Remedial Actions: 12.1, Work Agreement 300.

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YUCCA MOUNTAIN SITE CHARACTERIZATION PROJECT

WORK AGREEMENT (WA)

WA-0300

Revision 01

Three-Dimensional Rock Characteristics Models

Customer:

. S. Costin, 6852)

Date: 6/4/96

Supplier:

A. Rautman, 6115)

(W. Zelinski, 6115)

Supplier:

Supplier:

Technical Review:

QA **Review:**

(S. McKenna, 6115)

(Reviewer signatures above serve to document the review and resolution of comments; Customer and Supplier signatures include comment resolution and approval of the Work Agreement.)

Effective Date: _____6/14/96

Date: 6/4/41

Date: 10

96 Date

Date: 6/4/96

Date: June 4.

1736

<u>Scope:</u> This Work Agreement establishes responsibilities and interfaces between L. S. Costin (Customer), C. A. Rautman (Supplier and Principal Investigator) and support staff (S. McKenna and W. Zelinski) for activities conducted in support of the three-dimensional rock characteristics models study.

Specifically, the scope of this Work Agreement includes oversight, management of stated resources, and conduct of activities in the following summary accounts for FY96:

WBS#	Upper-Tier WA #	PACS Account #	PACS Account Title	Case #
1.2.3.2.2.2.2	WA-0340	TR32222EB1	Model 2-D and 3-D Thermal and Mechanical Rock Properties	0139.373
1.2.3.2.2.2.2	WA-0340	TR32222EB2	Model 2-D and 3-D Hydrologic Rock Properties	0139.372

<u>Objective:</u> The objective of the work prescribed by this Work Agreement is to conduct geostatistical and geometric modeling of thermal and mechanical properties, and hydrologic properties for a variety of purposes. Work will include:

- -- compilation and evaluation of available rock-property measurements and similar data;
- -- compilation and evaluation of available geologic and geometric information;
- -- integrate rock properties data with geologic/geometric information into an integrated site model;
- -- statistical and spatial continuity analyses of data;
- -- generation of appropriate geometrical and geostatistical models;
- -- validation of the geometrical and geostatistical models by verifying that the output is consistent with site data; and
- -- support writing of data synthesis reports.

The following models will be developed. Models will be validated by verifying that the output is consistent with site data.

- 1. Porosity and bulk density model(s) of the Topopah Spring Tuff for the extended site area, or as much of that region as the data allow. The "extended site area" is defined roughly as extending from the vicinity of Yucca Wash south to the latitude of drill holes WT-11 and WT-12, and from Windy Wash east to Fortymile Canyon.
- 2. Porosity and bulk density model(s) of the Calico Hills Formation and Prow Pass Tuff for the extended site area, or as much of that region as the data allow.
- 3. Thermal conductivity model(s) of Topopah Spring Tuff for the central repository block area.
- 4. Matrix saturated hydraulic conductivity model(s) of the Topopah Spring Tuff for the extended site area, to the extent that the data allow modeling of this region.
- 5. Geostatistical modeling of rock properties to support LBL site-scale unsaturated zone hydrologic model and SNL performance assessment activities.

<u>Tasks</u>: Tasks and responsibilities included in this Work Agreement are described in the matrix below.

<u>RESPONSIBLE PERSON</u>	<u>SUPPORT</u>	TASK DESCRIPTION	
C. A. Rautman	W. Zelinski S. McKenna	 Task 1: Develop computer-based 3-D models that integrate site geologic information integrate quantitative data on rock characteristics include compilation/evaluation of rock properties data include borchole geophysics data validation of models using site data 	
C. A. Rautman	W. Zelinski S. McKenna	Task 2: Support writing of rock properties, geotechnical and geophysical data synthesis and other reports.]
C. A. Rautman		Task 3: Provide technical oversight, management of resources, and interface/information exchange with M&O management and other organizations as needed.	7

Responsibility Matrix

Interfaces: As part of Task 3, technical interfaces will be maintained with USGS and SNL PIs responsible for thermal, mechanical, and hydrological properties testing. The supplier will also maintain an interface relationship with the M&O Office Manager for these activities. Internal management issues (personnel assignments, subcontracts, etc.) will be jointly addressed with the customer as part of the responsibilities delegated under upper-tier WA-0340.

