

Sandia National Laboratories

Albuquerque, New Mexico 87185

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November 15, 1986

WM-285
WM Record File

A1158
SNL

WM Project 10, 11, 16

Docket No. _____

PDR ☒

LPDR B, N, S

Distribution:

Coleman
Still

(Return to WM, 623-SS)

Joanne - Ticket

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Neil M. Coleman
Hydrology Section
Geotechnical Branch
Division of Waste Management
U.S. Nuclear Regulatory Commission
7915 Eastern Avenue
Silver Spring, MD 20910

Dear Mr. Coleman:

Enclosed is the monthly report on FIN A-1158, Repository Site Definition and Technology Transfer for October 1986. Please feel free to contact me at FTS 844-8368 or Charlene Harlan at FTS 844-8164 if you have any questions or comments.

Sincerely,

Robert M. Cranwell

Robert M. Cranwell, Supervisor
Waste Management Systems
Division 6431

RMC:6431

Enclosure

Copy to:

Office of the Director, NMSS
Attn: Program Support
Robert Browning, Director
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Health Siting & Waste Management Division
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A-1158 PDR

3549

PROGRAM: Task I, Repository Site Definitions

FIN#: A-1158

CONTRACTOR: Sandia National Laboratories

BUDGET PERIOD: 10/86 -
9/87

NMSS PROGRAM MANAGER: N. M. Coleman

BUDGET AMOUNT: - 0 -

CONTRACT PROGRAM MANAGER: R. M. Cranwell

FTS PHONE: 844-8368

PRINCIPAL INVESTIGATOR: C. P. Harlan

FTS PHONE: 844-8164

PROJECT OBJECTIVE

To develop RSDs for candidate host media and provide data for use in developing and testing performance assessment methodologies for the various media.

ACTIVITIES DURING OCTOBER 1986

No activity.

PROGRAM: Task II, Technology Transfer

FIN#: A-1158

CONTRACTOR: Sandia National Laboratories

BUDGET PERIOD: 10/86 -
9/87

NMSS PROGRAM MANAGER: N. M. Coleman

BUDGET AMOUNT: \$165K

CONTRACT PROGRAM MANAGER: R. M. Cranwell

FTS PHONE: 844-8368

PRINCIPAL INVESTIGATOR: C. P. Harlan

FTS PHONE: 844-8164

PROJECT OBJECTIVE

To provide technical support for the transfer of the capability to use the information, analytical techniques, and tools developed for the NRC under the Performance Assessment Methodology program (FIN A-1266).

ACTIVITIES DURING OCTOBER 1986

SWIFT II Self-Teaching Curriculum (STC)

Updates to the Self-Teaching Curriculum are being incorporated into the report. An additional analytical solution is being added to problem 2 verifying the SWIFT II results. This analytical solution came out of the SWIFT II Verification/Validation task also funded under FIN A-1158.

TOUGH User's Guide

Karsten Pruess (LBL) has completed the draft report incorporating comments from NRC and Sandia. As a result of these changes, both the TOUGH code and the sample problems have been modified. When Sandia receives the draft report, the formal internal review will begin. After review of the report, management sign-off will begin unless extensive changes are required. Dr. Pruess will receive the final comments and, if necessary, modify the camera ready originals before transmitting them to Sandia. Peer review (one reviewer and one referee) time, management sign-off time, and time required for Dr. Pruess to modify the camera ready copies if necessary, are heavily dependent on current staff and management commitments, and one to two month time estimates are typical.

When a tape containing the new version of the code and sample problems is received, QA will be repeated.

TOUGH Seminar

Karsten Pruess (LBL) has requested direction from NRC concerning a potential seminar next spring. Areas to be addressed are number of days involved, defining the intended audience, course objectives, determining whether theory or hands-on experience are preferred, materials to be provided, location of the seminar, and other areas of concern to the project manager.

