

Sandia National Laboratories

Albuquerque, New Mexico 87185

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A1158

SNL HL

WM Project 10, 11, 16

Docket No. \_\_\_\_\_

PDR

LPDR  (B, N, S)

Dr. Richard Codell  
Geotechnical Branch  
Division of Waste Management  
U.S. Nuclear Regulatory Commission  
7915 Eastern Avenue  
Silver Spring, MD 20910

Distribution:

RCodell

NStill

(Return to WM, 623-SS)

Jean-Ticket

C<sup>2</sup>

Dear Dr. Codell:

Enclosed is the monthly report on FIN A-1158, Repository Site Description and Technology Transfer for March 1985.

Please feel free to contact me if you have any questions or comments.

Sincerely,

*Margaret Chu For  
R.M. Cranwell*

Robert M. Cranwell, Supervisor  
Waste Management Systems  
Division 6431

RMC:6431:jm

Enclosure

Copy to:

Office of the Director, NMSS  
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Division of Waste Management  
Enrico Conti, Branch Chief  
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PDR WMRES EXISANL  
A-1158 PDR

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PROGRAM: Repository Site Definitions; FIN#: A-1158  
Short-term Technical Assistance Tasks I, III

CONTRACTOR: Sandia National Laboratories BUDGET PERIOD: 10/84 -  
9/85

NMSS PROGRAM MANAGER: R. B. Codell BUDGET AMOUNT: \$90K  
(Tentative)

CONTRACT PROGRAM MANAGER: R. M. Cranwell FTS PHONE: 844-8368

PRINCIPAL INVESTIGATORS: R. L. Hunter FTS PHONE: 846-6337  
M. D. Siegel FTS PHONE: 846-5448

#### PROJECT OBJECTIVE

To develop reference repositories in media other than bedded salt (i.e., basalt, domed salt, welded tuff, and granite).

#### ACTIVITIES DURING MARCH 1985

##### Repository Site Definition

A limited effort was devoted to updating the geochemistry data base for the RSD. We are waiting for NRC comments on the RSD for unsaturated tuff.

Most of the subcontractor charges of \$36K on this contract will be credited at a later date. A request for reclassification of about \$60K in funds for this project has been made but is requiring some time to get through the Sandia budgeting system.

PROGRAM: Technology Transfer FIN#: A-1158  
Task II

CONTRACTOR: Sandia National Laboratories BUDGET PERIOD: 10/84 -  
9/85

NMSS PROGRAM MANAGER: R. Codell BUDGET AMOUNT: \$277K  
(Tentative)

CONTRACT PROGRAM MANAGER: R. M. Cranwell FTS PHONE: 844-8368

PRINCIPAL INVESTIGATORS: R. L. Hunter FTS PHONE: 846-6337  
M. D. Siegel FTS PHONE: 846-5448

#### PROJECT OBJECTIVE

To insure through technical support, problem definition, and documentation the timely, thorough, and efficient transfer of the information, analysis techniques, and analysis tools developed for the U.S. Nuclear Regulatory Commission (NRC) by the methodology program.

#### ACTIVITIES DURING MARCH 1985

Work on finalizing of TOUGH proceeded on schedule in March. The treatment of binary diffusion has been completely reworked. We included air transport by this mechanism, and provided for a general pressure and temperature dependence of diffusivity. Also, provisions were made for domain-dependent tortuosity effects. Several modifications were made which will improve code performance for highly non-linear problems. Formation heat conductivity was generalized to allow for saturation dependence. Improvements in coding were made throughout the program. All code modifications were carefully tested and checked. Several runs have been made of prototype-sample problems.

Dick Codell, PM, has asked for an expanded explanation of the scaling of the Jacobian matrix to be included in the TOUGH code. Scaling of elements within the Jacobian matrix, better known as matrix pre-conditioning, is used to make the matrix better conditioned for solving equations. Typically, values of elements in the Jacobian matrix vary over as much as 20 orders of magnitude. The reason for this is the system of units that TOUGH uses. Energy typically has values of  $10^6$  joules, and pressure, typically,  $10^6$  to  $10^7$  pascals. These are much larger than air mass fraction, which may have large negative exponents. This wide range in the magnitude of the matrix elements results in a loss of precision in numerical computation, especially during addition and subtraction. The

scaling of the matrix elements reduces the range of values from as much as twenty orders of magnitude to about three orders. The result is better numerical stability and iterative behavior of the matrix. LBL is using a matrix preconditioning subroutine supplied by Harwell to scale the Jacobian matrix in the TOUGH code.

A-1158, Task II  
 0976.010  
 March 1985

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY SANDIA'S ACCOUNTING DEPARTMENT.

	Current Month	Year-to-Date
I. Direct Manpower (man-months of charged effort)	0.2	1.2
II. Direct Loaded Labor Costs	2.0	11.0
Materials and Services	0.0	0.0
ADP Support (computer)	0.0	0.0
Subcontracts*	-15.0	25.0
Travel	0.0	0.0
Other	-1.0	0.0
<b>TOTAL COSTS</b>	<b>-14.0</b>	<b>36.0</b>

Other = rounding approximation by computer

III. Funding Status

Prior FY Carryover	FY85 Projected Funding Level	FY85 Funds Received to Date	FY85 Funding Balance Needed
172K	277K	None	105K

\*Includes \$18K in new subcontractor charges and \$33K in reimbursed charges.

A-1158

TOTAL FOR 0976.010 and 0976.020

March 1985

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY SANDIA'S ACCOUNTING DEPARTMENT.

	Current Month	Year-to-Date
I. Direct Manpower (man-months of charged effort)	0.2	1.6
II. Direct Loaded Labor Costs	2.0	15.0
Materials and Services	0.0	0.0
ADP Support (computer)	0.0	0.0
Subcontracts	21.0	183.0
Travel	0.0	0.0
Other	-1.0	0.0
TOTAL COSTS	22.0	198.0

Other = rounding approximation by computer

III. Funding Status

Prior FY Carryover	FY85 Projected Funding Level	FY85 Funds Received to Date	FY85 Funding Balance Needed
172K	367K	None	195K

A-1158, Tasks I and III  
 0976.020  
 March 1985

THIS IS AN ESTIMATE ONLY AND MAY NOT MATCH THE INVOICES SENT TO NRC BY SANDIA'S ACCOUNTING DEPARTMENT.

	Current Month	Year-to-Date
I. Direct Manpower (man-months of charged effort)	0.0	0.4
II. Direct Loaded Labor Costs	0.0	4.0
Materials and Services	0.0	0.0
ADP Support (computer)	0.0	0.0
Subcontracts*	36.0	158.0
Travel	0.0	0.0
Other	0.0	0.0
<b>TOTAL COSTS</b>	<b>36.0</b>	<b>162.0</b>

Other = rounding approximation by computer

III. Funding Status

Prior FY Carryover	FY85 Projected Funding Level	FY85 Funds Received to Date	FY85 Funding Balance Needed
None	90K	None	90K

\*Most of this month's new charges will be reimbursed. The 60K referred to in previous monthly reports is still in Sandia accounting.