426.1/MJW/83/11/29/0

11/7/83

- 1 -

Distribution
WM s/f
WMRP r/f
NMSS r/f
CF
REBrowning
JOBunting
MJBell
MRKnapp
PSJustus
JTGreeves
PAltomare
HJMiller
LBHigginbotham
RRBoyle
MJWise & r/f
MWeber
POrnstein
MGordon
TMcCartin (RES)
PDR
LPDR (B, N, S)

File #426.1 (A1166
WM - 10, 11, 16

Dr. Nestor Ortiz
Sandia National Laboratories
Division 6431
P.O. Box 5800
Albuquerque, NM 87185

Subject: Response to October Progress Report (FIN A1166)

Dear Dr. Ortiz:

I have reviewed the October progress report and your attached responses to NRC comments on the SWIFT verification report. All responses are acceptable. As we discussed on November 14, the due date for the camera-ready copy of the SWIFT verification report is February 1, 1984.

NRC comments on the draft NWFT/DVM verification report are attached. Please provide your written responses to these comments by January 13, 1984.

The action taken by this letter is considered to be within the scope of the current contract SOEW 50-82-26. No changes to costs or delivery of contracted products are authorized. Please notify me immediately if you believe this letter would result in changes to costs or delivery of contracted products.

Sincerely,

M. J. Wise
Repository Projects Branch
Division of Waste Management

Enclosure:
As stated

cc: W. Snyder, SNL

	:WMRP:ejc	:WMRP	:WMRP	:	:	:
E	:MJWise	:RRBoyle	:HJMiller	:	:	:
E	:12/7/83	:12/ /83	:11/7/83	:	:	: : :

General Comments

1. It would be useful to present the input and output of both NWFT/DVM and SWIFT when the results of the two are compared.

2. Although the space and time steps are given for each problem, it is not clear why some are chosen by the user and others are set by the code. Please explain.

Abstract

1. Second sentence - Please reword to reflect our earlier discussions about the purpose of this report. That is, NRC supports this work to ensure that the codes are as error-free as possible, etc. (Also, a reference to "independent testing" may be misconstrued - please delete.)

2. The abstract should be more general, and references to INTRACOIN and SWIFT should be deleted.

Introduction

1. First paragraph, last sentence - This sentence is confusing. Rather than describing SWIFT as a "more general transport code," wouldn't it be more appropriate to say a "more complex flow code?" (Also, please provide a reference for the SWIFT code.)

2. Second paragraph, last sentence - Where, in leg 13, does migration begin?

3. Third paragraph, first sentence - See comment 1, Abstract.

4. Third paragraph, third sentence - Consider rewording as follows: "...necessary to simulate the system are correctly solved."

5. Third paragraph, third from last sentence - Consider replacing "validated" with "verified for a particular class of problems."

6. Third paragraph, second from last sentence - Is it not possible (or practical) to simulate a 1-D validation problem?

7. Paragraph 3 - Please include 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 unidirectional 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?

Chapter 2 (Problem 1)

1. Page 5, last paragraph - Please state where migration begins.

2. Page 6-7 - Please explain how a retardation of 9353 was calculated with a Kd of 7.793.

3. Page 7, DVM card - Why is the repository length 1.00E5 feet? Is this significant? The time and space steps given in Table 2-4 are not used as input on the DVM card. Were these values calculated by the code?

Chapter 3 (Problem 2)

1. Page 11, second sentence - This sentence is confusing.

2. Page 11, Results Section - Why are the results of the NWFT/DVM run compared with SWIFT results rather than the analytical solution?

3. Page 19, Table 3-8 - What percentage difference is allowed for good agreement? In particular, the Cmax values for the first case are not very close.

4. Pages 20-23 - These figures would be much more helpful if both the NWFT/DVM and SWIFT breakthrough curves were shown.

Chapter 4 (Problem 3)

1. Page 25 - Please explain the significance of two retardation sets.

2. Page 25, last paragraph - Please discuss the analytical solution in greater detail.

3. Page 27 - No Kds are shown for legs 13 and 10.

Chapter 5 (Problem 4)

1. Paragraph 1 - Why was a 13.5 inch borehole selected for this scenario? The inclusion of a diagram of the scenario would help to familiarize the reader with the physical framework of the system.

2. Paragraph 3 - If the borehole is simulated by legs 10 and 12, and flow from the repository is forced upward based on the imposed hydraulic 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?

3. Paragraph 3 - 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.

4. Paragraph 3 - What is the significance of the last sentence to the "verification" of the code?

5. Paragraph 3 - 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 from readers who are not familiar with the input structure of the NWFT/DVM code.

6. Paragraph 4 - 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 similiar? Does SWIFT account for speciation and complexation phenomena that may affect solubilities?

7. Paragraph 4 - 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 closeness 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.

8. Paragraph 4 - 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.

9. Should there be a reference for Figure 5-11?