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November 13, 1984

NRC FINB6985

Ms. Pauline Brooks, Project Officer
Division of Waste Management
MS 623 SS
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555

Subject: Contract No. NRC-02-81-026
Benchmarking of Computer Codes and Licensing Assistance

Dear Pauline:

As you requested, enclosed are three copies of the external QA comments on the waste package code benchmark problem report. Please contact me if you have any questions.

Sincerely,

Doug
Douglas K. Vogt
Project Manager

WM-RES

WM-Record File <i>B6985</i> <i>CorStar</i>	WM Project <i>10, 11, 16</i>
	Docket No. _____
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Enclosures

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WASHINGTON, D.C.

INCLINE VILLAGE

165.3

Dr. Roger W. Carlson, P.E.
640 Mabry Road
Atlanta, Georgia 30328
November 5, 1984

Mr. Doug Vogt
Vice President, CorSTAR
7315 Wisconsin Ave., North Tower 702
Bethesda, Maryland 20814

Dear Doug,

Enclosed is a list of the comments that I have as a result of reviewing the draft report documenting the development of a set of benchmark problems for computer programs for the evaluation of waste packages. In summary, I found this report to be extremely poorly written with paragraphs that were confusing, self contradictory and insulting to the project sponsor. The introduction is very wordy with many paragraphs that do very little to provide an understanding of the importance of the following sections. Many of the statements of the benchmark problems were confusing and did not convey the intent or details of the problem. The following pages provide detailed comments which expand upon these general comments. My recommendation is that this report be given to an editor to prepare substantial revisions which would improve the readability and impression of the project sponsor.

Agreement between the various authors should be reached about the format of the report. Items such as the identification of the units associated with the definition of variables and the content of the sections dealing with output specifications were treated differently in various sections.

I am also enclosing the invoice for the effort that I have expended during the review of the subject report. This invoice covers the efforts expended during the months of October and November 1984.

Mr. Doug Vogt
page 2

It has been a pleasure to work with you and your staff on this project
and I hope to continue this relationship in the future.

Yours truly,

A handwritten signature in cursive script that reads "Roger W. Carlson". The signature is written in black ink and is positioned directly below the typed name.

Roger W. Carlson

November 5, 1984

Review of Report
BENCHMARK PROBLEMS FOR WASTE PACKAGE
COMPUTER CODES

- | Page | Comment |
|-----------|---|
| 1. iv | There is no page iv. |
| 2. 4 | Top paragraph. The text "degradation of or" is confusing. |
| 3. 4 | Second paragraph. The word "transfer" should be "transient." |
| 4. 4 | Page 4 was present twice in this copy. |
| 5. 4 | Section 1.3. Computer codes to be tested by benchmark problems should be identified in all sections or none. |
| 6. 5 | The word "speciation" is unknown. Is this a typo? |
| 7. 6 | The previous efforts should be identified by reference. |
| 8. 7 | Why does section 1.5 start on a new page?
Third paragraph of section 1.6. The use of the pronoun "these" in the topic sentence of this paragraph is confusing because the reference is uncertain. |
| 10. 9 | Top. Listing "input specifications" and "output specifications" implies specific computer programs. Benchmark problems should be generic and apply to all programs that can solve the problem. |
| 11. 9&10 | Stating that benchmark problems haven't been run is admitting to an incomplete project. |
| 12. 11 | First two sentences are contradictory. |
| 13. 11 | Third sentence is garbled. |
| 14. 11 | Problem 2.1 does not make it clear that the source is a cylinder inside the cylinder that is the main part of the problem. It sounds like the source is a part of the wall of the storage canister. |
| 15. 12 | Figure 2.1-1. This shows only the specific case where r_m is equal to r_f . This figure would be more effective if a more general case were represented. |
| 16. 13 | Bottom. r_w should be defined. |
| 17. 15&16 | Present results in dimensionless form to make results more generic. |
| 18. 17 | Why is Figure 2.2-1 different from Figure 2.1-1? |
| 19. 17 | Title. The expression " $(0 < r < r_w)$ " should be " $(0 < r < r_w)$." |
| 20. 16&18 | Differential equation (8) should be stated as applying to all regions at the beginning of this section rather than limiting the equation to region c and then later saying that it also applies to regions a and b. |
| 21. 19 | Objectives. Specific code WAPPA should not be identified. A generic objective would be more useful. |
| 22. 20 | Assumptions. Complete text of second assumption. |

Review of Report
BENCHMARK PROBLEMS FOR WASTE PACKAGE
COMPUTER CODES

23. 21 Problem statement. This is the first problem statement where the cylinders have been described as infinite. However, the first three problems have been similar in the treatment of axial conduction of heat.
24. 21 Problem statement. Text "with time" is better stated as "as a function of time."
25. 21 Paragraph after problem statement. Remove the word "only."
26. 21&23 The fact that the cylinder is in equilibrium with the atmosphere prior to the transient is immaterial. The only significant fact is that the temperature in the cylinder is independent of position and less than the atmospheric temperature during the time of interest.
27. 24 Analytic solution. This is the first solution to be referenced. I think that the solutions to the previous problems should also be referenced unless a complete derivation of the solution is presented.
28. 24 My copy appears to have had a note attached under equation 28 which obscured some of the definition of symbols.
29. 24 I would like to see some recommendation as to the number of terms to be included in the infinite series of equation 27.
30. 27 Table at top of page. The top lines of this table appear to have missing entries.
31. 29 Figure 2.4-1. This problem is described as one dimensional so presence of boundary at $y=1$ is confusing.
32. 30 Assumptions. An important assumption in this problem is that the fluid is stationary prior to change of phase. Any convection would invalidate the solution that is presented.
32. 31 Output. One of the most important outputs of this problem is the location of the edge of the frozen region.
33. 40 Assumptions. Same comment as 22.
34. 40 This problem introduces the solution for the temperature distribution in the waste region. Why wasn't this included in previous problems?
35. 43 This problem needs to be referenced so that any details of the test or meaning of the tabular data can be verified by the user of the benchmark problems.
36. 49&50 Is the decay heat a function of axial position?

Review of Report
BENCHMARK PROBLEMS FOR WASTE PACKAGE
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37. 77 Analytical solution. A computer program model cannot produce an analytical solution.
A less complicated problem can be presented where the surface temperature of the canister is forced to endure a step change. The heat transfer should be assumed to be only radial. This problem will give results which are close to the results from problem 2.7 but it can be shown that the results are conservative for computing the thermal stress distribution.
38. 80 The output section of this benchmark problem is totally inappropriate. Instructions to the analyst do not belong in a benchmark problem. This benchmark problem demands a solution which will serve as the correct answer that is to be achieved by users of this problem.
39. 84 Figure 3.1-1 is identical to Figure 2.1-1 so why repeat it?
40. 88 Dimensionless plots of these results are available in many text books that present this solution.
41. 92 Top. Units are missing on shape. Mode shape should also be defined as the position dependent displacement of the beam.
42. 94-96 The output specifications start on page 94. The text identified as output specifications should be moved to page 94.
43. 96 Equation 66. The indication for equation 66 is misplaced.
44. 101 The text labeled Output Specifications should be moved to page 101.
45. 106-107 The equations developed for the relative displacement between the mass and container are wrong because the second derivative of the relative displacement equals $-g$ when time is zero. There cannot be any relative force or acceleration at the start of the free fall. I believe that the solution should show no relative displacement during the free fall.
46. 110 Bottom. Mass should not be expressed in slugs.
47. 111 Output Specifications. The type of program should not be specified.
48. 113 Top. I would prefer to see equations written in a form that more clearly identifies the forces acting on the masses.
49. 117 Output specifications. The text under this heading should be moved to page 117.
50. 118 Equation 123 is incorrectly written.
51. 129 Objective. The stated objective is inappropriate for a benchmark problem. This raises concern about the value of this entire problem as a benchmark problem.

Review of Report
BENCHMARK PROBLEMS FOR WASTE PACKAGE
COMPUTER CODES

52. 133 Figure 3.8-2. The curve for LMP=24000 appears distorted at the top. Also why use exponential notation for LMP when simple notation would take less room.
53. 134 Assumptions. The assumption of ovality is not consistent with the development of the equations that is presented on the previous pages.
54. 135 Objectives. The objective of a benchmark problem does not include demonstration of a method.
55. 139 Analytical solution. The statement about an analytical solution should not be based on any computer programs.
56. 142 Output specifications. This section should include the output that is expected when a computer program is used to solve this problem.
57. 145 Table. This table is incomplete.
58. 148 Analytical solution. The analytical solution should not be based upon a solution computed by ANSYS.
59. 150 Objectives. The objective of a benchmark problem is to provide a test which will verify the correct operation and use of any computer program that is capable of solving that type of problem. Preparing a comparison of measurements with calculations using various models is inappropriate for this project.
60. 155 Assumptions. This section should list assumptions that are made in the solutions that follow. Advice to the user of the problem should not be a part of assumptions.
61. 171 Table 4.3-1 is missing.
62. 182 Comments. These comments are inappropriate for reasons stated in comments 59.
63. 183 Same comment as 60.
64. 190 Figure 4.5-2. The text and tabular data in this figure is very difficult to read.
65. 193 The comments about the benchmark problems in this section parallel the comments about the problems proposed in the previous sections. Specifically, a benchmark problem is to present the necessary data to describe a problem and the correct solution of that problem. Any efforts or text that attempts to compare methods or evaluate alternate methods is not in concert with an effort to develop benchmark problems.
66. 204 I am not qualified to comment upon geochemical benchmark problems and as such no further review of this report was

QA Comments

Harden Engineering Company
Route 4 Box 66-2
Mocksville, N.C. 27028
October 26, 1984

Mr. Lyle R. Silka
Director of Hydrogeologic Services
CorSTAR Research, Inc.
7315 Wisconsin, North Tower #702
Bethesda, Maryland 20814

Subject: Quality Assurance Review of CorSTAR Draft Report
"Benchmark Problems for Waste Package Computer
Codes".

Dear Mr. Silka:

I have completed my review of Chapters 1-5 of the subject report. The purpose of this review was to determine (1) if the report is complete in providing the necessary input data to successfully run a model;

(2) whether the problems presented offer a means to adequately test models in areas important to the analysis of High Level Waste (HLW) repositories; and

(3) whether the problems present realistic sets of data. My conclusions are as follows.

(1) Except for the 4 cases discussed below, the report does provide the information needed to model the given problems.

(2) The problems presented offer a means to adequately test the computer program capabilities needed for a HLW repository analysis. However, since no solutions are given for the hypothetical and validation problems, it will be difficult to test some features. These include radiation and natural convection heat transfer across the air gaps in a repository, temperature dependent material properties, elastic-plastic thermal stress analysis, and source strength calculations. While these features are included in the benchmark problems, the only way they can be adequately tested is by analyzing the same problem by different means and comparing results. It would be helpful to the analyst to have solutions in the report.

(3) The problems do indeed present realistic sets of data. The problems appear to be based on actual designs that have been used in practice. One possible exception is the seven layer cylinder in problems 2.5 and 3.10.

The review copy of the report is enclosed, in which typographical errors have been indicated and minor comments made. The problems which appear to have incomplete input data are as follows.

In problem 2.6, the details of the fuel rods and the overall dimensions of the fuel bundle are needed to calculate the temperature distribution in the fuel assembly. The fuel rod surface temperatures must be calculated in order to determine the heat transfer through the fill gas to the outer cylinder. Although not necessary for calculating fuel assembly temperatures, it would be helpful to the analyst to have the locations of the other thermocouples for which results are given in Tables 2.6-4 through 2.6-27.

Analyzing the creep buckling problem in Section 3.8 using the COVE computer program would be a chore, since the creep input would have to be first generated from the isochronous stress-strain curves given in the report. The creep parameters for input to COVE should be included.

In problems 4.2 and 4.3, it is not clear where the radiation detectors are located, nor what the E-1 profile is. A sketch showing the detector locations would be helpful.

In problem 4.4, the non-fuel materials in the fuel assembly need to be specified. This data is necessary to calculate the source strength.

In general, the report is clear and well organized. It will be a valuable tool to the analyst testing computer programs for waste package analysis.

Sincerely,

William H. Harden

William H. Harden

August 17, 1984

Lyle R. Silka
CorSTAR
North Tower Suite 702
7315 Wisconsin Avenue
Bethesda, MD 20814

Dear Lyle:

Please find enclosed the draft chapter you asked me to read. I have made a number of comments directly on the text, many editorial and some substantive. I tried to indicate in the left hand margin each line for which a suggested change or comment was made. Additionally, the following comments refer to the given location in the text.

1,7 Awkward use of "input" and "analyses" (in a discussion of geochemical numerical models). Try "The results of geochemical model calculations may serve to guide investigations . . .", although this is admittedly very passive. The danger is to give the model human capabilities like "to provide, to evaluate, . . ."

1,19 - 1,23 Lab studies are useful. (Don't come down so hard here - you'll offend all experimentalists.)

2,28 - 2,31 First sentence is awkward. "analogs similar to processes"? Perhaps break into 2 or 3 sentences and expand some.

8,1 - 8,2 I think this is an overstatement. True, natural mineral assemblages with good evidence of equilibrium can be used to confirm or question thermo data. I'm not convinced that enough information exists to convince the reader for this system. Either elaborate greatly or leave out. Only a few minerals in the thermo data base could be tested at best - not even close to the entire data set.

Missing page of text between 15 and 23.

23 (general) It seems to me that a lot of retrograde metamorphism can occur in 2 MY at 50-150 deg C - - doubts about present vs. past mineral assemblage.

An attempt to reconstruct the solution chemistry from solid phase chemical/mineralogical information in order to then consider solution - solid reactions or equilibrium appears to be basing a story upon dependent data sets. But I don't think that taking the water chemistry from a different site is legitimate when the goal is quantitative modeling either.

The minerals are not really thermodynamically well-defined phases here if their composition is not pure (and known). The nuclides are substituting in trace amounts into all kinds of minerals, and in that situation no thermo description of the nuclide behavior is possible.

In the end, only possibility is to attempt to model the major aqueous species. Surely Oklo can be put to better use at least qualitatively to help us understand radionuclide behavior. I think better systems (geothermal or contact metamorphism) exist about which more is known independently and in situ for us to practice modeling major species on.

Table 6.3-2 missing.

27 - 33 general. First we extrapolate to original subsurface brine composition from the above-sediment sample (using certain assumptions in order to do so). Now we have two points. Use two points to calculate mass transfer along the flowpath. But only ever sampled one! If I've understood this, it sounds very circular. I think there is a real problem with this data set. Did you come across any high temp. systems where two points along the flowpath were independently sampled? I don't know of any.

By not allowing the overall chemical composition to change between the two samples, do you also not allow any mass transfer?

33,17 - 33,18 A kinetic model may assume homogeneous equilibrium (so aqueous speciation would be at equilibrium) but heterogeneous disequilibrium (mineral - solution disequilibrium). In fact, most do that. You might want to clarify here.

35,14 - 35,15 Is this equilibrium at the end of a long run just so that we observe the final mineral products? Do we observe any kinetic effects in the experiments (I presume that we do from the Figures) or do we just model them? I really don't understand the objectives here. You should try to clarify. I got to the end of the problem and I didn't know if the output would help me meet the objectives. How do we use Figs. 6.5-1 - 7? Elaborate if possible. Also, where do we get the rate constants? (From experiments like those described here, and very few have been done.) We can't even hope to do this for other than the major elements. I have to respect your attempt here, but we are SO FAR from being able to do this . . . I realize this is presented as an idea for later on, but the input data is insufficient to run a kinetics code.

I think that the first two problems look pretty reasonable for a start on testing simulation of high-temp. chemical interactions, in particular, aqueous speciation of major elements. I think the other three problems are less successful. There are too many unknowns about the two natural analog systems to provide definitive input and output to test a code. I particularly think that the reaction path code problem may not be a valid test for the reasons mentioned above. If I have misunderstood your statement of the problem, others might too. Do what you can to elaborate on it. The kinetics problem suffers from lack of all the necessary data, but I think that is the current state of affairs.

I know of no way that the thermo data can be benchmarked. I

believe that is up to the process of continuing use, critical evaluation, and new measurements by a number of scientists in different laboratories. I don't know of any mathematical way to approach the task.

If you can answer some of my questions and comments by refining or elaborating on your text I think that will help you improve the chapter.

Good luck, Lyle. Talk to you soon!

Sincerely,



Janet S. Herman

August 11, 1984

Mr. Lyle R. Silka
Director, Hydrological Services
CorSTAR
7315 Wisconson, North Tower
702
Bethesda, MD 20814

Dear Mr. Sylka:

The following is my evaluation of the draft chapter "Waste Package Geochemical Code Benchmark Problems". I hope that my comments will prove useful.

Let me preface my discussion by saying that I am *not impressed* by any of the existing general geochemical programs that purport to model the complex natural processes found in geothermal systems. They all have one or more shortcomings that I would gladly detail at your request. For example, a comparison of some existing programs, carried out by Nordstrom et al. (1979) A comparison of computerized chemical models for equilibrium calculations in aqueous systems, A.C.S. Symp. Ser. 93, showed significant disagreements between various programs for relatively simple cases at 25 degrees (no comparison was made between calculated results and real geologic or experimental observations). This suggests to me that high temperature models, which use even less reliable thermodynamic data bases, will be totally unacceptable for modelling radioactive waste disposal problems. None-the-less, there is a serious need for carefully crafted programs of this sort and I presume that the benchmark problems discussed in your report will serve as standards for developing better computer models.

First, let me deal with a few editorial problems. Page 2 and one or more pages before page 23 were missing from my copy; this clearly needs to be corrected in the final draft. I found no problems with the writing style/grammar but feel that the organization could be improved. For example, the introductory remarks make a strong case for considering well-studied geothermal systems as ideal benchmark problems but the first two problems are the only ones based on such systems. The third involves a rather inaccessible ore deposit; the fourth considers an expired natural reactor; and the fifth is based upon an experimental study. The rationale for selecting these other test

cases should be discussed or, better yet, all of the benchmark problems should be based on geothermal systems. There is a similar problem with the repository rock types. The introduction points out that at least four rock types will be considered yet the benchmark problems are heavily weighted toward basalt. Granites and tuffs are not even mentioned. This bias must be justified if it is retained. Also, I see no need for the output of the WATCH1 program listed in Table 6.2-2. The chemical data on page 8 are obviously of value as problem input data but the calculated ionic strength, ion balance, activity coefficients, activities, chemical geothermometers, etc. are model dependent and should be calculated by the test programs. Finally, the report ends rather abruptly after the fifth problem; I would like to see a short summary/conclusions section to round it off.

Before addressing the selected benchmark problems specifically, I think it would be useful to discuss the phylogony of geochemical computer models, their level of sophistication, the range of chemical species they consider, and the reliability of their thermodynamic data bases.

There are two basic types of geochemical computer programs, interpretative models and predictive models, the proposed benchmark problems cover both types. *Interperative models* give detailed information about the possible range of chemical conditions at a particular time instant. Examples include, mineral solubility, log activity-log activity, and P-T-X phase diagrams. By comparing the possible phase assemblages with those predicted by the models, the geochemist determines a unique set of physical and chemical parameters that define the natural system. A good example of this type of program is SOLUPLOT written by Craig Bethke. This program uses a table of free energy data to construct Eh-pH and log oxygen activity-pH diagrams. I would also include WATEQ, EQ3, REDEQL, and SOLMNEQ among others in this category because they are used to compare the consistency between water chemistry and the observed mineral assemblages. Because they do not consider reaction rates, these programs can only suggest which phases should be in equilibrium with the solution but slow kinetics may not allow equilibrium to be established. *Predictive models*, on the other hand, consider the evolution of ~~of~~ the system over time. PATHCALC, PATHI, and EQ6 are examples of this type of model. Their implementation is usually quite difficult because they must relate a large number of often poorly understood, ill-behaved, non-thermodynamic variables. In the simplest case, one variable such as temperature or the concentration of one component is changed with time and the rest of the system is equilibrated at each time step. This is really too naive to ~~be~~ give a very useful prediction of what might happen in nature because the rest of the system does not equilibrate instantaneously as is assumed. However, similar problems have already been addressed by chemical engineers, who have developed far more sophisticated numerical models than any that geochemists presently use. I expect that we will follow their lead in terms of programming techniques.

We need a way to express the range of ability and the level of sophistication of a particular geochemical program. The

problems presented in the report are clearly designed to test programs with an increasingly wider range of ability. For example, a program that could deal with problem 2 certainly would be able to handle problem 1. I would like to see a ranking of programs along this line:

1. Solid + solution equilibrium (interperative)
2. Solid + solution + vapor equilibrium (interperative)
3. Solid + solution, closed system, reaction path (predictive)
4. Solid + solution, open system, reaction along a flow path (predictive)
5. Solid + solution, open system, reaction along a flow path + mineral transformations (predictive)

There are clearly other types of computer models that could be developed but these five seem to represent the range needed to solve the problems presented here and I expect they would be of value in modelling radioactive waste problems. In addition to their range of abilities, programs have different levels of thermodynamic sophistication. Taking interperative models as an example. Models that might be used within the program from simplest to most complex:

Stoichiometric solids<Ideal solid solutions<Non-ideal solid solutions<Adsorption effects<Distribution coefficients

Ideal aqueous solutions<Debye-Huckel model<Ion pairing model<Sophisticated solution models (eg. Pitzer's model)

Ideal gases-Henry's law solubility<Salting-out effects<Specific interaction effects<Non-ideal gases

A similar ranking of rate laws in predictive models can be established. The point here is that you need to somehow define the minimum level of range and sophistication acceptable for each benchmark problem. For example, some of the product solids are not pure endmember compositions (smectite, for example) so it seems that all programs must be equipped with some way to approximate the properties of solid solutions.

A potentially serious problem that I see in the benchmark problems is the lack of distinction between major and trace elements. I will admit that none of the existing programs make this distinction but I feel that this is one of their greatest difficulties. The ten most abundant elements in the earth's crust are: O, Si, Al, Fe, Ca, Na, K, Mg, Ti, and H. The most important species in natural solutions are: hydrogen ion, Na, Ca, Mg, K, hydroxide, sulfate, chloride, and bicarbonate. I'm not sure which vapor species are most important but would expect nitrogen, oxygen, carbon dioxide, hydrogen sulfide, and sulfur dioxide to be in the list. All programs *must* be able to deal with these major species very thoroughly and accurately. They control the oxidation state, pH, major aqueous complexes, P-V-T properties, etc. of the

system. The trace elements (ie. all other species) only follow their lead; they never determine the basic chemical properties of the system. Furthermore, most rocks contain feldspars, quartz, micas (or clay minerals), and iron oxides. These minerals, along with any others that are expected to be common, must be considered thoroughly by any program. This is a special difficulty in problem 3, where a great deal of information about minor and trace elements is given but very little about major elements is available to define the overall system chemistry. From all of this, I conclude that someone must choose a *minimum* set of geologically abundant minerals (including solid solution species), aqueous species, and gases that must be included in all programs and *benchmark problems*.

Thorough evaluation of thermodynamic data is a difficult and time consuming task. The present data sets, with one exception, were accumulated by individuals on the basis of personal preference. This often gives an adequate, but not entirely dependable, set of data for geochemical calculations. Techniques for critically evaluating thermochemical data vary among geochemists so some data sets are quite reliable while others contain quite a few estimated, less reliable, values. The only consistent way to correlate a large data base was developed by John Haas and James Fisher (1976) Simultaneous evaluation and correlation of thermodynamic data, *Am. Jour. Sci.*, 276, 525-545. This method has been applied to produce an internally consistent set of data for a variety of minerals by G. Robinson et al. (1979) Thermodynamic and thermophysical properties of selected phases in the MgO-SiO₂-H₂O-CO₂, CaO-Al₂O₃-SiO₂-H₂O-CO₂, and Fe-FeO-Fe₂O₃-SiO₂ chemical systems, U.S.G.S. Open file report 83-79. This approach gives a least squares fit of a grid of calorimetric, solubility, and phase equilibria data so that any datum that does not conform to thermodynamic behavior is easily spotted and discarded. Furthermore, the final fit represents the best possible distribution of errors among the data to give the most reliable data base. Unfortunately, the method is quite cumbersome so it is reasonable to use it only for the most important, major species. Benchmark problems do provide a reasonable test of the adequacy of a thermodynamic data base. In addition, they can be implemented much more readily than Haas' method. However, they must be designed to test the data over a wide range of temperature and bulk composition.

The following are specific comments for each benchmark problem (there are a few additional comments on the manuscript):

PROBLEM 6.1--This is a good, well documented problem. It will test the capability of a program to handle simple major element and major species. If it is assumed that the geothermal waters flow from high to low temperature zones, this problem could also be used to test the ability of a reaction path-type program to predict the mineral zoning

shown in Figure 6.1-1. Unfortunately, there is no problem of this sort given for other rock types. I recommend that Cerro Prieto (see *Geothermics*, 13, no. 1/2, for starters) as a good example of a similar situation for sediments. The Salton Sea geothermal field is a well studied example that could be used for a highly saline situation (the Bureau of Mines has done a great deal of metal corrosion studies there that could be quite pertinent to radioactive waste). Finally, the hot dry rock work at Los Alamos (see *Jour. Volcanology and Geothermal Research*, 15, no. 1-3) could be a good basis for a problem involving granite.

PROBLEM 6-2. Again this is a good, well-posed problem. I would again like to see additional rock types considered. I know that boiling has been studied at Cerro Prieto (sediments) and in the New Zealand (tuff) geothermal systems.

PROBLEM 6-3. I am less enthusiastic about this problem. It is much less well defined. For example, saying that the composition of the groundwater at the Okla site was the same as that from the Grants Mineral Belt is rather speculative; this is not the kind of well-defined input data that I would want to use to test a program. Furthermore, the output can be compared with only a set of qualitative observations. Table 6.3-3 shows that such qualitative relationships can be inferred from simple Eh-pH diagrams without the aid of a sophisticated program. Furthermore, this problem requires a program to predict the redistribution of trace elements in a temperature field yet there is no previous problem to test whether the program can even deal with major element redistribution. Is there any geothermal system, like the hot dry rock system at Los Alamos or the New Zealand ones, where the distribution of both major and trace elements is well documented? If this problem is retained, I feel it should be accompanied by a cautionary note stating that it is not necessarily internally consistent.

PROBLEM 6-4. While the Red Sea deposits are geochemically interesting, I feel they represent an inappropriate model for any type of radioactive waste scenario. For your information, R. J. Pottorf (1980) Hydrothermal sediments of the Red Sea, Atlantis II Deep-A model for massive sulfide-type ore deposits, Ph.D. thesis, The Pennsylvania State University, had developed a rather extensive geochemical model of the processes involved in the deposition of the Red Sea sulfides. This model shows that mixing of the hot brine and Red Sea water is of some importance in this system so that simple cooling cannot account for the observed mineral assemblage. I doubt if such a situation would ever arise in conjunction with radioactive waste disposal. I would suggest that some geothermal scaling study might be a more useful basis for a cooling problem or perhaps, you could recast problem 6.1 in a way that requires the program to predict the mineral zones from the highest temperature part of the reservoir to the

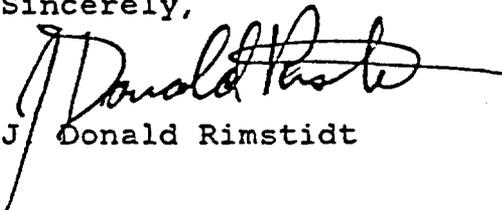
surface (low temperature) (there is a lot of information about fluid compositions and mineral assemblages at Cerro Prieto that might make a good cooling-path problem).

PROBLEM 6-5. On page 1 is a list of some of the many problems arising in experiments designed to model complex natural systems, and yet, such an experiment has been chosen to test a computer model that is supposed to be more reliable. While I understand the desire to include benchmark problems that look especially relevant to radioactive waste disposal, I feel that testing the reliability of a computer program with questionable experimental results will gain nothing. Note how the curves jump around in Figure 6.5-7; I doubt that a computer model would be able to predict such behavior even if it were true. I recommend dropping this problem altogether.

There is one final issue to be adressed: How can you quantitatively rate the performance of a particular program for each problem? Missed one mineral = 90%, missed two minerals = 80%, etc. or what? I do not have any clear ideas on this but you can be sure that someone will ask how you can say that program A is twice as good as program B. I think such an evaluation method should be pretty carefully laid out in the conclusions part of the report.

In conclusion, I feel that the benchmark problem idea is an excellent one and the use of well-studied geothermal systems as a basis for these problems is also quite good. I would like to see problems 6.3, 6.4, and 6.5 stick closer to well studied geothermal cases if at all possible. I think problems 6.1 and 6.2 show that you have made some real progress.

Sincerely,



J. Donald Rimstidt