Sandia National Laboratories

Albuquerque, New Mexico 87185

September 15, 1986

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 August 1986. Please feel free to contact me 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 Division of Waste Management Philip Justus Division of Waste Management Enrico Conti, Branch Chief Health Siting & Waste Management Division John Randall Division of Radiation Programs and Earth Sciences 6400 R. C. Cochrell 6430 N. R. Ortiz 6431 R. M. Cranwell 6431 C. P. Harlan 6431 G. F. Wilkinson

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PROGRAM: Repository Si	te Definitions	FIN# Task	: A-1158 I
CONTRACTOR: Sandia Nation Laboratories	nal	BUDGET PERIOD:	10/85 - 9/86
NMSS PROGRAM MANAGER:	N. M. Coleman	BUDGET AMOU	NT: - 0 -
CONTRACT PROGRAM MANAGER:	R. M. Cranwell	FTS PHONE:	844-8368
PRINCIPAL INVESTIGATORS:	G. F. Wilkinson C. P. Harlan	FTS PHONE: FTS PHONE:	844-0074 844-8164

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J 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 AUGUST 1986

No activity.

PROGRAM: Tech	nology Transfer	FIN# Task	: A-1158 II
	lia National pratories	BUDGET PERIOD:	10/85 - 9/86
NMSS PROGRAM MANA	AGER: N. M. Cole	man BUDGET AMOU	NT: \$115K
CONTRACT PROGRAM	MANAGER: R. M. Cran	well FTS PHONE:	844-8368
PRINCIPAL INVEST	GATORS: G. F. Wilk C. P. Harl		844-0074 844-8164

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 AUGUST 1986

# SWIFT II Self-Teaching Curriculum (STC)

Preparation of an errata sheet to the SWIFT II Self-Teaching Curriculum is currently underway. When complete, it will be transmitted to the Division of Technical Information and Document Control for distribution. We anticipate completion during the month of September.

# <u>SWIFT II Seminar</u>

A seminar on the capabilities and use of the Sandia Waste-Isolation Flow and Transport Model for Fractured Media (SWIFT II) was held at NRC in Silver Spring, MD on August 19-21, 1986. The objectives of this course were to provide a detailed description of SWIFT II (evolution, assumptions and equations, numerical implementation, code data input, quality assurance) and illustrate the use of structure, data input, quality assurate the code through sample problems. Documentation including the SWIFT II Data Input Guide, SWIFT II Theory and Implementation, "Theoretical Description of SWIFT II Self-Teaching Curriculum, Boundary Conditions" by Everdingen and Hurst, and a copy of the instructors' viewgraphs was provided to the twelve attendees, which consisted of NRC staff and contractors. The course was taught by P. A. Davis and E. J. Bonano, and a presentation on procedures for accessing SWIFT II on the INEL computing system was delivered by C. P. Harlan.

PROGRAM: Maintenanc	e of Computer Codes	FIN <b>#: A-11</b> 58 Task III
CONTRACTOR: Sandia Nat Laboratori		BUDGET PERIOD: 10/85 - 9/86
NMSS PROGRAM MANAGER:	N. M. Coleman	BUDGET AMOUNT: \$175K
CONTRACT PROGRAM MANAGE	R: R. M. Cranwell	FTS PHONE: 844-8368
PRINCIPAL INVESTIGATORS	: G. F. Wilkinson C. P. Harlan	FTS PHONE: 844-0074 FTS PHONE: 844-8164

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

**ACTIVITIES DURING AUGUST 1986** 

#### USGS 3-D Model Code

The USGS-3D model code has been read from tape onto the SNL Open NOS computing system in preparation for transfer to INEL. At the present time we are experiencing difficulties in compiling, which is probably due to some hardware incompatibilities. SNL computing center consultants are working with us on this matter. This code was developed for use on specific hardware and, consequently, is very machine-dependent.

As we had outlined in the April monthly report, there are many unknowns in implementing this code, which was developed by another agency entirely independent of SNLA's QA program. Ongoing progress will continue to be reported.

#### TOUGH Code

In the July monthly report we informed you that our output from running sample problems 3 and 6 on the Sandia NOS operating system compared poorly with the results contained in the draft user's guide. Karsten Pruess of these discrepancies. We have informed In discussions with him, we have resolved our concerns with sample results should have been plotted in mole fractions problem 6. Our instead of mass fractions and effective saturations instead of The fact that mole fractions instead of mass fractions, saturations. which is the TOUGH output, are used in Figure 19 of the draft documentation is not clear in the text but is listed on the y-axis of The use of effective saturation is indicated neither in Figure 19. the text nor on Figure 19 of the draft documentation. Dr. Pruess advised that he would expand the draft documentation to indicate that the mole fractions and effective saturations were used to construct Figure 19. We have revised the figure comparing the output from our TOUGH runs with Figure 19 of the draft documentation to reflect mole fractions and effective saturations and have noted excellent agreement

between the two. The discrepancy involving sample problem 3 has not been resolved as yet.

