

Sandia National Laboratories

Albuquerque, New Mexico 87185

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September 11, 1984

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

WM-RES

WM Record-File <u>A-1166</u> SNL	WM Project <u>10, 11, 16</u> Docket No. _____ PDR <input checked="" type="checkbox"/> LPDR <input checked="" type="checkbox"/> (P, N, S)
Distribution: <u>RCodell</u> <u>PHite</u> (Return to WM, 623-SS)	<u>Joc-Ticket</u> _____

Dear Dr. Codell:

Enclosed is the monthly report for FIN A-1166, Maintenance of Computer Programs, for August 1984. Please call or write if you have any questions or comments.

Sincerely,

Robert M. Cranwell

Robert M. Cranwell, Supervisor
Waste Management Systems
Division 6431

RMC:6431:jm

Enclosure

Copy to:

- Office of the Director, NMSS
- Attn: Program Support
- Robert Browning, Director
- Division of Waste Management
- Malcolm R. Knapp
- 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
- 6431 R. M. Cranwell
- 6431 P. A. Davis
- 6431 G. E. Runkle

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A-1166 PDR

PROGRAM: Maintenance and Validation of Computer Programs FIN#: A-1166

CONTRACTOR: Sandia National Laboratories BUDGET PERIOD: 10/83-9/84

NMSS PROGRAM MANAGER: R. Codell BUDGET AMOUNT: \$130K

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

PRINCIPAL INVESTIGATORS: P. A. Davis FTS PHONF: 846-5421

PROJECT OBJECTIVES

The objective is a maintenance task that will ensure that the Sandia computer programs remain consistent with current operating systems, are as error-free as possible, and have up-to-date documentation for NRC. There is also a validation assessment task to identify real physical situations which could provide data for validation of the Sandia computer program.

ACTIVITIES DURING AUGUST 1984

TOUGH Verification and Validation

The proposed tasks for the preparation of a self-contained document for the TOUGH computer code have been given preliminary approval by K. Pruess and the appropriate LBL management. A copy of these tasks is attached. Funding for all but Task 6 will be provided under FIN A-1158. Task 6, which is to provide assistance in the verification and validation of the TOUGH code, will be funded under FIN A-1166 and is included in the proposed FY 85 189 for this program.

SWIFT II Computer Code

Several problems have been encountered with the SWIFT II computer code causing delays in completion of documentation and quality assurance (QA) efforts for this code. For example, a copy of the code was received from GeoTrans, Inc. on March 27, 1984, and was accompanied by the appropriate GeoTrans QA documentation. However, in our efforts to use the code this past summer, multiple errors were discovered. GeoTrans was informed of these errors and a new version of the code, again accompanied by QA documentation, was sent on August 8, 1984. This new version contained two primary changes, in addition to corrections to the previous errors. These two changes were:

- (1) conversion from top-centered boundary conditions to block-centered boundary conditions
- (2) improved machine independence, making the code more portable from one computer system to another.

However, problems were again encountered with this new version of the code. For example, pressures-at-datum, which for a specified option (ITHRO = 2), are supposed to be a function of the variable density, are, in fact, based on reference densities and not variable densities.

Until an accurate version of SWIFT II can be obtained from GeoTrans, accompanied by accurate documentation, release of the SWIFT II code will be delayed.

PROPOSED TASKS FOR
DEVELOPMENT OF A SELF-CONTAINED CURRICULUM FOR THE TOUGH CODE

TASK 1:

Finalize a version of the TOUGH computer code and document. This version of the code should be similar to the code described in the seminar presented to the Nuclear Regulatory Commission in August, 1983. Additional capabilities should include: a) non-linear material properties, b) a scaling factor to adjust the units, and c) an extended library of capillary functions.

Time Schedule

September 1984 - December 1, 1984 -- Finalize version
December 1984 - January 1985 -- Rework final version
to be consistent with
sample problems
developed

TASK 2:

Assist Argonne Software Center in resolving the proprietary claim to the Harwell Subroutine Library MA28 package. This package is in the TOUGH computer code.

Time Schedule

September 1984 - November 31, 1984

TASK 3:

Develop sample problems for the purpose of illustrating capabilities of the TOUGH code. Provide a variety of problems from simple to complex. Consider problems which are meaningful and relevant to the intended use of the code. Include problems to demonstrate the following: 1) 1-D infiltration problem, 2) 2-D infiltration problem, 3) flow to a geothermal well, 4) radial heat flow problem around a canister for purposes of demonstration of code capability for two-component, two-phase fluid and heat flow, 5) similar to problem 4 only for fractured media, 6) demonstration of code capability for two-component, two-phase fluid and heat flow using 2-D stratigraphy from a real site, and 7) 3-D infiltration and heat problem, if feasible.

Time Schedule

September 1984 - February 28, 1985 -- Complete first four problems,
-- Detailed approach for problems 5 - 7

March 15, 1985 -- Status meeting to discuss problems 5 - 7.

TASK 4:

Draft a self-contained document for the TOUGH code. Include the following topics: 1) physical effects modeled by TOUGH, 2) governing equations, 3) mathematical and numerical methods, 4) architecture of code, 5) preparation of input data, 6) output of code, 7) description of sample problems.

All work performed under this task shall meet the standards of NUREG-0856.

Time Schedule

June 1985 - August 1985

TASK 5:

Revise draft self-contained document incorporating and addressing comments from Sandia National Laboratories and the NRC. Prepare final camera-ready document for publication by the NRC.

Time Schedule

June 1985 - August 1985

TASK 6:

Assist in verification and validation efforts of the TOUGH code. This would include furnishing appropriate analytical problems for purposes of verifying the code and supplying field data, laboratory experiments, etc. for use in validation activities.

NOTE: Tasks 1 - 5 will be funded with a ceiling price of \$80,000 from FIN A-1158.

Task 6 will be funded in FY 85 from FIN A-1166.

Monthly progress reports will be provided to Sandia National Laboratories by the 1st day of the following month.