3109.2/MFW/83/09/08/0

SEP 8 1983

Distribution:
WM file: 3109.2
WMHL r/f
NMSS r/f
REBrowning
MJBell
DJFehringer
MFWeber & r/f
HJMiller
JOBunting
PSJustus
JTGreeves
PDR

WM Record File 109.2

WM Project 1
Docket No.
PDR ✓
LPDR
Distribution:

(Return to WM, 623-SS)

MEMORANDUM FOR: M. J. Wise
High-Level Waste Licensing
Management Branch
Division of Waste Management

FROM: Michael F. Weber
High-Level Waste Licensing
Management Branch
Division of Waste Management

SUBJECT: REVIEW OF THE NWFT/DVM VERIFICATION REPORT

As requested by your memo of August 22, 1983, I have reviewed the subject document and am fowarding to you my comments. In my opinion, this report lacks some of the information that would be necessary to completely verify a computer code. In Section V, which I was specifically requested to review, the reader is refered to the preceding problems in the Verification report and the Users Manual for NWFT/DVM for the information that is vital to the verification effort. Many of my specific comments suggest information gaps in the report as written. To improve the value and technical credibility of the document, I suggest including this information.

The report also uses the term "verification" in a context that is slightly different than that presently used by the NRC staff (see NUREG-0856, NUREG-0960, and the Meeting Notes for the BWIP/NRC Performance Assessment Workshop of August 28-September 1, 1983). In a paraphrased definition, verification of a computer code attempts to determine whether the code correctly solves the governing equations upon which the code is based. Absolute verification should consist of the comparison of the exact solution to an analytical problem with the results of the same problem that are obtained by using the computer code. Problem Four of the verification report would be more appropriately refered to as a benchmarking problem, because an exact solution (closed form) to the problem does not currently exist. In the verification report the results of the NWFT/DVM model are compared to the results of a more complicated model of a similar problem. The more complicated problem was solved by using SWIFT. Benchmarking may be the only method of checking a codes accuracy in solving the governing equations, particularly in systems for which an exact solution is not currently available. Whenever benchmarking is substituted for absolute verification, therefore, the substitution should be explicitly stated and

OFC	:WMHL					
NAME	:MFWeber					
DATE	:09/ /83					

justified. My specific comments on the verification report are as follows:

Abstract

1. Comparisons on the output of computer codes do not constitute absolute verification problems and are not as rigorous as comparisons with exact solutions.

Chapter 1

1. Paragraph 1: Review of the Users Manual for the NWFT/DVM code indicates that the SWIFT code does not provide boundary conditions for the groundwater flow model used within NWFT/DVM (see Sample Problem No. 1 of the NWFT/DVM Users Manual). The concluding sentence of the first paragraph may be misleading to the readers who are not familiar with the Users Manual.

2. Paragraph 2: Where does migration begin within leg 13 of the framework? Does it begin at the upstream end of the leg, or in the middle of the leg, or at the downstream end of the leg?

3. Paragraph 3: Verification and validation do not assure the correctness of computed results. If the results of verification and validation tests are favorable, the correctness of the computed results in similar problems is supported but not absolute. The correctness (validity and accuracy) of computed results will always be subject to technical review on a model-specific basis, and cannot be generally assumed.

4. Paragraph 3: The question of whether or not code benchmarking is an alternative to or should be included in the rigorous verification of a code has not been resolved (see introductory remarks of this memo).

5. Paragraph 3: The report by Ward et al. (1983) does not validate SWIFT. The report does indicate that SWIFT has been verified for various groundwater flow and heat transport problems through porous media.

6. Paragraph 3: Producing comparable results is not necessarily a <u>strong</u> test of a code's ability to correctly simulate contaminant transport problems. The benchmarking of a computer code is one technique which can be used to build consensus within the technical community that

OFC	:WMHL	:	:	:	:	:	:
NAME	:MFWeber	:	:	:	:	:	:
DATE	:09/ /83	:	:	:	:	:	:

the results of a code are at least as accurate as the results of the code which is being benchmarked against.

7. Paragraph 3: I would add the comment that along any flow segment advection and dispersion of the contaminants are unidirectional.

8. Paragraph 3: This section does not justify the use of the multi-dimensional model to establish boundary/initial conditions for the unidirectioal transport model embodied in NWFT/DVM. Furthermore, the rationale behind the comparison of results from NWFT/DVM and SWIFT needs to be explicitly discussed.

