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MEMORANDUM FOR: Malcolm R. Knapp
High-level Waste Licensing
Management Branch
Division of Waste Management

FROM: Peter M. Ornstein
Michael F. Weber
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SUBJECT: VARIABLY-SATURATED, NON-ISOTHERMAL FLOW CODE ACQUISTION

Within the next several years, the NRC will conduct performance assessments of groundwater flow and transport from HLW repositories to the accessible environment for variably-saturated, non-isothermal flow systems (e.g. NNWSI). Although the data required to exercise complex numerical flow and transport codes may not be available by the time of licensing, such codes will be used to conceptualize the flow systems, determine important processes, and analyze system sensitivity to hydraulic parameters. These complex codes may also be used to justify simpler approaches to assess radionuclide transport within the unsaturated zone at NNWSI. Our present capabilities are limited to assessing isothermal, 2-D variably-saturated flow systems. The third dimension and non-isothermal treatment will be necessary to analyze the thermal effects of the decaying HLW, and the importance of corresponding data needs, in the immediate vicinity of the repository(ies). Therefore, it is our intent to aquire one or more 3-D non-isothermal variably-saturated flow codes to improve our present capabilities.

We intend to have these codes operational on the BNL system, and be experienced in applying it, by October 1. With these codes, Performance Assessment staff will conduct preliminary sensitivity analyses of processes within the vadose zone to support SCP review and DSCA preparation during the final quarter of 1983. These processes, which are expected to significantly affect repository performance in the vadose zone, should not be oversimplified by applying less sophisticated approaches without justification. Without this assessment, conceptual and numerical models of the flow system are limited to isothermal pre-emplacement conditions.

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Specifically, the processes and flow systems which must be simulated to assess repository performance in the variably-saturated environment include the following:

° Propagation of drying and wetting fronts away from the repository.

° "Wick effect" due to thermal perturbation of the vadose zone which may draw water upwards from the water table through the repository.

° Convection cells within the vadose zone.

° Heat transfer away from the repository due to conduction, advection, and phase changes.

° Formation of perched water lenses within the vadose zone under non-isothermal conditions.

° "Resaturation" of the repository after thermal flux from the repository decreases.

° Steam production and escape to the atmosphere.

The processes listed above cannot presently be modeled with any of the NRC codes. In addition to sensitivity analyses to support SCP review, Performance Assessment will use these codes to perform other appropriate numerical studies during the next several years.

As part of the NNWSI performance assessment program, DOE has been developing several non-isothermal, variably-saturated flow codes. Therefore we believe that it is conceivable for DOE to use results obtained from these codes to support the forthcoming SCP. Even though DOE might not include numerical performance assessments in the SCP, NRC review of the NNWSI site should evaluate DOE suppositions pertaining to post-emplacement groundwater flow in the vadose zone.

For the NRC staff to competently apply these codes in the SCP analysis, several months of experience are required to develop the necessary expertise. Consistent with the time schedule of the SCP release, we suggest that these codes are loaded on the BNL system early this summer. This learning period will allow NRC staff to execute several sample problems, delimit problems in applying the code, and prepare for SCP review of the NNWSI site. The following codes were selected for more detailed review by NRC staff through review of available literature.

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Using general criteria, we have identified two codes, MULKOM and TRACR3D, that meet our needs and are readily obtainable in the short term (3 to 6 months). TARGET and VIP appear to be capable of meeting NRC needs, but because of their proprietory nature, they may not be readily obtainable at reasonable costs, and there may be conflicts with code release to the public sector. The other codes listed do not meet our needs.

Code Name	Dimension	° of Saturation	Documentation	Acquire*
MULKOM (by LBL)	3D	Variable	1/2	9
TRACR3D (by LANL)	3D	Variable	>3/4	5
TARGET (by Dames & Moore)	3D	Variable	>3/4	P
VIP (by Nolen)	3D	Variable	>3/4	P
WAFE (by LANL)	2D	Variable	>3/4	5
Pollock's (by USGS)	2D	Unsaturated	0	0
SAGURO (by SNL/DOE)	2D	Variable	>3/4	5

*Acquire = is an estimate of the ease of obtaining the code on a 0 to 10 scale (10 highest) with P = proprietory.

The cost of obtaining TRACR3D is minimal compared to the potential benefits of obtaining this code. If DOE uses this code for performance assessment of NNWSI, it will be advantageous to the NRC and DOE programs to be able to review and execute this code in house. Furthermore, early review and benchmarking by the NRC may eliminate potential issues the NRC might raise about the application of the code during site licensing procedures. Sandia is in the process of acquiring this code for the NRC. MULKOM appears to be the best and most easily-obtainable code to analyze variably-saturated, non-isothermal flow systems. K. Pruess, the author of both MULKOM and SHAFT79, has informed us that MULKOM is not merely a modified version of SHAFT79, but is dissimilar in both code architecture and equations of state. We recommend that the NRC obtain this code.

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Please use this opportunity to comment on our plans for acquiring the two recommended non-isothermal, variably-saturated flow codes. The program that was suggested at the staff meeting on Friday, March 4, has been revised to expedite the acquisition of such codes. We request your prompt response to this memo so that we may prepare to use these codes for SCP review.

Original Signed By:

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