Sandia National Laboratories

Albuquerque, New Mexico 87185

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Distribution:

MJWise

November 15, 1983

Ms. M. J. Wise
Repository Projects Branch
Division of Waste Management
U.S. Nuclear Regulatory Commission
7915 Eastern Avenue
Silver Spring, MD 20910

Dear Ms. Wise:

Enclosed is the monthly report for FIN A-1166, Maintenance of Computer Programs, for October 1983.

Please call or write if you have any questions or comments.

Sincerely,

Nestor E. Ortiz

Nestor R. Ortiz, Supervisor
Waste Management System
Division 6431

NRO:6431:jm

Enclosure

Copy to:
Office of the Director, NMSS
Attn: Program Support
Robert Browning, Director
Division of Waste Management
Daniel Fehringer
Division of Waste Management
Cal Belote
Division of Risk Analysis
John Randall
Health Siting & Waste Management Division
3151 W. L. Garner
6431 N. R. Ortiz
6431 P. A. Davis

PROGRAM:	Maintenance and Validation of Computer Programs	FIN#:	A-1166
CONTRACTOR:	Sandia National Laboratories	BUDGET PERIOD:	10/83 - 9/84
NMSS PROGRAM MANAGER:	M. J. Wise	BUDGET AMOUNT:	$130K
CONTRACT PROGRAM MANAGER:	N. R. Ortiz	FTS PHONE:	844-5644
PRINCIPAL INVESTIGATORS:	P. A. Davis	FTS PHONE:	846-5421

PROJECT OBJECTIVES

The objective is a maintenance task that will ensure that the Sandia computer programs remain consistent with current operating systems, are as error-free as possible, and have up-to-date documentation for NRC. There is also a validation assessment task to identify real physical situations which could provide data for validation of the Sandia computer program.

ACTIVITIES DURING OCTOBER 1983

Responses to the review comments on the verification and validation report were formulated. On October 10, Mark Reeves, Nestor Ortiz and Paul Davis met to discuss the responses and resolve differences of opinion on what several of the responses should be. The final set of responses were discussed and then forwarded to M. J. Wise. A copy of these responses is included with this monthly report. A final report will be sent to NRC in February, 1984.

Response to Para. 2, Letter from M. J. Wise to Paul A. Davis:

We agree that the report should be published as a NUREG. However, we do not favor joint publication with NWFT/DVM verification/validation results. The codes are too dissimilar to fit together easily. However, the NWFT/DVM document will reference the SWIFT document.

Response to General Comments (M. J. Wise):

1) Agree - Reference to NUREG-0856 will be included. However, we feel that the document basically is already consistent with NUREG-0856.

2) Explanation - We shall report our code maintenance to M. J. Wise under separate cover.

3) Explanation - A review of the use of the words "model" and "code" will be made and the text will be revised accordingly. If a model is viewed as a mathematical formulation to simulate natural hydrologic processes or systems, then SWIFT is both a model and a code. A strong sentiment was expressed within the Sandia review, however, that the term "model" should be applied only to a particular site or problem, e.g., "a model of the Hanford site." In this case SWIFT would be a code only. Both views appear to be consistent with NUREG-0856. Mr. Silling's views on this matter would be helpful.

4) Agree - Reference to SWIFT II will be removed. Presently a separate document for SWIFT II is planned for the future. At the time of the draft it was thought that one document would suffice for both codes and would avoid duplication.

5) Agree - The computer-drawn figures were obtained from a "rough" hard-copy unit to avoid unnecessary expense. Final figures will be drawn on high quality vellum by a Versatec plotter.

6) Explanation - The proper name is SWIFT although we may, from time to time, refer to it informally as SWIFT I to distinguish it clearly from SWIFT II.

Response to Specific Comments (M. J. Wise):

1) Agree - Title page will be revised to reflect correct NRC division and office names.

2) Explanation - SWIFT, we believe, is uniquely suited for assessment of repository design performance because of the strong coupling of flow, heat and brine which is present in the model. Of course, it would have to be used in conjunction with waste-package and rock-mechanics models. We feel, however, that it would be inappropriate to expand upon this point in the document and will eliminate the sentence in question.

