical report review. There is no objective or evaluation for precision. The model developed by this task is a conceptual representation (i.e., assumed hydrogeologic conditions and hydraulic properties necessary to illustrate general characteristics) and quantification of potential error in representation of the natural system is not possible.

Electronic data will be controlled by limited access to the computers that will contain those data. Each computer will be password protected. Data will be backed up on a regular basis. Access lists will be established for authorized users and these lists and the types of access will be listed in the applicable scientific notebooks.

## DATA RECORDING, REDUCTION, AND REPORTING

Data will be developed or used and controlled electronically in accordance with QAP-3.1, "Control of Electronic Data," to prevent tampering. Data will be recorded in electronic form, backed up to prevent loss, and verified when converted, transferred or input manually.

Data considered established fact by the scientific community need not undergo qualification. It is expected that most if not all of the groundwater temperature data near the LHG are unqualified. This task will produce a qualified conceptual model simulation that will be compared to unqualified reported data for corroboration purposes only. Unqualified data will be clearly labeled "unqualified" and traceability to their origin will be maintained.

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 UCCSN QAP's are controlled in accordance with QAP-17.0, "Quality Assurance Records". Quarterly report deliverables are 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.

University and Community College System of Nevada (UCCSN)

# Scientific Investigation Plan (SIP)

| | |
|---|---|
| **Task Title:** | Groundwater Flow and Thermal Modeling to Support a Preferred Conceptual Model for the Large Hydraulic Gradient North of Yucca Mountain |
| **Task Number:** | ORD-FY04-018 |
| **Document Number:** | SIP-DRI-039 |
| **Revision:** | 0 |
| **Effective Date:** | November 8, 2004 |

**Author:**

[redacted]
Phil Oberlander — Date: 10/25/04

**Approvals:**

[redacted]
Technical Reviewer
Greg Pohll — Date: 10/25/04

[redacted]
Technical Task Representative
Drew Coleman — Date: 11/04/04

[redacted]
Project Director
Raymond Keeler — Date: 01 Nov 2004

[redacted]
QA Manager
Amy Smiecinski — Date: 8-Nov-2004

**REVISION HISTORY**

| Revision Number | Effective Date | Description and Reason for Change |
|---|---|---|
| Rev. 0 | 11/08/2004 | Initial Issue |

## INTRODUCTION

Phil Oberlander is the principal investigator (PI) for the task Groundwater Flow and Thermal Modeling to Support a Preferred Conceptual Model for the Large Hydraulic Gradient North of Yucca Mountain, ORD-FY04-018, under the DOE Cooperative Agreement DE-FC28-04RW12232,. The PI and project staff will evaluate postulated conceptual hydrogeologic configurations of the large hydraulic gradient (LHG) north of Yucca Mountain. There are multiple conceptual models of the hydrogeology that may cause hydraulic heads similar to the (LHG). There are sufficient uncertainties in the hydrologic interpretation and range in hydraulic properties, such that a certain interpretation of the LHG is not indicated based solely on water level evidence. By combining groundwater temperature information with the water level information, a more rigorous numerical interpretation is formulated that should indicate the more likely conceptualization(s) of the LHG.

## SCOPE AND OBJECTIVES

The title of this task is Groundwater Flow and Thermal Modeling to Support a Preferred Conceptual Model for the Large Hydraulic Gradient North of Yucca Mountain.

This task will create a two-dimensional, saturated zone, vertical cross-section model of groundwater flow and thermal transport through the LGH. This model is referenced herein as the thermal model. The scope of this study is limited to presenting postulated hydrogeologic configurations of the LHG. These conceptualizations will include the use of postulated hydrogeologic structures and material properties. The thermal model will be spatially limited to the area immediately upgradient and downgradient of the LHG and will not reproduce the many hydrogeologic features of the existing regional and site-scale models. The thermal model will be orientated north to south approximately along a saturated zone streamline.

The results of the thermal modeling will be compared to temperature data reported for site wells by the U.S. Geological Survey (USGS) and in peer-reviewed journals. Most, if not all, of this reported data is non- qualified. This task will not qualify the reported data and the reported data will be used only as a basis of comparison for the model simulations.

Model results will support selection of LHG conceptualization(s) that is in best agreement with the observed conditions. A discussion of the relative merits and inconsistencies of the other conceptualizations will provide supporting documentation for the selection. This modeling may also provide information for a refined representation of the LHG for other YMP modeling activities.

This work is subject to University and Community College System of Nevada (UCCSN) Quality Assurance (QA) Program requirements. This Scientific Investigation Plan presents an independent confirmatory study supporting previously gathered information.

## APPROACH

Modeling the coupled groundwater processes of flow and thermal transport should provide greater insight into the flow dynamics and hydrologic properties of the LHG. Groundwater flow is a major component in distributing the thermal energy migrating upwards from depth and downwards from precipitation. The groundwater temperature distribution therefore reflects groundwater flowpaths, flow rates, and the thermal and hydraulic properties of the surrounding rock. By simulating alternative horizontal and vertical conceptualizations of the LHG, the conceptualization(s) that best matches the observed water level and water temperature information can be identified. This will support the saturated zone modeling by indicating the most likely configuration of the LHG structure. The basis of comparison for the model-predicted groundwater temperature will be non-qualified data reported by USGS and peer reviewed journals.

This task will use a two-dimensional, reduced form, of the saturated zone base case model reported on 9 April 2003 and documented as LA0304TM831231.002. That model was produced with the FEHM groundwater code and is in the project baseline as FEHM V2.20, STN/CSCI 10086-2.20-00.

Persons conducting this project will have 3 to 5 years experience in groundwater modeling.

The sequence of work is described below.

### *Data Collection*

The current interpretations of stratigraphy, hydrologic properties, thermal properties, and the most recent site-scale and regional-scale modeling will be evaluated for formulating the thermal models. The hydrogeologic property data will be obtained from the Yucca Mountain Project, Technical Data Management System (TDMS). Comparison and collaborative data will be obtained from journal articles and U.S. Geological Survey reports. Data will be managed according to QAP-3.1 Control of Electronic Data.

### *Model Formulation*

Hydrologic parameters will be derived from the site-scale and regional-scale models. Spatial discretization may be finer than regional-scale models for computational purposes. Hydraulic and thermal properties will be generalized within hydrostratigraphic layers. The model will use a single porosity and permeability within each model element. The model will not include any postulated repository affects and only ambient groundwater temperatures will be considered. The base-case model of the LHG will be approximate to the current saturated zone regional interpretation.

The thermal model will be steady state for both groundwater flow and thermal transport. The top of the model will be a prescribed hydraulic flux and temperature at the water table. The model will extend to the depth of the Paleozoic carbonate aquifer or deepest thermal log. The bottom of the model will be simulated as a prescribed hydraulic head and a spatially variable thermal flux. The upgradient and downgradient boundaries will be prescribed hydraulic fluxes or hydraulic heads based on the requirements for numerical stability. Both the hydraulic heads and groundwater temperatures will vary with depth. Hydraulic head at the water table surface and any hydraulic heads at depth will be the calibration parameters. The spatial thermal distribution between the upgradient and downgradient boundaries will be the evaluation parameters.

Thermal rock properties will be extracted from the project database. Because there is less thermal data at distance from the potential repository location, generalized information will be used in the thermal model. The methodology of Rautman (1995) may be used to assign thermal conductivity unless data that are more explicit are available.

The groundwater modeling code FEHM will be used for the simulations. This software was baselined 28 Jan 2003, as FEHM V2.20, STN/CSCI 10086-2.20-00.

Software will be managed according to QAP-3.2 Software Management.

### *Alternative Conceptualizations*

There are alternative conceptual combinations of hydraulic properties that may be the cause of the LHG. The alternative conceptualizations to be simulated are:

1. A vertical fault that acts as a low-permeability groundwater flow impediment (this conceptualization will form the base case),

2. Relatively lower hydraulic conductivity of the volcanic units upgradient of the LHG and relatively higher hydraulic conductivities downgradient of the LHG, and

3. A stratigraphic layer of low vertical permeability, causing the water table to "perch" above the low-permeability layer.

Informal discussions will he held with LANL staff performing the saturated zone modeling to ensure the physical extent and geometry of the postulated features are reasonable and that the alternative conceptualizations are viable in light of other information. These alternative conceptualizations will be theoretical constructs and will consist of assumed hydrogeologic properties and configurations. Therefore, the alternative conceptualizations will be non-unique and will not be supported by independent geological information.

### *Hydraulic Flow Calibrations*

A groundwater flow model of each conceptualization will be calibrated to hydraulic heads. The PEST code may be used for the calibration as needed. The PEST code is within the project's software baseline as PEST V 5.5, (STN)/CSCI Number 10289-5.5-00. The hydraulic parameters will be allowed to vary over a wide range to represent alternative conditions. The calibrated hydraulic properties will be compared to the observed hydraulic properties (i.e., hydraulic conductivity and porosity) to evaluate differences and the reasonableness. However, the properties of the postulated alternative hydrogeologic systems may be quite different compared to the current interpretations. Modeling will be performed according to QAP-3.3 Models.

### *Thermal Transport Modeling*

Adding thermal properties and heat transport to the calibrated groundwater flow models will simulate the spatial distribution of temperature. Temperature at water table and upgradient boundaries will be prescribed based on observed conditions. Neither the previously-simulated hydraulic properties nor these thermal properties will be adjusted in a calibration process to better match the observed groundwater temperature. Rather, the resulting spatial distribution of simulated temperatures within the body of the model will be the basis of comparison for evaluating how well each conceptualization matches the observed temperature conditions and trends. Statistical measure of the fit of the simulated temperatures to the observed temperature data will also be provided for each alternative conceptualization. Microsoft Excel spreadsheet functions will be used for the statistical analysis. Modeling will be performed according to QAP-3.3 Models.