NEFTRAN User's Manual

Work has begun on the User's Manual for the dual-porosity NEFTRAN computer code. This code is an extension of the NWFT/DVM code with

new capabilities added (generalized flow network, leg-transfer capability, new source term, and matrix diffusion). This report is being funded jointly by FIN A1266 and A1158. Primary effort in the near future will be to develop sample problems that verify/validate the model.

PROGRAM: Task III, Maintenance of Computer Codes

FIN#: A-1158

CONTRACTOR: Sandia National Laboratories

BUDGET PERIOD: 10/86 -
9/87

NMSS PROGRAM MANAGER: N. M. Coleman

BUDGET AMOUNT: \$180K

CONTRACT PROGRAM MANAGER: R. M. Cranwell

FTS PHONE: 844-8368

PRINCIPAL INVESTIGATOR: C. P. Harlan

FTS PHONE: 844-8164

PROJECT OBJECTIVE

To implement a quality assurance program to maintain computer codes, report errors, document changes, and inform the NRC staff.

ACTIVITIES DURING OCTOBER 1986

Three codes have gone through QA during October. LHS (Latin Hypercube Sample) was converted from the standard VAX version to CDC and the sample problems rerun. These conversions have been saved in an Update format to document the modifications. DNET was made less machine dependent by adding subroutines to the code that previously were pulled in from external libraries. These changes have been saved in Update format to document the additions. The sample problems were rerun and report results reproduced. USGS was adapted to the current CDC hardware and out-of-date system calls updated. The four sample problems were run and the report results reproduced.

Within the next few weeks, plans are to transmit LHS, DNET, and USGS to the INEL computer system for QA. When the QA is complete, these three codes will be added to the interactive on-line help currently available in the library area 'CRH' at INEL. The on-line help for these three codes will supply users with as much documentation and system use as possible to make them self sufficient. Copies of the on-line code documentation for LHS, DNET, and USGS are attached. In addition, under separate cover, a copy of the USGS manual will be forwarded to the NMSS PM.

PROGRAM: Task IV, Code Validation and Verification FIN#: A-1158

CONTRACTOR: Sandia National Laboratories BUDGET PERIOD: 10/86 -
9/87

NMSS PROGRAM MANAGER: N. M. Coleman BUDGET AMOUNT: \$25K

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

PRINCIPAL INVESTIGATOR: C. P. Harlan FTS PHONE: 844-8164

PROJECT OBJECTIVE

To assemble the various tests that have been performed to help validate and verify various portions of relevant codes and recommend any additional feasible tests.

ACTIVITIES DURING OCTOBER 1986

SWIFT II Verification/Validation

Dave Updegraff (SAI) has assembled existing verification and validation for the SWIFT II model. These results are summarized in a draft report. In addition, recommendations for areas to be developed are being added. Very little time was allocated to this task during October because of corresponding effort in updating the SWIFT II Self-Teaching Curriculum (STC). The STC is being used as research material for the verification and validation effort. In addition to adding an analytical solution to the STC verifying SWIFT II results, this use of the STC has been helpful in developing the updates to the report.

TOUGH Verification/Validation

As was presented in the January 1986 Program Review for FIN A1158, verification and validation of the TOUGH code is being performed through the development of sample problems in the User's Manual. NRC's comments of the earlier draft have been incorporated into this report.

PROGRAM: Task V, Short-term Technical Assistance

FIN#: A-1158

CONTRACTOR: Sandia National Laboratories

BUDGET PERIOD: 10/86 -
9/87

NMSS PROGRAM MANAGER: N. M. Coleman

BUDGET AMOUNT: \$25K

CONTRACT PROGRAM MANAGER: R. M. Cranwell

FTS PHONE: 844-8368

PRINCIPAL INVESTIGATOR: C. P. Harlan

FTS PHONE: 844-8164

PROJECT OBJECTIVE

To provide general technical assistance on waste management matters relating to Tasks I-IV.

ACTIVITIES DURING OCTOBER 1986

No activity.