3) Explanation - Solute transport is a special case of radionuclide transport, namely one specie without decay. To clarify, we shall state: "radionuclide, or solute, transport."

4) Explanation - The introduction will be changed extensively to reflect the deletion of SWIFT II and to add definition of crucial terms and discussion. The criticisms of flow and awkwardness will be removed at that time.

5) Explanation - The radiation submodel permits a radiation boundary condition to be prescribed at, say, the ground surface in order that the heat generated by the repository may be transferred to the atmosphere. This explanation along with an explanation of other submodels will be included in the text.

6) Agree - Footnote will mention Appendix N.

7) Agree - Reference to Benchmark Problem 3.1 in NUREG/CR-3097 will be included.

8) Explanation - There should be no reference.

9) Agree - Wording will be changed to read: ". . . boundary/initial conditions on drawdowns and flow rate Q are:". Other such changes will also be included as indicated by review of the document. However, we do not want to include a comprehensive list of symbols within each problem. We feel that such would detract from the clarity of the document and would add unnecessary bulk to the document.

10) Agree - Mention of the Theis solution will be included and the appropriate expression for W(u) will be given. However, we shall use the more general exponential integral rather than the approximate series expansion.

11) Agree - The order of the sections on assumptions and analytical solution will be inverted throughout the document.

12) Explanation - Parameters such as pipe roughness and heat transfer coefficients are not necessary since the well-bore submodel is not invoked. The well index is only necessary to calculate well bottom-hole pressure from the average grid-block pressure at the injection well and the bottom-hole pressure is not subject to verification in this problem. Thus the well index for a specified pumping rate is unnecessary. The well index is necessary, however, for Problem 2.2 and is given on p. 2-17.

13) Disagree - The comparison here is with the Theis solution, not the Carter-Tracy method. As stated ". . . the effects of this approximate condition [Carter-Tracy] should be negligible." Also, the Carter-Tracy method is somewhat complicated, and thus its presentation here would detract from the principal objective. A reference both to the SWIFT II Theory and Implementation Document and to the original Carter-Tracy paper will be included for the sake of the energetic reader.

14) Agree - Clarification of boundary conditions for the Cartesian grid will be included.

15) Agree - The dependent variable is missing from one side of the equation due to a typographical error.

16) Agree - See response to Specific Comment 6.

17) Explanation - Figure 2-5 should not have a reference because it represents general hydrogeological information.

18) Explanation - We prefer to modify the sentence here to read: ". . . flow rate G() is tabulated . . . and is generated herein using the algorithm supplied by Reed [1980]."

19) Agree partially - Discussion of well index will be expanded. We feel, however, that no more can be done for the Carter-Tracy condition other than to reference the Theory and Implementation Document and the original paper.

20) Explanation - Page 2-20 is intentionally blank so that new sections will start on an odd number, thus positioning text on the right as report is opened. The same comment applies for pp. 4-20 and N-8.

21) Agree - Reference to Benchmark Problem 3.3 in NUREG/CR-3097 will be included.

22) Explanation - Coordinate axes are aligned with principal axes of transmissivity tensor (see top of p. 2-22).

23) Agree - The assumption of a principal-axis transformation will be placed before Equation (2-14).

24) Agree - See response to Specific Comment 11.

25) Agree - Brackets will be included around the transmissivity.

26) Explanation - The solution for this equation is invariant to a simple rotation of the coordiate system.

27) Agree - Sentence will be removed.

28) Agree - Text will be changed.

29) Explanation - Firstly, the cone of depression for an anisotropic aquifer will be elliptical, thus requiring a larger domain in the direction of the major axis, namely the x-direction. Secondly, on purely physical grounds, the cone of the depression should have the dimensions of the right-hand sides of inequalities (2-19). Thus, the x-dimension of the cone of depression is significantly less than 65 km. Finally, a Cartesian grid is chosen, rather than a radial grid, since the problem does not have radial symmetry. This explanation will be included within the text.

30) Agree - Reference to Benchmark Problem 3.2 in NUREG/CR-3097 will be included.

