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August 15, 1984

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
Monthly Letter Progress Report for July 1984

Dear Pauline:

This letter contains a management level summary of progress during the month of June. Attached to the report is a copy of the technical status summary that provides further discussion of work performed during this period. We are submitting a cost summary report under separate cover.

Task 1 - Literature Search - Waste Package Codes

The data set report for the waste package codes has been typed in final form. Approximately six figures are now being redrafted and the report will be proofread before submittal to NRC. As discussed in the last report we are still waiting to review the report with C. Sastre of Brookhaven and to obtain permission from all the publishers regarding all the tables and figures used in the report.

Task 3 - Benchmark Problem Report - Waste Package Codes

This report has been completed with the exception of certain figures that are now being drafted in final form. The report will be submitted to NRC and for concurrent external QA review when those figures are completed.

Tasks 4&5 - Siting Codes

During July comments from the NRC and all external reviewers were received. These comments are enclosed with the technical status summary report. We are now reviewing the comments and developing options for responding to those comments. They will be discussed with you before we take actions to respond to the comments.

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Tasks 4&5 - Radiological Assessment Codes

During July we continued evaluating and comparing the results from the codes CELTRANS, PATH1/DOSHEM, BIODOSE and LADTAP. Input cards for the ORIGEN runs at ORNL were also prepared and debugged. During August we expect to start making significant numbers of ORIGEN runs. A total of some 30 runs will be required for the benchmarking of this code. The ORIGEN runs should be completed by the end of August or first part of September.

Tasks 4&5 - Repository Design Codes

No new codes were received during the month. Informal contact was made with Mr. K. Wahi at Sandia regarding the codes that NNWSI will use for repository design analyses and the possibilities of using ADINA/ADINAT at Sandia. Mr. Wahi could not add anything beyond the list of codes previously transmitted to us by NRC. Although Mr. Wahi has not used ADINA/ADINAT he believes that Sandia has the 1978 version of that code.

During July the codes MATLOC and COYOTE were installed on the CDC 7600 at BNL. One analytical and one hypothetical problem were run successfully using the code DOT. Three other problems were set up but not yet run using the code COYOTE. The technical status summary report includes a more detailed discussion of each of these items.

Task 8 - Earth Sciences Data Base

During July there was no significant effort on this task.

Problem Areas

The following problem areas that were identified in the July monthly progress report have the potential to impact project schedule or budget. The status of these problem areas is updated below:

- Comments on the Task 4&5 report for the siting codes are being reviewed. Upon completion of that review by the end of August we will meet with the NRC to discuss options for incorporating NRC and QA review comments and submittal of a final report.

- The availability of the codes ADINA/ADINAT were discussed at a meeting at the NRC on August 1. At the meeting we agreed to pursue potential sources outside the NRC for use of the code including Lawrence Livermore Laboratory, Sandia National Laboratory and the Basalt Waste Isolation Project. CorSTAR and Acres will pursue the Sandia option and the NRC the Lawrence Livermore Laboratory and BWIP option. Separately, the NRC will investigate acquiring the codes for use at the Brookhaven facility. In order to have minimal scheduling impact access to these codes should be obtained by September of 1984.

- We are reviewing the availability of the SPECTROM codes and will make a recommendation to the NRC

See folder for Ltr.
to Brooks frm. Vogt
8-10-84

B6985

TECHNICAL STATUS SUMMARY

TECHNICAL STATUS

Tasks 4&5 - Siting Codes

Comments from the external QA reviewers, Dr. Mary Anderson and Dr. Chin Fu Tsang on the draft Task 4&5 report are attached to the Technical Status Summary. CorSTAR is in the process of reviewing these comments and preparing a plan for responding to them. We will be prepared to discuss this material with you by the end of August.