MANAGEMENT TECHNICAL ISSUES:

Your letter dated October 2, 1986, requests recommendations concerning NRC contractor needs for consulting with cognizant Sandia staff on questions relating to SWIFT II and other Sandia codes made available to them through NRC. They have expressed a wish to have direct access to the staff rather than directing questions through NRC. Since FIN A1158 is not currently funded to address this responsibility, it would be desirable to have a task specifically assigned to track the manpower and associated dollars. Task V, Short-term Technical Assistance, could provide the means to budget and report this effort.

LHS INTERNAL DOCUMENTATION:

```
*****
*
*   CODE NAME       -   LHS
*
*   VERSION         -   RELEASE MARCH 1984
*                   -   CONVERTED FROM VAX TO CDC CYBER 7600
*                   -   SEPTEMBER 1986
*
*   DESCRIPTION     -   THE LATIN HYPERCUBE SAMPLING PROGRAM
*                       GENERATES EITHER LATIN HYPERCUBE OR RAN-
*                       DOM MULTIVARIATE SAMPLES. THE GENERATION
*                       OF THESE SAMPLES IS BASED ON INFORMATION
*                       SUPPLIED TO THE PROGRAM BY THE USER
*                       DESCRIBING THE VARIABLES OR PARAMETERS
*                       USED AS INPUT TO THE COMPUTER MODEL. THE
*                       ACTUAL SAMPLED VALUES ARE USED TO FORM
*                       VECTORS OF VARIABLES COMMONLY USED AS IN-
*                       PUT TO COMPUTER MODELS FOR PURPOSES OF
*                       SENSITIVITY AND UNCERTAINTY ANALYSIS
*                       STUDIES.
*                       NOTE: IT IS IMPORTANT FOR THE USER TO
*                       REMEMBER THAT THE LHS PROGRAM UTILIZES A
*                       RANDOM NUMBER GENERATOR TO CREATE THE MONTE
*                       CARLO SAMPLE, AND THEREFORE THE EXACT
*                       SAMPLE CREATED WILL VARY FROM MACHINE TO
*                       MACHINE.
*
*   LANGUAGE        -   ANSI STANDARD FORTRAN, VERSION 77
*
*   HARDWARE        -   CDC CYBER 7600 MACHINES
*
*   LIBRARIES       -   NONE USED
*
*   EVOLUTION       -   LATIN HYPERCUBE SAMPLING, SANDIA
*                       NATIONAL LABORATORIES, 1980
*
*   DOCUMENTATION   -   LHS USER'S MANUAL, NUREG/CR-3624,
*                       SAND/83-2365
*
*   SANDIA CONTACTS -   GINGER F. WILKINSON, DIVISION 6431
*                       CHARLENE P. HARLAN, DIVISION 6431
*                       MICHAEL J. SHORTENCARIER, DIVISION 6415
*
*****
```

LHS FILES:

```
LHS      - CYBER 855 VERSION OF LHS (UPDATE FORMAT)
LHSSRC   - LHS SOURCE TO UPDATE PROCESSOR
LHSCMP   - LHS FORTRAN 77 COMPILE FILE
LHSLGO   - LHS COMPILED BINARIES
LHS01    - LHS SAMPLE PROBLEM 1
LHS02    - LHS SAMPLE PROBLEM 2
LHSDOC   - FILE CONTAINING DOCUMENTATION ON LHS
```

LHS EXECUTION PROCEDURE:

```
(EXAMPLE USING LHS01)
GET,LHSLGO/UN=CRH      (ATTACH THE EXECUTABLE BINARIES)
GET,TAPE5=LHS01/UN=CRH (SELECT LHS01 AS THE INPUT DATA FILE)
LHSLGO                (EXECUTE JOB)
.
.                      (EXECUTION IN PROGRESS)
.
RETURN,*,TAPE6         (RELEASE ALL FILES EXCEPT OUTPUT TAPE6)
```