<u>Ouality Assurance Controls:</u> The work defined in this Work Agreement is related to Site Characterization/Performance Assessment. The following matrix lists the QA procedures that are determined to be applicable to the work defined within this Work Agreement, and identifies the parties in this Work Agreement responsible for complying with the controls. (Note that this table does not replace QAIP 2-5 training assignments).

QA Procedure Matrix

PROCEDURE #	DESCRIPTION ,	CUSTOMER	SUPPLIER
QAIP 1-5	Establishing Work Agreements	x	All*
QAIP 2-5	Training		· · · · · · · · · · · · · · · · · · ·
QAIP 2-6	Qualification and Certification of Personnel	X	
QAIP 4-1	Procurement		Rautman
QAIP 6-2	Reviewing, Approving, and Issuing Technical Documents	X	All
QAIP 6-3	Conducting Document Reviews	X	All
QAIP 17-1	Protecting, Preparing, and Submitting YMP QA Records		
QAIP 19-1**	Software Quality Assurance		All
QAIP 20-2	Scientific Notebooks		
APQ-16.1Q	Performance/Deficiency Reporting	X 1	All
APO-16.20	Corrective Action and Stop Work		· All

* "All" indicates that procedure applies to all suppliers named in this WA.

****** Procedure may apply after QARD Rev. 5 is implemented. Under QARD Rev.4 Procedure is not required.

No hold points or quality verification points are defined for this work. QA surveillances and process checks included in procedural controls are used to verify quality

Readiness Review Prerequisite: Not Applicable.

<u>Records</u>: The QA records generated by activities described in this Work Agreement result from implementing the QA procedures in the preceding matrix. Completed records will be reviewed, authenticated, and submitted to the SNL YMP Records Center by the Supplier. The file code(s) to be used for records packages resulting from work in this WA is YMP:1.2.3.2.2.2.2:WA-0300:XX:YY, where XX is either QA or NQ and YY is a descriptor for the record (see NWMC File Code, 4/7/95). Records related to the production, review, and approval of a formal report (SAND or SLTR) will be filed under code YMP:1.2.3.2.2.2.2:PUB:XX:(SAND# or SLTR#).

<u>Deliverables:</u> Report input and records shall be completed and transmitted in accordance with the deliverable dates in the Project Baseline as modified by the SNL Basis of Estimate and identified on the following matrix.

Deliverables Matrix

RESPONSIBILITY	DESCRIPTION	MILESTONE LEVEL	<u>DUE DATE</u>
C. A. Rautman	Submit letter with attachments to M&O Office Manager containing input on 2-D and 3-D hydrologic rock properties modeling for inclusion into site geotechnical report, and use in other performance assessment models.	4	5/15/96
C. A. Rautman	Submit letter with attachments to M&O Office Manager containing input on 2-D and 3-D thermal and mechanical rock properties for inclusion into site geotechnical report, 3D geologic framework model, and use in other performance assessment models.	4	3/15/96
C. A. Rautman	Submit letter with attachments containing integrated site model to M&O Office Manager in support of M&O Level 3 milestone.	Supports Level 3 Milestone	6/3/9 6

<u>Other Customer Requirements</u>: The Supplier will provide weekly technical status updates to the Customer, as well as input to monthly cost and schedule updates. The Supplier is responsible for identifying, developing, and issuing all lower-tier Work Agreements necessary to support the conduct of the work and deliverables described.

All personnel participating in the work described in this Work Agreement are responsible for complying with all safety, ES&H, and other requirements.

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<u>Schedule:</u> The schedule and due dates for the activities described in this Work Agreement are identified in the Deliverables matrix. Additional information may be obtained from the Project and Control System.

Budget: The estimated budget for this effort is \$239,139.

•<u>Training</u>: Personnel assigned to this Work Agreement shall be qualified to QAIP 2-6 and trained to the appropriate procedures as identified in the QA Procedure Matrix and in accordance with QAIP 2-5 as assigned by the Task Manager (see WA-0340).

Acceptance Criteria: The work shall be accepted as complete when the three deliverables defined in the matrix above are delivered to the M&O Office Manager and associated records packages have been submitted to the SNL local records center. The submittals must meet the criteria established for the deliverables in the Participant Planning Sheets (kept on file in the SNL project control office.)

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Investigative Actions: 18.1, Memo from R. Richards to M. Brady, dated 5/30/96.

Sandia National Laboratories

Albuquerque, New Mexico 67165 WBS 9,1,3,2

OA:

date: May 30, 1996

to: Michaele C. Brady, 6850, M/S 1399

from: R. R. Richards, 6812, M/S 1333

subject:

Investigative Action for Deficiency Report (DR) YMQAD-96-D044 Concerning Model Validation

The subject DR included an investigative action as follows, "All other Work Agreements (other than WA-300) that deal with model development will be reviewed to determine the extent that they meet the requirements for specifying the approach and criteria for the model validation portion of the activity." I have completed that evaluation; the results are presented in the attachment to this memo.

This evaluation, together with reviews of reports concerning model application and validation done for the Burn-up Credit effort, made clear to me that there is a wide conceptual difference between how our investigators think about validation and the concept behind the cited DR. The concept (and requirements) embodied in the DR is that to determine that a mathematical model is "valid" (i.e., an adequate representation of actual physical phenomena), some specific criteria must be applied in the comparison of the model output to real-world data. That, in turn, implies that those criteria be established before the comparison is made. This approach to model validation seems rigorous and reasonable, being a specific application of the concept of determining if something is "good enough" or "meets specifications" by comparing to a standard.

However, the idea of using criteria in determining whether a model is valid for a given purpose is not a concept that is readily and inherently applied by our investigators, if the text of the evaluated Work Agreements is any indication. As the attached results show, the existing approach to validating models is uniformly different in practice than the concept embodied in the DR (which arises from QARD requirements). That suggests either that the concept embodied in the DR is <u>not</u> appropriate for validation (although we ought to establish why the existing practice can be considered rigorous enough), or that we should take some action to cause our investigators to be more structured and demanding in their validation efforts.

copy to:

M/S 1326	H. A. Dockery	6851
M/S 1325	L. S. Costin	6852
M/S 1333	C. P. Jaramillo	6812

Model Validation Approach and Criteria

An evaluation was made of existing Sandia National Laboratories Work Agreements for activities supporting the Civilian Radioactive Waste Management Program. This evaluation was performed as investigative action arising from Deficiency Report YMQAD-96-D034. Specifically, the investigative action portion of that Deficiency Report states that , "All other Work Agreements (other than WA-300) that deal with model development will be reviewed to determine the extent that they meet the requirements for specifying the approach and criteria for the model validation portion of the activity."

The results of the evaluation are shown below. The Work Agreements (WAs) listed are those currently active[®] WAs that involve model development in some way, except for WA-300.

WA Number	WA Title	Comments
040, rev. 2	Development and Validation of Flow and Transport Models	Activity includes 3 main activities that are said to involve model devel, and validation. The work description covers data generation in detail, is sketchy on model development efforts, and silent on validation approach. No validation criteria are provided.
106, rev. 4 	Numerical Climate Model Validation	Approach to validation well described. No specific criteria stated (or intended); desired result was to simply state the qualitative comparison between model results and data.
119, rev. 2	Empirical Model of Ground Motions from Underground Nuclear Explosions	Activity is wholly devoted to development of a model for ground motion prediction. Validation not addressed (may have been intended to be covered in another WA that was never developed).
132, rev. 0	Conduct Studies to Support Calculations of Ground Water Travel Time	Activity involves model development. Approach to validation is either absent or unclearly stated (step 7 of sec. 9?). No criteria specified for validation.
165, rev. 0 _.	Analysis Code Validation	Validation approach not clearly described; no criteria for successful validation are specified.
166, rev. O	Numerical Validation of Rock- mass Thermal Expansion, Stiffness, and Strength	Approach to validation specified for all 3 parameter models. However, no criteria for determining that the models are 'valid' are specified.

^{*}Active* in this sense means that the WA remains open as a controlled document. In several cases, the work is complete, or otherwise ended,

181, rev. 0 Enhance Groundwater Travel Time (GWTT) Modeling Capabilities

192, rev. 0 Develop Bounding Representations of Unsaturated Fracture Flow Activity calls for enhancing existing models, then using the models for analysis of GWTT. No validation actions are included.

Activity includes modifying or enhancing existing models. 'Validation' not addressed, <u>per se</u>. However, 'evaluation' of models, via benchmark analysis comparisons required; no criteria for these comparisons is specified.

Action to Preclude Recurrence: 20.-1, Copy of QAIP 2-4.