MEMORANDUM

TO: CorSTAR Research, Inc. DATE: July 25, 1984
Attention: Doug Vogt

FROM: Chin Fu Tsang

SUBJECT: Comments on the two-volume report: "Benchmarking of Flow and Transport Codes for Licensing Assistance"

Introduction

I have studied the whole two-volume report and have considered the inputs and results of various calculations and associated arguments and discussions that are in the report.

The comments below include reactions and thoughts I have during this review and I believe that they are of a constructive character. The specific questions that are asked by Lyle R. Silka, Quality Assurance Manager, are also answered. However, since details of the codes are not given, my answers are somewhat tentative, based on information contained in the report and my general experience in modeling.

General Comments

The report is very impressive and represents a substantial amount of work. As any modeler knows, to perform careful benchmarking calculations, especially with codes developed by others, is a laborious task. I would like to compliment the authors that they have done an admirable job.

Of course, improvements can be made to the report, mainly in the presentation, and also some clarity in the execution of the work is desired. These are given in

the next section, entitled "Major Suggestions". Some of these should probaby be addressed in a follow-up project.

The details of the codes used in this report are not described. Based on information available and general modeling experience, the following questions may be answered:

(a) Is the report complete in identifying all the input data and output results so that the problem could be run by another as an independent check? The authors have made a conscientious effort to provide all needed input data. I believe with the data provided and usual information, an independent check can be made. Output results tend to be representative and not complete. However, one should not expect complete outputs. Often, in code comparison work, a discrepancy requires one to go back to detailed computer outputs to find intermediate results to understand its cause.

(b) Where code comparisons are made, are the data and model set-up specification descriptions sufficient to allow an evaluation of the comparison and the interpretation of causes for discrepancies? For comparing codes covered in the report, the data and model set-up specification descriptions appear to be sufficient to allow an evaluation of the comparison and interpretation of causes for discrepancies. However, when compared with codes not in the list to be benchmarked in this report, the input and model set-up data for these "external" codes are not sufficient. Discussions of causes for discrepancies are given by the authors; however, I believe that it will be impossible for a reader not completely familiar with all the codes to be able to identify possible causes for discrepancies based on information in this report alone.

(c) Where model results are compared to other modeled data, field or lab data, are points of comparison the same in time or space? Yes, and in cases where they are not, they have been carefully pointed out.

(d) Although you cannot independently check the results, is the output reasonable and representative of probable repository conditions? I have looked fairly carefully at all the output graphs. They look reasonable. One or two minor comments are given in the sections below for particular cases. The hypothetical repository problems are representative of certain aspects of repository conditions.

Major Suggestions

These are given in no particular order, and some of them, as mentioned earlier, could be carried out in a small follow-up project.

(1) The report is currently arranged according to codes. But for the stated purpose of determining the adequacy of description and data input for the problems chosen and testing the capabilities of the chosen codes (p. 1), it would be much better for the reader if the report is arranged according to problems that are solved. Results of different codes solving the same problem will then be grouped together, making comparison much easier. This will also help to avoid frequent references to earlier sections, that "Statement and objectives of this problem were described previously in Section —".

(2) A paragraph or a section needs to be written on why and on what basis these particular codes are chosen for benchmarking. Do the general capabilities of these codes together cover all NRC's needs? Are some of these codes similar so that one or the other can be dropped? Are there other codes of interest to NRC but are covered by other NRC projects? One example of the latter is the TRUST code documented by PNL for the NRC.

(3) A discussion should be given on what basis a code is used to solve a selected subset of the benchmark problems. Does it mean that the particular code does not have the capability of solving other problems in the benchmark set?

(4) In the brief description of the codes on pp. 2-6, key references and dates of the development of these codes should be given. Then NRC personnel or other readers can get more into them if they wish by studying these references. So carefully chosen reference materials for each code are very useful. For each code, earlier validation studies must have been made and it is good to reference that too. Also, their application into different areas of heat and mass transport research should be described, which will give the readers a feeling of the flexibility of their use.