PROCEDURE TO GET A HARDCOPY OF THIS DOCUMENTATION:

```
GET,LHSDOC/UN=CRH
(SEND THIS FILE TO YOUR PRINTER)
```

DNET INTERNAL DOCUMENTATION:

```

* .....
* CODE NAME      - DNET
*
* VERSION        - RELEASE OCTOBER 1981
*                  - CONVERTED FROM CDC 7600 TO CYBER 180/855
*                  - SEPTEMBER 1986 (IDENTIFIER IS SEP86)
*
* DESCRIPTION    - THE DYNAMIC NETWORK MODEL SIMULATES SALT
*                  DISSOLUTION IN BEDDED SALT FORMATIONS.
*                  INCLUDED IN THE MODEL ARE THE CAPABILITIES
*                  FOR SIMULATING PROCESSES SUCH AS SALT
*                  CREEP, SUBSIDENCE, AND THERMOMECHANICAL
*                  EFFECTS, ALL OF WHICH CAN AFFECT THE SALT
*                  DISSOLUTION PROCESS.
*
* LANGUAGE       - ANSI STANDARD FORTRAN 66
*
* HARDWARE       - CDC CYBER 180/855 MACHINES
*
* LIBRARIES      - NONE USED
*
* DOCUMENTATION  - DNET USER'S MANUAL, NUREG/CR-2343,
*                  SAND81-1663
*                  - DNET SELF-TEACHING CURRICULUM,
*                  NUREG/CR-2391, SAND81-2256
*
* SANDIA CONTACTS - LARRY R. SHIPERS, DIVISION 6431
*                  CHARLENE P. HARLAN, DIVISION 6431
*                  GINGER F. WILKINSON, DIVISION 6431
* .....

```

DNET FILES:

```

DNET      - CYBER 855 VERSION OF DNET (UPDATE FORMAT)
DNETSRC   - DNET SOURCE TO UPDATE PROCESSOR
DNETCMP   - DNET FORTRAN 66 COMPILE FILE
DNETLGO   - DNET COMPILED BINARIES
DNET01    - DNET USER'S MANUAL & STC PROBLEM - BASE CASE
DNET02    - DNET USER'S MANUAL & STC PROBLEM 2
DNET03    - DNET USER'S MANUAL & STC PROBLEM 3A
DNET04    - DNET USER'S MANUAL & STC PROBLEM 3B
DNET05    - DNET USER'S MANUAL & STC PROBLEM 4
DNETDOC   - FILE CONTAINING DOCUMENTATION ON DNET

```

DNET EXECUTION PROCEDURE:

```

ATTACH,DNETLGO/UN=CRH      (EXAMPLE USING DNET01)
GET,TAPE5=DNET01/UN=CRH    (ATTACH THE EXECUTABLE BINARIES)
DNETLGO,TAPE5,TAPE6        (SELECT DNET01 AS INPUT DATA FILE)
                             (EXECUTE JOB)
                             (EXECUTION IN PROGRESS)
RETURN,*,TAPE6             (RELEASE ALL FILES EXCEPT OUTPUT TAPE6)

```

PROCEDURE TO GET A HARDCOPY OF THIS DOCUMENTATION:

```

GET,DNETDOC/UN=CRH
(SEND THIS FILE TO YOUR PRINTER)

```

USGS MODIFICATIONS:

MODIFICATIONS TO USGS3D (POSSON VERSION) WERE MADE IN ORDER TO REMOVE SOME MACHINE DEPENDENCIES. THE FOLLOWING MODIFICATIONS WERE MADE TO THE USGS3D UPDATE SOURCE FILE.

