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

FROM: Peter M. Ornstein
High-Level Waste Licensing Management Branch
Division of Waste Management

SUBJECT: TRIP REPORT

During the week of January 17, 1983, I was in Denver, Colorado to attend the NNWSI pre-SCR hydrology workshop. In addition to attending the workshop, I met with the modeling staff from Dames & Moore's Denver office to discuss Dames & Moore's modeling capabilities and also attended meetings in Tucson, Arizona with NRC contractors from the University of Arizona to discuss the applicability of the U. of A. work to the NRC's role in NNWSI. Summary and highlights of each of these meetings are presented below.

Dames & Moore

On January 17, 1983, I met with Dames & Moore's Advanced Technology Group to discuss Dames & Moore's modeling capabilities and modeling experience in the unsaturated zone. An agenda is attached.

The discussions focused on the TARGET code which is the primary code Dames & Moore employs for saturated/unsaturated simulations. TARGET is an integrated finite difference code which may be used in 1, 2, or 3 dimensions. It is capable of simulating nonisothermal flow through variably saturated (saturated and unsaturated) media and also transport multiple radionuclides with multiple decay chains. The most appealing aspect of TARGET is its high degree of versatility. Any number of physical phenomena (i.e., fluid flow, heat transport, vapor flow, transport) can be coupled and solved either interdependently or sequentially so long as each physical phenomena is mathematically stated in a certain format. For one dimension, this format is

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$$\frac{\partial}{\partial t}\left\{a\phi\right\} + \frac{\partial}{\partial x}\left\{bV\phi\right\} = \frac{\partial}{\partial x}\left\{C\left[D\frac{\partial\phi}{\partial x} + E\frac{\partial\theta}{\partial x}\right]\right\} + d$$

where the variables a, b, c, d, E, ϕ, and θ, are defined according to the respective physical phenomena (see Table 1). Contrary to the apparent complexity of the code, Dames & Moore insists that TARGET is an easy code to use. They also insist that the code is numerically unconditionally stable (i.e., transport through large grid blocks might not need to be restricted).

Several case studies were described where this code was used. In one study TARGET was used to delineate the extent of an ice/water interface around a subsurface liquified gas pipeline. The code simulated the heat transfer, groundwater flow, and ice/water phase change. In West Germany, TARGET was used to predict radionuclide transport through the unsaturated zone from a low level waste disposal site. The transport of 130 radionuclides with 10 to 50 chains for each radionuclide were simulated.

The case studies appear to indicate that TARGET could be applied to Yucca Mountain where nonisothermal multiple phase (air, water, vapor) processes will be important.

The code has been documented, but has not been released to the public since Dames & Moore has retained propriety over it. They appeared interested in contracting with the NRC for the release of the code. Towards that end, Dames & Moore suggested providing us with a comprehensive seminar on the code's capabilities. A full evaluation of the code cannot be made with the amount of information presently available.

NNWSI Hydrology Workshop

The NNWSI hydrology workshop provided a forum for candid discussion between DOE and NRC on the contents of the forthcoming SCP. The USGS, under contract to DOE, initiated the discussions by presenting preliminary results of studies they have been conducting as well as preliminary descriptions of studies being planned. Thus, the workshop provided the NRC with a preview of some SCP contents and enabled the NRC to provide the DOE with immediate feedback. Highlights of the USGS presentations are outlined below.

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The USGS has the lead responsibility of characterizing the Yucca Mountain site and developing a conceptual groundwater flow model. They are performing hydrologic tests on the rock strata and analyses on core samples to establish a conceptual flow model and to obtain parameter values for their computer modeling. The computer models will then be used to refine the conceptual flow and transport models, the results of which will be used by SNL as the basis for subsequent performance assessment analysis.

The computer code being employed by the USGS for the flow model is a code written by R. Cooley (of the USGS). It differs from conventional codes in that it solves for transmissivity values instead of water level values. A potentiometric surface is produced in similar fashion to conventional codes. This code is being used to model a regional area which encompasses the entire Nevada Test Site. A subregional modeling study (i.e., the Yucca Mountain block and vicinity) using this code is being planned.

A code written by J. Tracy (formerly of the USGS), will be used to model transport around the repository and on a subregional scale. The code will incorperate a sensitivity analysis routine to quantify parameter uncertainty. Both the transport and flow codes employ the Finite Element Method and neither code is fully documented.

The computer code CHEMTRN will be used by the USGS to analyze and simulate the Yucca Mountain area hydrogeochemistry. The physical processes simulated by CHEMTRN include:

- precipitation of solids,
- dissociation of water (pH independent),
- advection (1-D steady state),
- diffusion/dispersion,
- dissolution of solids along flow path,
- sorption by ion exchange, and
- sorption by surface ionization-complexation.

The USGS outlined very preliminary plans to characterize the hydrogeologic properties of the unsaturated rock strata of the repository block. These plans include:

2 shallow boreholes (UZ 4 and 5)
 ° Estimate flux in the upper clastic unit
 ° 300 feet deep

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- One in center of Drillhole Wash
- One at margin of Drillhole Wash

3 deep boreholes (UZ 1, 2, and 3)
- To determine:
  - vertical permeability to air
  - horizontal permeability to air and water
  - tortuosity
- Array of air piezometers in UZ 1
- Gas samples for fluorocarbon analysis
- Injection tests (air or nitrogen, trace gases, water) (UZ 2 and 3 only)

Exploratory Shaft
- Bulk permeability tests
  - determine fracture interconnectivity and conductivity
- Packer injection tests (air)
  - determine pressure/permeability relationships under various saturation conditions
- Hydrologic infiltration tests
  - determine water transport rates under controlled conditions
- Vertical borehole into lower clastic unit
  - determine hydrologic properties and evaluate possible perching of groundwater
- Laboratory analysis of water samples
- Analysis of blocks obtained during excavation
  - evalute effects of fractures on a controlled volume

The Performance Assessment for NNWSI will be performed by SNL. A definitive choice of computer codes does not appear to have been made. The codes listed for possible use are as follows: NWFT, WAPPA, ARRAYF, UNSAT, GETOUT, TOSPAC, SAGUARO, TRACR3D, FEMWATER, FEMWASTE, VTT, SWENT, TRUST, MMT, and other analytical solution codes developed at U.C.B. Since the base case flow path will be defined by the USGS, the performance assessment will be limited to consequence analyses of scenarios affecting the flow path.

University of Arizona

At the University of Arizona, T. Verma, J.Pohle, and I met with S. Neuman and D. Evans (U. of A.) to discuss the NRC's impression of the NNWSI workshop. Specific topics discussed included the USGS plans for modeling and characterizing the unsaturated zone. It appears that the work being performed for the NRC by the U. of A. is similar to the work planned by the USGS. Similarities include some of the characterization techniques for unsaturated and fractured rock parameters. The USGS effort will be on a larger scale than the U. of A. effort, and is likely to employ techniques and equipment developed under the NRC's U. of A. contract.

Very little progress had been made along on Phase II of the U. of A. research since their presentation on Phase I in Silver Spring last November. This was attributed to contractual problems at the NRC which has subsequently been worked out.

Discussions with Dr. S. Neuman also focused on NRC's interest in obtaining a non-isothermal flow code for the unsaturated zone. Dr.Newman was not familiar with several of the codes the NRC was considering.

Also, the U. of A. was interested in providing the NRC with technical advice during NRC's review of the NNWSI SCP. This work would be a natural extension of the work already being provided to the NRC by the U. of A. in understanding flow through unsaturated fractured media, and would be similar to the technical assistance provided to the NRC on the BWIP SCR by other contractors. Details of the proposed technical assistance will be worked out at a later date.

ORIGINAL SIGNED BY
Peter M. Ornstein
High-Level Waste Licensing
Management Branch
Division of Waste Management

Enclosure:
As stated

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TABLE I

TERMS USED IN THE FORMULATION OF THE GOVERNING EQUATIONS OF FLOW AND TRANSPORT

Symbols in Basic Equation	Terms in Variably Saturated Flow Equation	Terms in Saturated Flow Equation (in terms of pressure head)	Terms in Saturated Flow Equation (in terms of total head)	Terms in Mass Transport Equation
Φ	ψ	ψ	$(h={}^{h}\psi+z)$	c^{1}
a	$S_r S_c$	S_c	S_c	$Rn+R_s(1-n)\frac{c_s^{1}}{c^{1}}$
b	0	0	0	Rn
c	$K_r K_{ij} RM$	$K_{ij} RM$	$K_{ij} RM$	Rn
D	1	1	1	D_{ij}
E	—	—	(R-1)	—
θ	—	—	z	—
d	$\frac{\partial}{\partial x_i}\{K_r K_{ij} R^2 M \frac{\partial z}{\partial xj}\} - Rn\frac{\partial S_r}{\partial t} + \frac{\dot{m}'''}{\rho_o}$	$\frac{\partial}{\partial x_i}\{K_{ij} R^2 M \frac{\partial z}{\partial xj}\} + \frac{\dot{m}'''}{\rho_o}$	$\frac{\dot{m}'''}{\rho_o}$	$\frac{\dot{m}'''}{\rho_o}[c_o - c]$

(From Sharma, 1981. Refer to NUREG/CP-0030, P. 188)

SUBJECT: Informal discussions with U.S. N.R.C. staff on mathematical models of fluid dynamics, heat transfer and mass transfer in variably-saturated porous media.

LOCATION: Dames & Moore office, Denver, Colorado

DATE: Monday, January 17, 1983

Time: 10:AM

AGENDA

1. Introductions:
   - NRC staff;
   - Dames & Moore staff

2. NRC Goals regarding mathematical models.

3. Dames & Moore Approach:
   - Mathematical model framework;
   - Coupled flow and heat transfer;
   - Mass transfer;
   - Applications to projects.

4. Discussions

5. Further actions