### *Comparison of Results*

The conceptualization that is most consistent with the observed flow and temperature data will be identified. The selection of the preferred alternative(s) will be based on the statistical comparison of observed and predicted temperatures as well as the correspondence of spatial temperature trends. The sensitivity of the hydrologic parameters of the most consistent conceptualization will be evaluated to measure the robustness of the temperature match to variation in hydraulic conductivity.

### *Prepare Final Report*

A final report will be prepared that discusses the technical approach, groundwater flow and thermal transport model, and modeling results in the format prescribed in QAP-3.4 Technical Reports.

The deliverable associated with completing this task is the final report. If a subtask is later evaluated as non-quality affecting, the DOE Technical Task Representative will be notified in writing and a revised SIP will be written and sent to the QA Manager.

**SCHEDULE**

| Deliverables for Task ORD-FY04-018 | Completion Date |
|---|---|
| Quarterly Reports | Ongoing |
| Complete model analysis | 1-May-05 |
| Submit the final data to the TDA | 15-May-05 |
| Submit the final report | 23-Jun-05 |

**INTERFACE CONTROLS**
Internal Interfaces: Phil Oberlander, DRI
External Interfaces: Drew Coleman, DOE/YMSCO

Information will be transferred across interfaces by electronic methods.

**STANDARDS**
There are no special standards and criteria for this task. No specific job skills are required beyond those stated in the position descriptions filed with the HRC.

## IMPLEMENTING PROCEDURES

No implementing procedures will be prepared for this task.

## SAMPLES

No samples will be collected.

## SCIENTIFIC NOTEBOOKS

One scientific notebook will be kept for this task.

## EQUIPMENT

No field or laboratory equipment will be used.

## SOFTWARE AND MODELS

Programs such as Excel, PowerPoint, and Word are used to create reports, presentations and documents. Model simulations will be performed according to QAP-3.3. The groundwater modeling code FEHM will be used for the simulations. This software was baselined 28 Jan 2003, as FEHM V2.20, STN/CSCI 10086-2.20-00. Parameter estimation may use the PEST code to estimate hydraulic conductivity. The PEST code is within the project's software baseline as PEST V 5.5, (STN)/CSCI Number 10289-5.5-00. The model will be managed according to QAP-3.3. The model simulations performed will be numeric representations of hydrogeologic conceptualizations and cannot be quantitatively validated. The use of these models is limited to comparison to non-qualified reported thermal data to indicate which conceptualization(s) best match the observed data.

## PROCUREMENTS AND SUBCONTRACTS

No procurements or subcontracts are necessary.

## HOLD POINTS/DECISION POINTS

There are no hold points/decision points as defined in the UCCSN QA Program for this work.

## QUALITY CONTROL

Error associated with data reduction performed by task personnel will be minimized by verifying the accuracy of the reduced data to the raw data and that the reduction processes are accurate. Data verification will be performed by someone other than the originator. These reviews will be documented in the scientific notebooks for this task and in conjunction with the technical report review. There is no objective or evaluation for precision. The models developed by this task are conceptual representations (i.e., assumed hydrogeologic conditions and hydraulic properties necessary to illustrate general characteristics) and quantification of potential error in representation of the natural system is not possible.

Electronic data will be controlled by limited access to the computers that will contain those data. Each computer will be password protected. Data will be backed up on a regular basis. Access lists will be established for authorized users and these lists and the types of access will be listed in the applicable scientific notebooks.

## DATA RECORDING, REDUCTION, AND REPORTING

Data will be developed or used and controlled electronically in accordance with QAP-3.1, "Control of Electronic Data," to prevent tampering. Data will be recorded in electronic form, backed up to prevent loss, and verified when converted, transferred or input manually.

Data considered established fact by the scientific community need not undergo qualification. It is expected that most if not all of the groundwater temperature data near the LHG are unqualified. This task will produce qualified conceptual model simulations that will be compared to unqualified reported data for corroboration purposes only. Unqualified data will be clearly labeled "unqualified" and traceability to their origin will be maintained.

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." QA records produced as a result of the UCCSN QAP's are controlled in accordance with QAP-17.0, "Quality Assurance Records". Quarterly report deliverables are 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.

## REVIEWS AND VERIFICATIONS

Scientific notebooks started under this task will be reviewed at the end of the subtask, or earlier as needed. The data and final report developed under this task will be technically reviewed according to QAP-3.3 Models and QAP-3.4 Technical Reports respectively before submission. Technical and planned QA reviews will be conducted when the report is completed.

## RECORDS AND SUBMITTALS

QAP-17.0, "Quality Assurance Records", will be used for the protection and transmittal of QA records. Data will be transmitted as QA records under QAP-3.6.Documents or items that will be produced and submitted to DOE will be produced in accordance with QAP-3.3 Models.

## REFFERENCES

There are no references for this SIP other than the QAP's.