- (1) THE FOLLOWING PLOT SUBROUTINES WERE INSERTED JUST BEFORE "*DECK,FORCIO". THESE PLOT ROUTINES ARE NOT AVAILABLE AT ALL INSTALLATIONS. THE EFFECT OF THIS CHANGE IS TO SUPPRESS PRINTER PLOTS.

```
SUBROUTINE PLOTS (X,Y,N)
RETURN
END
SUBROUTINE SCREEN (W,X,Y,Z)
RETURN
END
SUBROUTINE VWPORT (W,X,Y,Z)
RETURN
END
SUBROUTINE WINDOW (W,X,Y,Z)
RETURN
END
SUBROUTINE NUMBER (V,W,X,Y,Z,L)
RETURN
END
SUBROUTINE SYMBOL (W,X,Y,I,Z,L)
RETURN
END
SUBROUTINE PLOT (X,Y,N)
RETURN
END
SUBROUTINE XUNLOAD (I)
RETURN
END
```

- (2) ALL FIVE REFERENCES TO THE STRING "=MEM(" ARE COMMENTED OUT BY PLACING A "C" IN COLUMN 1. THIS FUNCTION IS NO LONGER SUPPORTED AND THE USER NOW REQUESTS THE EXTENDED MEMORY.
- (3) ALL FOUR REFERENCES TO THE STRING "CALL RQUEST" ARE COMMENTED OUT BY PLACING A "C" IN COLUMN 1. THIS SYSTEM COMMAND IS NO LONGER SUPPORTED AND THE USER MUST NOW SAVE AND RETRIEVE THE RESTART FILES IF DESIRED.

USGS FILES:

```
USGS      - USGS AFTER INSTALLATION, IN UPDATE FORMAT
USGSSRC   - USGS AFTER INSTALLATION (SEE MODIFICATIONS LISTED ABOVE),
            SOURCE TO UPDATE PROCESSOR
USGS3D    - POSSON VERSION BEFORE INSTALLATION (SEE MODIFICATIONS LISTED
            ABOVE), SOURCE TO UPDATE PROCESSOR
USGSUPD   - INPUT TO UPDATE PROCESSOR TO DEFINE HARDWARE, DIMENSIONS,
            PROBLEM SIZE, OPTIONS, ETC (SET UP FOR SAMPLE PROBLEMS)
USGSLGO   - USGS COMPILED BINARIES (FOR SAMPLE PROBLEMS)
FLECSM    - FLECS FORTRAN FILE
FLECSLG   - FLECS COMPILED BINARIES
USGS01    - USGS USER'S GUIDE PROBLEM 1
USGS02    - USGS USER'S GUIDE PROBLEM 2
USGS03    - USGS USER'S GUIDE PROBLEM 3
USGS04    - USGS USER'S GUIDE PROBLEM 4
USGSDOC   - FILE CONTAINING THIS DOCUMENTATION
```

USGS SAMPLE PROCEDURE TO CREATE BINARIES FOR SAMPLE PROBLEM EXECUTION:

```
GET,USGSUPD/UN=CRH
ATTACH,USGS/UN=CRH
UPDATE,P=USGS,I=USGSUPD,N=0,C=FLECSIN,F,8,L=0
REWIND,ALL
ATTACH,FLECSLG/UN=CRH
FLECSLG,FLECSIN,FLECSLS,FLECSOU
REWIND,ALL
FTN4,I=FLECSOU,B=LGO,LCM=I,L=0
REWIND,ALL
DEFINE,USGSLGO
COPYBF,LGO,USGSLGO
RETURN,ALL
```

USGS SAMPLE EXECUTION PROCEDURE FOR PROBLEM 1:

```
GET,USGS01/UN=CRH
ATTACH,USGSLGO/UN=CRH
RFL,0,400
LDSET,PRESET=0
    USGSLGO,USGS01,USGS01P
```

```
RFL,0
    (USGS01P IS OUTPUT FILE FOR PROBLEM 1)
```

USGS SAMPLE EXECUTION PROCEDURE FOR PROBLEM 2 (CREATES A RESTART):

```
GET,USGS02/UN=CRH
ATTACH,USGSLGO/UN=CRH
RFL,0,400
FILE(BAKOUT,SBF=NO)
LDSET,PRESET=0
    USGSLGO,USGS02,USGS02P
```

```
RFL,0
    (USGS02P IS OUTPUT FILE FOR PROBLEM 2)
    (BAKOUT IS RESTART FILE - SAVE FOR RESTART)
```