# INEL Computing System

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Procedures for submitting a batch job during an interactive session and re-dimensioning SWIFT II for larger problems were added to QUAHELP, the on-line help procedure on the INEL computing system. Information on using these features is included as attachments to this report.

PROGRAM:	Code Validati	on and	Verification		FIN# Task	
CONTRACTOR:	Sandia Nation Laboratories	al		BUDGET	PERIOD:	10/85 - 9/86
NMSS PROGRAM	MANAGER:	N. M.	Coleman	BUDG	ET AMOU	NT: \$87K
CONTRACT PRO	GRAM MANAGER:	R. M.	Cranwell	FTS	PHONE:	844-8368
PRINCIPAL IN	VESTIGATORS:		Wilkinson Harlan		PHONE: PHONE:	844-0074 844-8164

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 AUGUST 1986** 

Work continued on the SWIFT II verification/validation effort. We performed a computerized literature search of the DOE, NTIS, and GEOREF databases through DIALOG Information Services. This search yielded a few references to SWIFT II, but none were related to either verification/validation or other lab or field problems.

In addition, we began preparation of a rough draft of the SWIFT II verification/validation report. The planned format is as follows. Any verification/validation problems that have been previously described in literature will be summarized in the report. Any verification/validation problems we found or will find that are not described in the literature will be explained in more detail than those problems found in the literature. Finally, any problems we recommend to complete a SWIFT II verification/validation effort will be explained in detail and cited with the appropriate references. Current plans are to complete a rough draft of the report by September 30, 1986.

-PROGRAM:	Short-term Te	echnical Assistance	e FIN# Task	
CONTRACTOR:	Sandia Nation Laboratories	nal	BUDGET PERIOD:	10/85 - 9/86
NMSS PROGRAM	MANAGER:	N. M. Coleman	BUDGET AMOU	NT: \$39K
CONTRACT PRO	GRAM MANAGER:	R. M. Cranwell	FTS PHONE:	844-8368
PRINCIPAL IN	VESTIGATORS:	G. F. Wilkinson C. P. Harlan	FTS PHONE: FTS PHONE:	844-0074 844-8164
PROJECT OBJE	CTIVE			

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

ACTIVITIES DURING AUGUST 1986

No activity.

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SWIFT II EXECUTION PROCEDURE - BATCH EXAMPLE USING SIISTC1:

(1) CREATE ONE FILE CONTAINING THE FOLLOWING RECORDS. SAVE THE FILE UNDER SOME NAME, FOR EXAMPLE, 'MYJOB'.

> /JOB XYZ. (XYZ is your USERID) /USER CHARGE, 123456789, X. (Enter your charge number) /NOSEQ ATTACH, SWIILGO/UN=CRH. RFL(EC=1000). LDSET, PRESET=0. SWIILGO. /EOR (SIISTC1 DATA SET)

/EOR /EOF

2) HOW TO SUBMIT YOUR BATCH JOB DURING AN INTERACTIVE SESSION:

GET, MYJOB SUBMIT, MYJOB, TO (BATCH SYSTEM RESPONDS WITH 'JSN IS ABCD' ENQUIRE, JSN=ABCD

QGET, ABCD

WHERE ABCD IS YOUR SYSTEM JOB NAME) (TO ENQUIRE ON PROGRESS) (TO PULL OUTPUT INTO YOUR LOCAL AREA AFTER ENQUIRE SHOWS 'WAIT QUEUE')

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- (1) Examine page 5 of output file for a table entitled 'UTILIZATION OF COMMON ARRAY STORAGE'
- (2) Compare current core dimensions with your data requirements for arrays G, G2, G3, and IG.
- (3) Create and save your own binaries with the following interactive control stream:

  - (a) GET, SWIIDIM/UN=CRH(b) BEGIN, SWIIDIM (This procedure prompts you for sizes)
  - (Select a name for binaries, ex, MYLGO) (c) DEFINE, MYLGO
  - (d) COPYBF, LGO, MYLGO (Save your binaries in your area)
  - (e) ROUTE, MYLIST, DC=PR, ST=MOI, UN=NRC, UJN=XYZ. (where XYZ is your userid. WARNING this route is optional and sends a very large compile listing to your printer)
- (4) Use your binary file MYLGO in place of the library binary file SWIILGO.
- (5) The request for extended memory at execution time should be increased to reflect the added memory. An estimate of this number is printed out from the procedure in step (3). As an example, the RFL,0,472 requirements for the QA version of SWIFT II were determined by:
  - G array G2 array G3 array IG array
    - 48000 + 30000 + 58000 + 20000156000 =

472 K Octal

- (6) INEL system limitations:

  - (a) A single common block size is 131071 maximum(b) The total of all four array sizes must not exceed 262144 (1000K octal)

A-1756 1646.010 August 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 
<b>I.</b>	Direct Manpower (man-months of charged effort)	0.4	12.2
II.	Direct Loaded Labor Costs Materials and Services ADP Support (computer) Subcontracts Travel Other (computer roundoff)	3 0 1 24 0 0	125 2 3 149 8 0
	TOTAL COSTS	28	287

III. Funding Status

Prior FY	FY 86 Projected	FY 86 Funds	FY 86 Funding
Carryover	Funding Level	Received to Date	Balance Needed
None	365K	365K	None

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)	4.9	23.2
11.	Direct Loaded Labor Costs Materials and Services ADP Support (computer) Subcontracts Travel Other (computer roundoff)	34 0 2 19 0 1	189 0 14 * 70 1 4
	TOTAL COSTS	56	278

\* Some of these charges are accruals. III. Funding Status

Prior FY	FY 86 Projected	FY 86 Funds	FY 86 Funding
Carryover	Funding Level	Received to Date	Balance Needed
\$150K	\$486K **	\$336K **	- 0 -

\*\* \$70K of these funds were transferred to A-1755 by NRC Form 173 dated April 4, 1986.

A-1158, Task I 0976.010 August 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 
1.	Direct Manpower (man-months of charged effort)		0.0
11.	Direct Loaded Labor Costs Materials and Services ADP Support (computer) Subcontracts Travel Other (computer roundoff)	0 0 0 0 0	0 0 0 0 0
	TOTAL COSTS	0	0

III. Funding Status

Prior FY	FY 86 Projected	FY 86 Funds	FY 86 Funding
Carryover	Funding Level	Received to Date	Balance Needed
None	None	None	None

A-1158, Task II 0976.020 August 1986

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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)	4.0	11.0
II.	Direct Loaded Labor Costs Materials and Services ADP Support (computer) Subcontracts Travel Other (computer roundoff)	28 0 0 6 0 0	90 0 *33 0 1
	TOTAL COSTS	34	124

\* Some of these charges are only accruals.

III. Funding Status

Prior FY	FY 86 Projected	FY 86 Funds	FY 86 Funding
Carryover	Funding Level	Received to Date	Balance Needed

\$115K

A-1158, Task III 0976.030 August 1986

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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)	0.7	9.5
II.	Direct Loaded Labor Costs Materials and Services ADP Support (computer) Subcontracts Travel Other (computer roundoff)	5 0 2 7 0 1	79 0 14 *12 0 3
	TOTAL COSTS	15	108

\* Some of these charges are only accruals.

III. Funding Status

Prior FY	FY 86 Projected	FY 86 Funds	FY 86 Funding
Carryover	Funding Level	Received to Date	Balance Needed

\$175K

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

		Current Month	Year -to- Date 
Ι.	Direct Manpower (man-months of charged effort)	0.2	2.1
II.	Direct Loaded Labor Costs Materials and Services ADP Support (computer) Subcontracts Travel Other (computer roundoff)	1 0 6 0 0	15 0 *25 1 1
	TOTAL COSTS	7	42

\* Some of these charges are accruals.

III. Funding Status

Prior FY	FY 86 Projected	FY 86 Funds	FY 86 Funding
Carryover	Funding Level	Received to Date	Balance Needed

\$87K

A-1158, Task V 0976.050 August 1986

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

		Current Month	Year -to- Date 
1.	Direct Manpower (man-months of charged effort)	0.0	0.6
II.	Direct Loaded Labor Costs Materials and Services ADP Support (computer) Subcontracts Travel Other (computer roundoff)		5 0 0 0 0
	TOTAL COSTS	0	5

III. Funding Status

Prior FY Carryover	FY 86 Projected Funding Level	FY 86 Funds Received to Date	FY 86 Funding Balance Needed

\$39K