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MEMORANDUM FOR: Malcolm R. Knapp, Chief
Geotechnical Branch
Division of Waste Management, NMSS
FROM: Peter Ornstein, Project Manager
Geotechnical Branch
Division of Waste Management
SUBJECT: TRIP REPORT - TOUGH MEETING
NNWSI HYDROLOGY DATA REVIEW

WM-RES

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PDR

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On July 22 - 23, 1984, I met with representatives from SNLA and LBL to discuss documentation of the TOUGH code in Berkeley, California. A detailed report of this meeting is attached.

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Peter Ornstein, Project Manager
Hydrology Section
Geotechnical Branch
Division of Waste Management, NMSS

Enclosure: As stated

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OFFICER	: WMGT	: WMGT	:	:	:	:	:
NAME	: PO	: MFliegel	:	:	:	:	:
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Berkeley Meeting, July 22-23, 1984

On Sunday, July 22, 1984, I met with G. Runkel (SNLA) and D. Updegraff (SNLA-SAI) to clarify our objectives for the following days' meeting with K. Pruess (LBL) on the development of a Self Teaching Curriculum (STC) for TOUGH. The key topics of discussion were the sample problem set that will be used in the STC and keeping the subcontract cost at \$80K. We decided that the sample problem set (discussed below) should have the dual purpose of educating the user as well as establishing the code's veracity through verification, validation, or benchmarking. Since a verification-validation-benchmarking document was planned under FIN A-1166, the two efforts can be combined into the STC. If, due to preparation of the verification-validation-benchmarking problem sets, subcontract costs exceed \$80K, additional money may be available through FIN A-1266.

On Monday, July 23, 1984, we met with Karsten Pruess to discuss the exact form and content of the TOUGH STC. The first item discussed was identifying which version of TOUGH should become the Standard Version. Karsten had made several modifications to the code since NRC had acquired the code in September. These modifications include: 1) inclusion of the "vapor pressure lowering" phenomenon; 2) modifications of computational aspects of the code to enhance its speed and stability; and 3) an increased number of moisture characteristic functions in the code library. Vapor pressure

lowering occurs under high-temperature low moisture conditions and is responsible for the existence of a liquid component even at very high negative matric potentials. The version TOUGH containing this phenomenon is still in the experimental stage and would require substantial development to fully implement. Also, preliminary work by Karsten in this area seems to indicate that vapor pressure lowering is not significant with respect to the overall thermal-hydrologic regime. In light of the questionable value of inclusion of this phenomenon and the developmental work it would require, it will not be incorporated into the Standard Version of TOUGH. The other two modifications will be incorporated since they enhance the useability of the code and require no additional developmental work.

It was also agreed that the Standard Version will be less machine dependent than the present versions and will have a more descriptive output. These modifications are not viewed to be significant.

The proprietary nature of the MA28 subroutine was discussed and Karsten indicated that he had made an unsuccessful effort to find a replacement subroutine. Planned resolution of the proprietary restriction is as follows: For a one time fee of \$3,000 to Harwell, the Argonne Code Center will have unlimited license to distribute the code. Since public availability of the code is in LBL's interest, LBL will pay the fee and not charge it to this contract. This arrangement will allow for public availability of the code solely through the Argonne Code Center. We agreed that the code would not be released to Argonne until it has been verified-validated-benchmarked. It was tentatively decided that there will be seven sample problems.

These problems, ranging from very simple to very complex, are as follows:

<u>Problem</u>	<u>Description</u>	<u>Comments</u>
1	1-D Column Infiltration	Verification problem
2	2-D Infiltration	Benchmark Problem
3	Garg's Problem (Geothermal)	Verification Problem
4	Waste Package Problem	Benchmark Problem
5	Waste Package Problem w/Fractures	
6	2-D Complex Stratigraphy	
7	3-D Problem	

Problems 1-4 were set up and run at the NRC TOUGH seminar last August. Since it is desirable to validate the code, if suitable validation problems are found they will be either added or substituted for problems 5-7. The exact problem set will be finalized by January 31, 1985.

In addition to the sample problems, the STC will contain discussions of physical processes simulated by the code, assumptions inherent in the governing equations, code architecture, input data, and code output. The STC will be consistent with NUREG 0956; "Final Technical Position on Documentation of Computer Codes for High-Level Waste Management." The subcontract between LBL and SNLA will begin on October 1, 1984, and be completed by August 31, 1985. A mid-term status review meeting between NRC, SNLA, and LBL will be scheduled for mid-February and a draft final STC will be submitted for SNLA and NRC review by June 30, 1985. The LBL-SNLA subcontract is expected to be in place in approximately 5 weeks.