USGS SAMPLE EXECUTION PROCEDURE FOR PROBLEM 3 (INPUTS A RESTART):

```
GET,BAKIN/UN=YOUR AREA (MUST BE LOCAL FILE, WAS BAKOUT)
GET,USGS03/UN=CRH
ATTACH,USGSLGO/UN=CRH
RFL,0,400
FILE(BAKIN,SBF=NO)
LDSET,PRESET=0
    USGSLGO,USGS03,USGS03P
```

```
RFL,0
    (USGS03P IS OUTPUT FILE FOR PROBLEM 3)
```

USGS SAMPLE EXECUTION PROCEDURE FOR PROBLEM 4:

```
GET,USGS04/UN=CRH
ATTACH,USGSLGO/UN=CRH
RFL,0,400
LDSET,PRESET=0
    USGSLGO,USGS04,USGS04P
```

```
RFL,0
    (USGS04P IS OUTPUT FILE FOR PROBLEM 4)
    (TRFILE IS BINARY OUTPUT TRANSIENT LEAKAGE DATA FILE)
```

PROCEDURE TO GET A HARDCOPY OF THIS DOCUMENTATION:

```
GET,USGSDOC/UN=CRH
    (SEND THIS FILE TO YOUR PRINTER)
```

A-1158

Total for 0976.010, 0976.020, 0976.030, 0976.040 and 0976.050
October 1986

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)	2.6 ---	2.6 ---
II. Direct Loaded Labor Costs	20	20
Materials and Services	0	0
ADP Support (computer)	4	4
Subcontracts	93	93
Travel	0	0
Other (computer roundoff)	1	1
	-----	-----
TOTAL COSTS	118	118

III. Funding Status

Prior FY Carryover -----	FY 87 Projected Funding Level -----	FY 87 Funds Received to Date -----	FY 87 Funding Balance Needed -----
\$224K *	\$377K	\$0K	\$266K

* \$224K carryover less approximately \$113K of FY86 expenses incurred
but not costed out of project in FY86 leaves a balance of \$111K.

A-1158, Task I
0976.010
October 1986

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 ---	0.0 ---
II. Direct Loaded Labor Costs	0	0
Materials and Services	0	0
ADP Support (computer)	0	0
Subcontracts	0	0
Travel	0	0
Other (computer roundoff)	0	0
	---	---
TOTAL COSTS	0	0

A-1158, Task II
0976.020
October 1986

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)	0.5 ---	0.5 ---
II. Direct Loaded Labor Costs	3	3
Materials and Services	0	0
ADP Support (computer)	0	0
Subcontracts	24	24
Travel	0	0
Other (computer roundoff)	0	0
	---	---
TOTAL COSTS	27	27

A-1158, Task III
0976.030
October 1986

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)	2.0 ---	2.0 ---
II. Direct Loaded Labor Costs	16	16
Materials and Services	0	0
ADP Support (computer)	4	4
Subcontracts	37	37
Travel	0	0
Other (computer roundoff)	1	1
	---	---
TOTAL COSTS	58	58

A-1158, Task IV
0976.040
October 1986

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)	0.1 ---	0.1 ---
II. Direct Loaded Labor Costs	1	1
Materials and Services	0	0
ADP Support (computer)	0	0
Subcontracts	32	32
Travel	0	0
Other (computer roundoff)	0	0
	---	---
TOTAL COSTS	33	33

A-1158, Task V
0976.050
October 1986

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 ---	0.0 ---
II. Direct Loaded Labor Costs	0	0
Materials and Services	0	0
ADP Support (computer)	0	0
Subcontracts	0	0
Travel	0	0
Other (computer roundoff)	0	0
	---	---
TOTAL COSTS	0	0