31) Explanation - Second bullet will be clarified to read "coupling of vertical flow through an aquitard with horizontal flow in an aquifer."

32) Explanation - Reference is not necessary for Figure 2-10.

33) Agree - See response to Specific Comment 11.

34) Explanation - See response to Specific Comment 12.

35) Agree - However, this problem does test a different section of the code than does the radionuclide transport.

36) Agree - Initial and boundary temperatures will be presented in text (in addition to computer input/output on microfiche).

37) Explanation - The difference in length scales for Problems 3.1 and 3.2 arises from the different retarded velocities in each case. Retardation within the fluid; results from the heat capacity of the rock. For the two linear cases, the movement of the front is given, approximately, by $x = vt$ where x is the distance traveled, v is the retarded interstitial velocity and t is the time. For the radial case the retarded velocity varies inversely as the radius r, i.e., $v \sim v_o/r$. In this case the approximate formula is $r^2 = 2v_o t$. In both cases the numerical grid is taken sufficiently large to contain the fronts and their smearing due to conduction. This explanation will appear within the text.

38) Agree - Reference to Ros et al. will be included.

39) Agree - Legend is to be revised.

40) Disagree - Limitations due to numerical criteria are treated by the Theory and Implementation Document and by the SWIFT Self-Teaching Curriculum. In Problems 4.1, 4.2 and 7.1 the time scales are controlled by problem specifications or by the field data - not by numerical criteria. Also numerical limitations are highly problem dependent. A few tens of decades for the near-surface aquifer surrounding the Babylon landfill, where the interstitial velocity is approximately 1 ft/da could, perhaps, correspond to a few tens of millennia at a high-level nuclear waste site, which has been specially selected for small fluid velocities. Thus, this report does not provide a proper basis from which to comment upon the limitations of the numerical criteria. We shall attempt to provdie some clarifying remarks either in the problem discussion or in the introduction.

Disagree - It is not necessary to restrict SWIFT to far-field applications since it is also useful to assess repository-design performance.

Response to Specific Comments (S. A. Silling)

1) Explanation - The present use of the term "verification," as indicated on page ii, is consistent with NUREG-0856. Verification as defined by NUREG-0856 assures that a "computer code correctly performs operations specified in a numerical model." One of the best ways to assure correctness is to compare with known analytical solutions. Thus Problems 2, 3, and 4 were chosen.

We believe that the term "validation" should be reserved strictly for those comparisons between simulated results and field (or, perhaps, laboratory) measurements which would involve only minor parameter adjustments. This rarely is the case in simulating geohydrologic systems. Therefore, we propose that the term "field application" be substituted for the term "validation."

2) Agree - The present text will be restricted to SWIFT only. At the time of writing the draft, it was our thought that both SWIFT and SWIFT II could be included in the same report to avoid duplication. The executive summary and introduction will be revised. The sections entitled "Models Used" will also be revised.

3) Explanation - Two issues are apparently raised here. The first one concerns the Sandia Verification/Validation Project and the document under review, and the second concerns the Teknekron/GeoTrans Benchmarking Project. Relative to the first, the reviewer notes that several of the problems chosen for verification of SWIFT are also benchmarking problems. To be exact, 5 of the 11 problems were taken from the benchmarking document of Ross, et al. [1982]. It is our opinion that these benchmarking problems, as well as other standardized problem sets, e.g., INTRACOIN AND HYDROCOIN, should be used as widely as possible to facilitate the assessment of repository siting codes.

Relative to the second issue, the reviewer notes that two of the authors work for GeoTrans, which might raise the perception of SWIFT having an unfair advantage in the benchmarking study. Such a perception, we feel, is incorrect. The two authors in questions joined GeoTrans in October 1982 and December 1982. As such, they had no input at all to the Benchmarking Document, which was completed in November 1982. In our opinion, the benchmarking study should not be perceived as a competitive event. We see it as a exercise by NRC in providing some necessary quality assurance for codes which are, or potentially may be, used in the licensing process.

4) Agree - Additional details concerning the GeoTrans QA program will be added.

5) Agree - The wording referred to by the reviewer will be made more specific.

