

APR 23 1984

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MEMORANDUM FOR: Malcolm R. Knapp, Chief  
Geotechnical Branch

FROM: Richard Code11  
Hydrology Section  
Geotechnical Branch

SUBJECT: TOUGH CODE CHECKOUT, OPS PLAN COMMITMENT 5313121

I have developed a plan for performing the requested checkout of the TOUGH code OPS Plan 5313121. The plan at this point is highly tentative and I welcome your comments on it. I hope to make use of both NRC and contractor personnel to accomplish the task.

The NRC people working on the project will be Pete Ornstein, Tim McCartin and myself. Pete and Tim have been running the code for several months. I am just now becoming familiar with it. We plan to have regular meetings to discuss the progress of our experiments with TOUGH. Our discussions will also serve to familiarize us with unsaturated media and serve as a forum to monitor the progress of the contractor work.

Sandia National Laboratories and Lawrence Berkley Laboratory will be undertaking the task of preparing documentation in the form of a self-teaching curriculum under FIN A1158 in late FY 84 and early FY 85. In their pursuit of this task, they will be performing much of the debugging and code testing with test problems. Work on running and checking the TOUGH code will also be performed under A1266 (Research).

We will have input to SNL under these contracts and will be able to direct their choice of problems for the self-teaching curriculum. I expect that we will be able to choose one or several test problems which will partially satisfy the aim of checking out the program for our needs. For a more thorough checkout, I expect to take advantage of A1166 "Maintenance of Computer Programs". The current contract makes no explicit mention of the TOUGH code. As mentioned in the April 13, 1984, memo from Browning to Brown accepting the SNL Proposal for A1166, we will solicit a new proposal from SNL for FY 85 and 86. At this time, we could specifically include TOUGH code validation and verification. I don't think it will be necessary to have any work on TOUGH in FY84, because the work on this code under A1158 will not start until late FY84.

The time table for a thorough verification and validation of TOUGH will be late FY 85 under my proposed plan. The type of work which we hope to see carried out is included in the attached outline, prepared by Pete Ornstein.

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The NRC staff participation will be limited to running the TOUGH code in order to become familiar with it, and its application to unsaturated media so that we can do an effective job of monitoring the three contractor efforts, A1158, A1166 and A1266. Most of the work however will be borne by the contractors. We are also investigating available test problems and field data which would be suitable for the verification and validation.

I feel the approach I have outlined is the most efficient use of the staff's time and of our contractor resources. The original OPS plan date for TOUGH code checkout was July 30, 1984. I propose that by this date, the status of the contract work on the TOUGH code be defined in detail for FY 85 and possibly FY86 and presented in a letter report. The results of the staff's experimentation with TOUGH up to that date will also be reported.

Richard Codell  
Hydrology Section  
Geotechnical Branch

Attachment:  
Draft outline for TOUGH  
Code Evaluation

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PLAN TO DEBUG & EVALUATE TOUGH  
AND PLAN TO ASSESS NRC MODELING NEEDS

TASK

1.0 DEBUG TOUGH

- 1.1 Identify bugs in TOUGH.
- 1.2 Identify source of bugs within code.
- 1.3 Correct bugs by modifying code (if appropriate).
- 1.4 Document bugs along with any corrections made.
- 1.5 Establish a master log along with a procedure to track documentation (1.4).
- 1.6 Repeat 1.1 - 1.4 as new bugs are discovered.

2.0 EVALUATE TOUGH

- 2.1 Review problem sets developed by LBL (under FIN 3109) to compare with NRC unsaturated flow benchmark problems.
- 2.2 Modify problem sets as appropriate.
- 2.3 Execute TOUGH using above data sets.
- 2.4 Document results.
- 2.5 Identify additional problems to test non-isothermal properties of TOUGH.
- 2.6 Develop data sets and execute code.
- 2.7 Document results.

3.0 TOUGH POST-PROCESSOR

- 3.1 Complete development of a post-processor for TOUGH.
- 3.2 Prepare draft documentation for post-processor.

4.0 MODELING NEEDS (UNSATURATED ZONE)

- 4.1 In-depth review of NRC in-house capabilities for modeling groundwater flow and transport (radio-nuclides) through the unsaturated zone.
- 4.2 Recommend additional model development (if appropriate).