(5) The report, while including some fracture problems mainly in double-porosity approach, does not put sufficient emphasis on fractured-porous medium. A good follow-up project will be to do benchmarking for codes that can be made to model fracture flow. The report also seems to emphasize on decay chain modeling. I believe it is over-emphasized.

(6) A number of times in the report, comparisons are made with "external" analytic or numerical results, e.g., those from INTRACOIN project. However, these "external" results are not tabulated or plotted, and only qualitative discussions are given. I believe these results, including INTRACOIN results, are not proprietary. They should be presented as graphs, and tabulated if possible. Otherwise it will be difficult for readers to evaluate the results.

(7) In code comparison and benchmarking, two factors are involved. One is the code capability and accuracy, and the other is the cleverness and experience of the user in designing inputs to adapt the code to solve a given problem. These two things need to be separated. For example, an earlier work on geothermal model intercomparison study (Stanford University Report SGP-TR-42, December 17, 1980) took great care only to address the first factor. The current report appears to mix the two factors together. It will be good and advisable to clearly discuss which part is code capability based on straightforward inputs to the code and which part is the adaptation and maneuvering of inputs that an experienced modeler can cleverly design to solve the problem.

(8) After this report, perhaps one can define the limits of applicability or optimal areas of application for each code. In other words, summarize the types or classes of problems each code can handle readily. Also, perhaps the benchmark problems can be modified so that the inputs to code do not require special adaptation.

Specific Comments and Minor Errors

p. 1, middle:	List of codes misses FEMWATER, FEMWASTE and CCC.
p. 1, 4th line:	"from the repository" whould be better "from the repository to the biosphere".
p. 5:	It seems NWFT/DVM and NUTRAN have similar approaches and capabilities, why choose both?
p. 5, 15th line:	"saturated porous media" should be "variably saturated porous media".
p. 8:	SWIFT is repeated twice. NWFT/DVM (generalized version); generalized version is not referred to in text — need explanation.

p. 13, equation (2.6b): $\int_u^\infty$ should be $\int_{u'}^\infty$. Also, S')3S should be S'/3S.

p. 16: Δt, for first and second runs are not that different, why not use 100 sec for both?

p. 18: I think perhaps Run #2 is confusing and can be dropped. Run #1 can cover both short and long times.

p. 19: Drawdown units should be "feet"?

p. 20: Analytic solution should also be listed for comparison.

p. 21: Symbols are too small.

p. 23: It will be good to test codes against cases where Txy ≠ 0. This will be a more stringent test!

p. 25: Upper curve should have also label Y = 0. Lower curve should have also label X = 0.

p. 74: Discrepancy corresponds to mesh size, which is reasonable. The upper broken line has a strange wiggle near radial distance = 80m. Why? Is it an error or is it physical?

p. 75, 2nd para: The discrepancy could perhaps be due to mesh size and not numerical solution methods?

p. 92: I believe the solution assumes infinitely thick cap and bedrock. If so, this should be pointed out.

Also RHS of (3.15) is not obvious from (3.14).

p. 93: (3.4.2) should be (3.6.2).

p. 93: PORFLO seems to have quite a number of structural limitations. These should be summarized.

p. 96: "λ_D = ." should be "$\lambda_D = \infty$."

p. 100: The two line curves should be labeled. PORFLO results switching from one to the other could be due to boundary effect in numerical calculations?

p. 106, eq. (3.19b): r_c should be C_r(?)

p. 110: In discretization data for x_i, "240" is repeated – an error (?)

p. 114: Please display results of Harada et al.

p. 121: (3.16) should be (3.21).

p. 124:	Note: "$_L$ and $_T$" should be "α_L and α_T".
p. 125:	Middle: "e^{-t}" should be "$e^{-\lambda t}$" "Section 3.5.2" should be "Section (3.7.1)"
p. 137 y_im:	"-55." should be "-50."(?)
p. 138:	Please show INTRACOIN results.
p. 171:	For clarity, perhaps use solid lines for SWIFT (with river) and broken lines for SWIFT (without river).
P. 196:	Need to label upper figure, (a), and lower figure, (b).
p. 221, middle of figure:	 should be
p. 223:	Conceptualization is a bit stretched. Last line: "degredation" should be "degradation".
p. 257:	Horizontal axis needed labeling.
p. 267:	Bottom: need conclusions(?)
p. 287:	Should be Figure 5.2-5(a). Last line: "mtrix" should be "matrix".
p. 304:	Please present in graphs. Please display INTRACOIN results.
p. 308 middle:	"a large as" should be "as large es".
p. 361:	SWIFT results are not shown and should not be in the symbol labeling list.
p. 377, 2nd line from bottom:	"Forth" should be "Fourth".
p. 393:	Please also show analytic solutions for comparison.
p. 403 last paragraph:	Why NUTRAN does not use the same three values of dispersivities?
p. 411:	NUTRAN implicitly allows dispersion backforwards. This may be common practice, but is it not wrong physically?
p. 411 last paragraph:	Is the bug taken out?
p. 415:	Please display the comparison in graphs.

p. 448:	Perhaps it is not fair to compare FEMWATER with the code of Reeves and Duguid, since the former is developed based on the latter.
p. 455 equation (8.8):	"$\frac{\partial}{\partial}$" should be "$\frac{\partial}{\partial x}$"
p. 488, 3rd line:	"accutrately" should be "accurately"
p. 499:	In figure labeling list, "x_{max}" should be "Δx_{max}"
p. 517:	Need a much more complete reference list, covering key references of all the codes being benchmarked.

2602 Arbor Dr. #220
Madison, WI 53711
June 14, 1984

Mr. Lyle R. Silka
CorSTAR
7315 Wisconsin, North Tower #702
Bethesda, Maryland 20814

Dear Mr. Silka:

Enclosed are my comments on the draft document "Benchmarking of Flow and Transport Codes for Licensing Assistance", which you requested me to review in your letter of May 15, 1984. Also enclosed please find my invoice as per the statement of work form dated May 22, 1984.

In doing my review I kept in mind the 4 questions outlined in your letter of May 15th. Comments in the pages that follow address these questions in reference to specific items in the report. However, I would like to make some general observations about the report as a whole and the adequacy with which it meets the concerns outlined in the 4 questions in your letter.

a) For many problem simulations, the report does not provide all the input data required to run the simulation. In particular, information about the design of the grids used in the simulations is incomplete in some of the simulations. I recommend that enough figures as well as tables be provided to show the configuration of the grid in all relevant dimensions. That is, for three-dimensional problems, a three-dimensional grid needs to be defined. This will require at least two figures, as well as a table to specify the exact nodal spacing in all three dimensions.

Another difficulty in reporting simulations done with a specific model concerns various modeling "tricks" that often are code specific. Of the codes used in benchmarking, the only one with which I am very familiar is USGS3D. In the chapter which reports on the USGS3D simulations (Chap. 2) I was able to detect places where I suspect that certain modeling options and tricks had been employed to generate the simulation. These options and tricks were not described in the report. I suspect that similar omissions occur in the other chapters but because I am not familiar with the documentation for these codes I was not able to pick out this sort of thing. Whether or not it is desireable or even possible to specify everything necessary to run a simulation is a point that could be debated.

b) Although several codes are used to solve the same problem, serious attempts to compare codes are not made in this report. Exceptions to the previous statement are some comparisons presented in Chapter 6 where results from SWIFT and NUTRAN are listed along with the INTRACOIN study results for Problem 8.2. Also in Chapter 8, the results of FEMWATER/FEMWASTE are compared with UNSAT2 and with SATURN. Note that UNSAT2 is discussed in the Thomas et al. benchmark report but was not selected for benchmarking in the present report. SATURN is a proprietary code and no details on this code are available in the open literature. Hence, the comparisons in chapter 8 are of limited usefulness.

c) It is impossible to compare results from different codes on a node-for-node or time-for-time basis because different nodal spacings and different time steps were used for each of the codes. For example, compare tables on p. 132 and p. 258 for problem 8.2 and tables on p. 19, 62 and 163 for prob. 3.2. Even when results are graphed, comparisons cannot always be made. For example, compare the

figures on p. 131 and 257. The axes are oriented quite differently, making a direct comparison difficult. I find it hard to believe that the authors of this report were charged to make code comparisons because it is evident that no effort at all was made to facilitate code comparisons of simulation results. I do think that code comparisons would be a good idea but can appreciate that it may be difficult to get the codes to generate output at the same points in time in space.

I should also point out that similar types of output forms are not always provided. For example, a table of values is provided for the SWIFT simulation of Prob. 3.4 (pp. 172-173) but a similar table is not provided for the USGS3D solution of this problem. Similarly, some simulations have graphs but no tables, while others have tables but no graphs. In general, a comparison is made with an analytical solution when one is available. But this is not always the case. For example, in Chap. 6, the NUTRAN simulation is compared with the analytical solution for Prob. 8.1. PORFLO and NWFT/DVM were also used to solve Prob. 8.1 but no comparison with the analytical solution is made for these codes. Sometimes the analytical solution is provided in graphical form but not in tabular form. For each simulation there should be a table of values as well as a graph of the results. When an analytical solution is available, the table should include the analytical results as well as the numerical results.

Another thing I found surprising is that except for a comparison with NUTRAN in Chap. 6, p. 388, the results of the INTRACOIN study are not presented for comparison. When appropriate, reference is made to the fact that the INTRACOIN results are available and in some cases we are told that the comparison is "good" (e.g., p. 415) or "excellent" (e.g., p. 422) but the comparison with INTRACOIN data is not shown. Why not present the results of the INTRACOIN study?

d) The output of results is reasonable in all cases.

In the enclosed report you will note that I have mixed editorial comments with technical comments. It is my belief that both are of equal importance. The utility of the NRC Benchmarking reports will depend on whether the presentation is clear, consistent and complete. In discussing the "how-to's" of a simulation, there is enormous potential for confusion. Hence, it is critical that all statements be as specific as possible, even if it is necessary to be repetitive. It is essential to help the reader by continuous reference to other sections in the report and to relevant Tables and Figures. It is also imperative that a heroic effort be made to eliminate all typos from the final version of the report. To my dismay, I find that the earlier Benchmark Report by Ross et al. (1982) is rife with typos.

It is also unfortunate that the draft Benchmark report now under review does not consistently use the notation introduced by Ross et al. I also find it unfortunate that the Ross et al. report is not internally consistent with respect to notation which, I must remind you, is something I pointed out in my Aug. 1982 review of that report which was then in draft form. In particular, at that time I commented that many different symbols are used for the same parameter. The authors of the present report have reverted back to the most widely accepted symbol for most parameters. For example, in the present report the commonly accepted symbol psi is used for pressure head while Ross et al. used the non-standard symbol h for pressure head. Also, in the present report either alpha or epsilon is used for dispersivity. Alpha is the standard symbol. However, Ross et al. use the non-standard chi for dispersivity. In my Aug.

1982 comments I suggested that Ross et al. use consistent and standard notation for parameters. Evidently my suggestion was not accepted. I really think that this sort of inconsistency will drive readers wild.

In the enclosed comments I point out several examples of inconsistency and typos but I'm sure I didn't catch them all. Someone needs to go through both reports and make sure they are consistent and free from typos. An errata sheet should be prepared for Ross et al.

I assume that you are aware that the present draft report is incomplete in that the writeup for the CCC simulation of Prob. 5.3 is missing from Chapter 9.

Please feel free to call me if you have any questions about my report.

Sincerely,

Mary P. Anderson

Mary P. Anderson, Ph.D.
Hydrogeologist

COMMENTS ON: BENCHMARKING OF FLOW
AND TRANSPORT CODES FOR LICENSING ASSISTANCE

BY MARY P. ANDERSON

CHAPTER 1

p. 5 on FEMWATER: change "to simulate ground-water flow through saturated porous media" to "to simulate water flow through variably-saturated porous media"

p. 8, Table 1.1: Many entries in this table are incorrect.
NWFT/DVM: delete 8.2 and 8.4
SWIFT, second entry: delete 10.1 and 10.2
(also explain why there are two entries for SWIFT)
USGS3D: add 3.3
PORFLO: add 3.3 and 9.1; delete 3.4, 3.5, 5.3 and 8.4
CCC: add 3.1

List the entries in order of Chapters--i.e. Chap. 2, USGS3D should be listed first and CCC (Chap. 9) should be last.

It would be useful to provide another table as a companion to Table 1.1 which provides the same information in another form. I prepared such a table for my own use:

PROBLEMS	CODE USED TO SOLVE PROBLEM
3.1	CCC
3.2	USGS3D, SWIFT, PORFLO, CCC
3.3	USGS3D,PORFLO
3.4	USGS3D, SWIFT
3.5	USGS3D, SWIFT
3.6	SWIFT
4.1	FEMWATER
4.2	FEMWATER
4.3	FEMWATER
5.1	PORFLO, CCC
5.2	PORFLO, CCC, SWIFT
5.3	SWIFT, CCC*
6.1	SWIFT
7.1	SWIFT
8.1	PORFLO, NUTRAN, NWFT/DVM
8.2	PORFLO, NUTRAN, SWIFT
8.3	PORFLO, NUTRAN, NWFT/DVM
8.4	NUTRAN,SWIFT
9.1	PORFLO, SWIFT
9.2	SWIFT
9.3	SWIFT
10.1	FEMWASTE
10.2	FEMWASTE

*Information about the CCC simulation of Prob. 5.3 is not provided in the draft report.

Note that none of the codes were used to solve problems 5.4 and 8.5 in Ross et al. (1982).

GENERAL COMMENTS ON CHAPTERS 2 - 9

(1) Example mass balance checks should be provided for all simulations.

(2) Nodal grids with scales should be shown for each simulation.

(3) Because this benchmarking report is to be used as a companion volume to the report by Ross et al. (1982), "Benchmark Problems for Repository Siting Models", it is imperative that the notation used in the two reports be consistent. Unfortunately this is not the case for many of the simulations reported. Inconsistency will make it very difficult for the user to sort out notation. This problem is complicated by the fact that there are many bad typo's in the Ross et al. report. Furthermore, it appears that new ideas about the benchmark problems were incorporated in the present report. For example, a long term solution to Prob. 3.2 is presented in the benchmarking of codes report (Chap. 2) but only the short term solution is mentioned in the Ross et al. report. Another example is for Prob. 9.1. Ross et al. present a simple equation for a single nuclide while the correct equation for a nuclide with chain decay is presented in the present report. I list the inconsistencies and typos in the Ross et al. report that I happened to notice in the following pages of my comments. An errata sheet for the Ross et al. report should be prepared.

CHAPTER 2
BENCHMARKING OF USGS3D

(1) The USGS recommends that when designing a grid, nodal spacing not be increased or decreased by more than a factor of 1.5 from one node to its nearest neighbors. The reason for this guideline is related to the use of a harmonic mean for hydraulic conductivity and to concern over maintaining the accuracy of the finite difference approximation for irregular nodal spacing. The grids used in the example often violate this guideline (e.g., p. 15, 16, 49). Some discussion is needed on this point.

(2) The version of the USGS three-dimensional flow model that was tested is being phased out by USGS in favor of their new "modularized" model that has just been released. These problems should be re-run with this new version of the USGS model.

PROB. 3.2: The notation used in the equations is not consistent with the notation presented in the earlier NRC report by Ross et al. (1982) on "Benchmark Problems for Repository Siting Models". Some specific examples of discrepancies are noted below. All equations and notation should be consistent between the two reports.

Eqn. 2.1 has Ss on the RHS while Eqn. 3.5a in Ross et al. has an S on RHS. A typo in Ross et al. omits the ' on the RHS of eqn. 3.6.

In Ross et al. B is written without the '. Compare eqn. 3.7 in Ross et al. with Eqn. 2.6a in the present report. Also note that the leaky well function is called "H" in Ross et al. and "W" in the present report.

p. 14, Fig. 2.2: The equations on Fig. 2.2 appear in a different form when compared to the equations presented in the text on p. 13. This creates confusion and forces the reader to take the time to check that the equations are indeed consistent. Especially confusing is the introduction of a new and undefined symbol, S', on Fig. 14 in the definition of B'. The reader must wonder if this is some sort of typo or if S' = Ss' b. Write all equations on Fig. 2.2 in the same form as they appear in the text.

There is an inconsistency in the definition of the short term time limit between Ross et al. and the present report. In Ross et al. (p. 16) b' is squared, whereas it is not in the present report (bottom of p. 12). Furthermore in the equations on p. 159 of the present report b' is squared in the short term as well as the long term time limit definition.

p. 13: There is a typo in the definition of u'. Should be (1 + S'/ 3S) u not (1 + S')3S) u. Should use u' on Fig. 2.2 when defining the long-term solution.

Fig. 2.2: What is the meaning of the dashed line with the bars around it?

- Top of p. 15: Should give the value of the thickness of the aquifer, b. Is it 50 m?

p. 15, section 2: "to accurately represent" is a split infinitive.

Bottom of p. 15: Should emphasize that k=1 indicates the bottom layer. Is the thickness of the 2nd layer really 46 m? This represents a large increase in Δz from layer 1 to 2 and a large decrease from layer 2 to 3. See comment on this under "General Comments" section above.

p. 16: It is not a trival exercise to take advantage of the symmetry of the problem and simulate only one quadrant. Because of the way the model includes no flow boundaries along the edges of the grid blocks, it is necessary to adjust hydraulic conductivities for the blocks along the boundaries and to divide Q by 4. You should explain the procedure for these adjustments in complete detail. This will create enormous confusion for the uninitiated unless you are careful to explain each step completely.

p. 16, top of page: Talking about layers of unit thickness here will create confusion for those not familiar with the tricks associated with using the USGS3D model. You really need to explain about the two modes of operation of the code: basic mode (input K and Ss and true Δz's) and standard mode (input T and S and set Δz's equal to one).

p. 16, middle of the page and Fig. 2.3. The origin (i.e., x = y =0) is not shown clearly on Fig. 2.3. Moreover, the origin as defined in the figure is at the lower LHS of the grid. In the USGS code the origin is always defined to be the upper LHS. This will create confusion. Grid blocks should be shown and numbered on Fig. 2.3.

p. 16, middle of the page: Should explain what you mean by "active block".

p. 17, the weighted average and bottom of p. 15: Why was it necessary to use so many layers? You evidently used the USGS3D model in so-called "basic" mode, where you input values of K and set Δz such that the thickness of the hydrogeologic unit equals the sum of the Δz's for the layers that represent that unit. However, if you use the USGS3D model in the standard mode, you represent each hydrogeologic unit by one layer and input values of T and set Δz for all layers equal to one. In standard mode it is still possible to represent an aquitard by one layer of nodes and to assign a storage coefficient to that layer. This can be done without using the so-called TK option. (Use of the TK option eliminates the layer of nodes that represents the aquitard and forces one to assume that the aquitard has no storage.) Use of the standard mode without the TK option would seem to be a better and simpler way to represent this problem.

p. 19 and 20: Present the results from the analytical solution as well.