6) Agree - The brine equation has been verified for first and third type boundary conditions and compared to the analytical results of Problem 3.1. The subroutines ITER and ITERC do yield virtually identical results. Inadvertently, we omitted this problem from the report. We shall clarify our wording on this point. Direct verification of the nonlinear density aspects of the code is planned for a later document, perhaps for the verification of SWIFT II.

7) Agree partially - I note the Berg and McGregor [1966], Elementary Partial Differential Equations uses the "type 1", "type 2", and "type 3" designations for boundary conditions. However, we shall include some clarifying terminology.

8) Disagree - Equation (4-5) is a transformation which factors out the decay-production components. The resulting differential equation for $\theta(3)$ is exactly the partial differential equation of Coats and Smith [1964]. We will try to clarify this point.

9) Explanation - The term "infinite leach" in this context implies an infinite inventory, as is necessary to produce the boundary condition in Equation (4-3c). This explanation will be included in the text.

10a) Explanation - The grid is nonuniform with 20 @ 8.2, 3 @ 5.47 and 9 @ 8.2 ft. We shall state this in the text.

10b) Explanation - The source is in grid-block 1. We cannot impose this source precisely upon the boundary, as is done in the analytic solution, c.f., Equation (4-3c). However, since the source-block width is much less than the observation length, this is an acceptable approximation. There is no upstream diffusion from the source in the numerical solution, and this fact is consistent with the analytical solution with which we are comparing. This explanation will be included in the text.

10c) Explanation - Beyond 640 years, the concentration gradient within the system dissipates. The concentration for all components at 1123 years is virtually uniform (less than 3% variation from source to breakthrough point). In the absence of sharp concentration gradients, overshoot does not appear in the solution since the convection term causing the overshoot disappears. This, of course, would be expected due to the controlling complementary error function, erfc ((x-vt)...). This explanation will be included in the text.

11) Agree - Legend will include a solid line representing the analytical solution.

12) Explanation - For flow through a constant-pressure boundary, SWIFT assumes convective radionuclide transport, i.e., a concentration gradient of zero.

13) Explanation - A well is not used at the observation point. Neither fluid nor contaminant is removed from the system. Thus no boundary condition or sink term is involved.

14) Explanation - The factor results from the second-order CIT criterion, in which the term $(1 + 2\alpha/\Delta x) = 11$ arises. A note of explanation will be added to the text.

15) Disagree - We stand by the statement in the text (Section 4.2.9, second sentence). All curves in Figure 4-4 <u>do</u> have approximately the same shape except that the breakthrough curve for U-230 is shifted <u>horizontally</u> toward lower values of time due to its lower value of retardation (see Table 4-4 for retardations). Note also, from the half lives in Table 4-7 that the condition for secular equilibrium holds more strongly for Th and Ra than for U and Th. We shall expand the discussion in the text.

16a) Explanation - Source data on location and time of use of the various piles comes from historical records. See Sentences 2 and 3, top of Page 7-2 and references cited on the previous page. Source concentrations were inferred.

16b) Explanation - The distance coordinate in Figures 7-10a, b is along the y-axis. We shall so state on these figures.

16c) Explanation - Dilution by recharge and effects of recharge on the flow field are assumed to be neglibible due to a relatively large saturated thickness and a relatively high ground-water velocity. We shall clarify this point in the text.

16d) Explanation - Trial-and-error was used to refine the source-concentration data.

17) Explanation - The SWIFT profile at Well 11 does go down with increasing time. For the deepest Sampling Stations C the observed data also decreases. Although measuring very close to background concentrations, Stations A and B increase with time and differ from the SWIFT results. One possible explanation is the presence of a near-surface source for the chloride ion.

Well 11 is located near a street where salting would occur during the winter months. Another possible explanation is the fact that Well 11 is located near the outer periphery of the plume, which we found to be quite sensitive to the geometric details of the source. Possibly there are other explanations.

18) Explanation - The vertical details of the source should have very little effect on the plume beyond 5-10 dispersion lengths down dip, which is the region in which we are making the comparisons. We shall include this explanation within the text.

19) Agree - We shall include some tic marks on the figures to indicate the SWIFT gridding.