9. Paragraph 4: The last sentence is ambiguous and not justified in Chapter V. How does the comparison of the results from NWFT/DVM and SWIFT test the solubility-limited source model? How are source models in these two codes similar and different? Are there any reasons to expect that the source models will behave differently?

10. Is there a reference for Figure 1-1?

<u>Chapter V</u>

1. Paragraph 1: Why was a 13.5 inch borehole selected for this scenario? I recommend the substitution of the word "borehole" for "feature" in the second sentence. The inclusion of a diagram of the sceanrio would help to familiarize the reader with the physical framework of the system.

2. Paragraph 2: The last sentence is too weak as presently written. I recommend deleting it or expanding the discussion to justify the use of two retardation factors.

3. Paragraph 2: The reader needs the input and output from the SWIFT model of this problem before the two sets of results can be adequately compared. Why was the SWIFT code chosen for the comparison?

4. Paragraph 3: Why are different retardation factors used in the model? Do they correspond to the sorptive characteristics of different rock types? What are the rock types? Why is K_d set to zero for all radionuclides in legs 13 and 12?

5. Paragraph 4: If the borehole is simulated by legs 10 and 12, and flow from the repository is forced upward based on the imposed hydraulic

OFC :WMHL	:	:	:	:	:	:
NAME :MFWeber	:	:	:	:	:	:
DATE :09/ /83	:	:	:	:	:	:

gradients, why are the radionuclides transported down into the lower aquifer (i.e. down leg 12) rather than up leg 10? How is this flow path consistent with the description of the problem? The text should explain why leg 12 is entered as a negative integer in the flow path.

6. Paragraph 4: The author should explicitly demonstrate how the space and time steps, which are chosen by the code, are consistent with the numerical criteria for the NWFT/DVM code.

7. Paragraph 4: What is the significance of the last sentence to the "verification" of the code?

8. Paragraph 4: Other important input parameters (e.g., dispersivity, brine concentration, cross-sectional areas, etc.) are not described in the input specifications section. They should be included for completeness of the problem description, especially for readers who are not familiar with the input structure of the NWFT/DVM code.

9. Paragraph 5: Comparison of the results of the NWFT/DVM and SWIFT models of this problem does not verify the NWFT/DVM code.

10. Paragraph 5: How does the execution of this problem with NWFT/DVM and comparison of the results with SWIFT results verify the solubility source model of NWFT/DVM? How are the two source models different? How are they similar? Does SWIFT account for speciation and complexation phenomena that may affect solubilities?

11. Paragraph 5: In addition to supplying the reader with a graphical comparison of the output from the NWFT/DVM and SWIFT models, tabular output should be provided for comparison of the actual numerical output. This would allow the reader to calculate the difference between the two models (e.g., RMS, % difference, etc.) and determine the precision of the computed results. If acceptance criteria are proposed in the future of the code verification/validation/benchmarking program, tabular results could be evaluated directly.

12. Paragraph 5: What features of the NWFT/DVM code does this benchmarking problem test? Why was the problem executed? Would the reader be justified in concluding that NWFT/DVM performs equally as well on diffusion dominated transport systems? Or does this problem only evaluate the code's capability to accurately simulate convection/dispersion dominated systems.

OFC	WMHL					
NAME	MFWeber					
DATE	09/ /83					

13. Should there be a reference for Figure 5-1?

14. Table 5-3: The text should explain how the solubility limits of the radionuclides were determined. The discussion should justify why a solubility of 10.0 g/g is used for Cm246.

15. REFERENCES: The cited references are not in alphabetical order, do not need to be numbered, and do not use standard abbreviations for the referenced publications. I recommend alphabetizing the references, deleting their numbers, and using the full (i.e. unabbreviated) name of the cited reference.

I appreciate the opportunity to review the draft of the NWFT/DVM verification report. If you need additional assistance in clarifying my comments, I would be happy to meet with you at your convenience.

Original Signed By:

Michael F. Weber
High-Level Waste Licensing
Management Branch
Division of Waste Management

OFC :WMHL MW	:	:	:	:	:	:
NAME :MFWeber	:	:	:	:	:	:
DATE :09/8/83	:	:	:	:	:	: