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July 4, 1984

Dr. Malcolm R. Knapp
Division of Waste Management
U. S. Nuclear Regulatory Commission
Washington, DC 20555

Dear Dr. Knapp:

Thank you for the opportunity to review the draft report "Benchmarking of Flow and Transport Codes for Licensing Assistance," Volumes I and II, by CorSTAR. My comments are given below.

1. My main concern is that in its present form this report may not be as useful to the NRC and the public as it could be. My reason for saying this is that the report contains few if any comparisons between the results from the various codes. In other words, the report gives no conclusions. I thought that comparison between the codes was one of the purposes of the contract.

2. The level of proficiency which the authors display in running the simulations seems to vary between the codes. For example, the authors seem very skilled at running SWIFT, but they do not convince me that they have done all one can to get the best results out of PORFLO. Perhaps the authors could obtain assistance from Rockwell in running PORFLO.

3. I think that the report should be organized by problem rather than by code. This would make it easier for the reader to compare the results from the different codes.

4. Considering what I remember as Teknekron's claimed prowess in computer graphics, I find the graphics in this report disappointing. Tabulations of numerical data are notoriously difficult for readers to interpret in presentations of computer results.

5. To help ensure the reproducibility of the work, I recommend including input file listings, perhaps in an appendix.

6. Some techniques used in doing the computations seem inapplicable to the complex repository models that will be used in licensing. I am referring particularly to the adjustment of simulation times in USGS3D and PORFLO (see pages 18 and 63) and to the use of curvilinear coordinates in SWIFT and CCC (see pages 197 and 500). If I am correct in thinking that these techniques may not be applicable to repository models, perhaps they are not appropriate for use in benchmarking problems.

7. I also have some detailed comments, which are as follows:

p. 1. The term "hypothetical problems" should be explained.

p. 2. The reference by Thomas (1982) does not appear at the end of the report.

Sec. 1.3. The features mentioned for the different codes are not always consistent. For example, the text mentions that CCC has a feature for modeling temperature dependence of viscosity, but it does not mention that SWIFT has the same feature.

p. 11. The caption is the first place that the name Hantush appears. This should appear in the text as well. Also, axes should be shown on the figure.

p. 13. In eq. (2.6b) should the lower limit of integration be u'? In the last equation on this page, there is an unmatched parenthesis. Also, the definition of W is so complex as to be unclear.

p. 15. Give values for K and b.

p. 16. A time-step growth factor of 41.4% per cycle seems rather high. Is this within the limits, if any, recommended for the code?

In the last paragraph, I don't understand the reasoning behind adjusting the simulation time when comparing numerical results with the analytic solution. How will a user know how to adjust the simulation time when doing more complex models?

p. 21. Was the no-flow boundary placed far enough from the area of interest to avoid influencing the results significantly?

p. 22. A picture of the problem geometry would be helpful.

p. 23. In eq. (2.10) I think u_{xy} and U_{xy} may be confused.

p. 24. The grid block sizes double with each row or column. Is this within the recommended range for the code? Also, how were the time-steps chosen?

p. 25. It is not completely clear at what point the results are measured. (Are they on the axes?)

p. 35. There is undoubtedly a good reason why Kevin Lake was not included in the simulation, but I don't know what it is. (I am aware that Pinder and Bredehoeft did not include it either in their 1968 paper.)

p. 43. It would be helpful to have an isometric view of the geometry, since Figures 2.16-2.18 do not tell the whole story. For example, one cannot tell what aquifer 2 looks like underground except along the particular cross-sections shown.

p. 52-53. Some of the head contours appear to intersect no-flow boundaries at angles other than 90 degrees. This is not physically reasonable, but perhaps it is caused by the plotting program.

p. 54. What does the term "vertical slicing" mean?

p. 58. The view that PORFLO is inherently less accurate than USGS3D because PORFLO uses the alternating direction implicit (ADI) method of integration is not sufficiently supported by the authors. Clearly a noniterative method would be expected to require more time steps than an iterative method, but that does not mean the noniterative method is using an "excessive" number of time steps. There are many possible reasons why in this particular benchmark problem the PORFLO solution shows worse agreement than the USGS3D solution.

p. 63. I don't understand the reasoning behind the time scale adjustment.

p. 68. Eq. (3.1) should make it clear that the third term on the right-hand side is to be evaluated at z=b.

I don't see any justification for ignoring radial conduction in the bedrock and caprock, but I suppose this is a comment on the original analytic solution rather than on the current work.

p. 70. Should λ be τ?

p. 72. What is the value of b'?

p. 75. The authors again attribute the difference between the PORFLO solution and the analytic solution to the ADI technique without sufficient justification for this view.

p. 79. In eq. (3.9) what is γ? Also, eq. (3.8c) is unnecessary for an initial value problem with a parabolic second order PDE on a infinite domain.

p. 81. In eq. (3.10c) what are κ, κ', and λ'?

p. 90. I have the same comment for eq. (3.11) as for (3.1) above.

p. 92. Eq. (3.13c) is unnecessary for an initial value problem.

p. 94. Thermal conductivity should have units of BTU/(ft-day-degF).

p. 95. Is Figure 3.11 a plot of temperature at the withdrawal well?

p. 96. I don't understand why PORFLO can model only one particular set of the input parameters.

p. 99. The author attributes the numerical instability shown in Figure 3.13 to use of the alternating direction implicit (ADI) method of integration by PORFLO. The ADI method for parabolic PDE's is unconditionally stable, so I don't understand this conclusion. (See L. Lapidus and G. F. Pinder, Numerical Solution of Partial Differential Equations in Science and Engineering, Wiley (1982) p. 246.)

p. 103. Should B_r be B_s in the last term of eq. (3.17)?

p. 106. Eq. (3.19a) is unnecessary for an initial value problem. I don't see what the boundary condition (3.19b) corresponds to physically.

p. 151. I don't understand the comment that "the ADI technique cannot correctly simulate large contrasts in properties over small areas... without undo (sic) discretization" since ADI is a method for integration over time rather than a method for spatial differencing.

p. 164. I don't understand section 4.3.2 at all.

p. 187. I would hesitate to conclude that the SWIFT result proves that the site is stable, since SWIFT does not account for the feedback effect that salt solutioning has on the flow properties of the site (as a model such as DNET does).

p. 223. The difference between the first and second steps is not clear. Is the first step a steady-state calculation? If so, how can the authors talk about "initial conditions?" On p. 223 the text states that in the first step heat loading is at a maximum. But on p. 227 it says "a heat loading was added to the repository" in the second step.

p. 229. The trajectory of particle F appears to move from the rubble zone into a region of undisturbed salt. Does this make sense?

p. 257. It is surprising that the curvilinear and rectangular grids give significantly different results far from the singularities. Is this reasonable?

p. 268. Since there was already a 2D SWIFT grid set up for the hypothetical basalt site (see section 4.7), why bother setting up a new 1D model?

p. 276. The boundary condition in eq. (5.2-2c) is unnecessary for an initial value problem.

p. 276 (continued). Eqs. (5.2-1a) and (5.2-1b) appear to describe the pseudo-steady-state approximation. This approximation was the one used in the analytic solution. Since the SWIFT results using the dual-continuum model show worse agreement than with the pseudo-steady-state model, I would like to see some comment on the relative merits of the two models.

p. 278. The parameter θ_1 is defined but not used.

p. 281. Is the conversion factor g_c needed when metric units are used?

p. 295. The first term in eq. (5.3-1a) should have a minus sign in front.

p. 299. How were the fractures and the matrix modeled?

p. 308. What are "spherical units?"

p. 309. The first term in eq. (5.4-2a) should have a minus sign in front.

p. 312. Eqs. (5.4-5b) are not the Bateman equations. The Bateman equations are solutions to (5.4-5b). (See I. Kaplan, Nuclear Physics, Addison-Wesley (1962) p. 243.)

p. 315. I don't think it's appropriate to use separate runs for Cm245 and the other pair of nuclides, since this would not ordinarily be done in the simulation of a real repository. If SWIFT can't do the entire chain, too bad.

p. 317. I still don't know what "sphere" the authors are talking about.

p. 359. The reference for Headworth (1980) is missing from the end of the report.

p. 363. I don't understand what Figure 5.5-3b is supposed to mean.

p. 414. NWFT/DVM contains two distinct methods for simulating radionuclide migration, namely NWFT and DVM. Which was used?

In the tables it would help to list the Peclet numbers for each case, since this parameter bears on the accuracy of the DVM model.

The Δx value of 1.64 ft results in a very fine grid, since L=1640 ft. How was this increment chosen?

p. 500. In eq. (9.5-1) the θ's need subscripts.

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Please note that I cannot comment on the sections of the report dealing with unsaturated flow, since I know even less about that subject than I do about saturated flow.

If you have any questions, please call me at (818) 449-0718 or (818) 356-4489.

Best regards.

Sincerely,

S Billing

Stewart A. Silling

cc: R. Codell, NRC
N. Ortiz, SNL