PROB. 3.3: There is a typo in eqn. 3.9a in Ross et al. (p. 17). On the RHS of the eqn., "h" should be "s".

p. 23: There is a mix of upper and lower case u below eqn. 2.10. Use all lower case. Also note that in Ross et al. (p. 18) the variable of integration is designated by "v" instead of "u". Be consistent in notation between the two reports.

p. 23, bottom of page: As with prob. 3.2, you need to explain that in order to treat one quadrant of the problem it is necessary to adjust the hydraulic conductivities of the boundary blocks as well as divide Q by 4.

p. 24: Need to show a figure illustrating the grid, as well as provide the information on exact grid dimensions currently given on p. 24.

p. 27 and 28: Present the results of the analytic solution as well.

PROB. 3.4: p. 29, last paragraph: Change "the Meguma ground and" to "the Meguma Group of Precambrian age and"

p. 33, eqn. 2.9: Need to explain that the 3-D model can be used to solve 2-D problems by using only one layer. Eqn. 2.9 should be labelled 2.11; refer to p. 23. where you will see equation 2.10 .

p. 33, middle of the page: When you talk about bottom and top boundaries as well as side boundaries, you are defining boundaries of a three-dimensional problem domain. This is confusing because you have introduced a two-dimensional equation (eqn. 2.9) as the governing equation. Need to separate true boundary conditions for the two-dimensional problem from assumptions one implicitly makes as a result of conceptualizing the system in two dimensions.

p. 33, 3 lines above section 2.4.2: Change "in the river stage (L)" to "in the river (L)".

p. 34: The symbol for the pumped well is missing from the legend.

p. 35, 1st full paragraph: Change "USGS3D requires the use of two extra rows and two extra columns of grid blocks" to "USGS3D requires the use of two extra rows (rows #1 and 23) and two extra columns (columns #1 and 24) of grid blocks".

p. 38, Fig. 2.13: Change "Frind & Pinder" to "Pinder & Frind". Also explain the citation to "SEFTRAN" and give a reference.

PROB. 3.5: p. 46, 3 lines above section 2: Change "nodes was added" to "nodes (layer #11) was added". Also note that "to more correctly place" is a split infinitive.

p. 46, Section 2: You say the grid is 21x10x10, yet on p. 49 there are 11 layers. Moreover, on p. 48 you show a plan view grid that is 21x10 without boundary nodes. It would seem that the actual dimensions of the grid are 23x12x11, including the inactive boundary nodes and the ficticious top recharge layer.

p. 49, Table 2.5: the total number of nodes is 23x12x11 or 3036, instead of 2000.

p. 50, beginning of section 2.5.3: You don't rigorously (i.e., mathematically) define boundary conditions. Refer to Figures 2.16-2.18 to guide reader to "the aforementioned natural boundary conditions".

p. 50, end of 1st full paragraph: Why isn't the easterly flow of water in the upper aquifer simply due to the constant head boundary that penetrates only the upper aquifer? This boundary would cause water to be directed toward it. Why do you suspect that the highly transmissive vertical zones play a role in deflecting the flow lines? A seemingly different explanation of the flow patterns is given on p. 176 for the SWIFT simulation of the same problem.

p. 50, the water balance: It would be useful to present the discharge to each node along the constant head boundary. It would also be useful to present the breakdown of water flowing upward from the lower aquifer to the boundary nodes and the amount of water flowing through the upper aquifer to the constant head boundary (the river). Perhaps this would give a better sense of the three-dimensional aspects of this problem.

p. 50, bottom of page: Why is it "of interest to note" the mass balance error, other than the fact that one is always interested in the mass balance error?

p. 50, bottom of page: Change "with discharge being greater than sources" to "with outflow being greater than inflow".

p. 50, bottom of page: You need to explain what you mean by restart. Also Why does this particular problem exhibit asymptotic convergence?

p. 54, top of page: Need to explain what you mean by "using vertical instead of horizontal slices". Refering to SSOR (slice successive over-relaxation) and pointing out its similarities to LSOR might help. Give a reference for either or both SSOR and LSOR. Are you sure that only "minor" changes would need to be made to the USGS3D code. What is your idea of "minor"?

CHAPTER 3
BENCHMARKING OF PORFLO

PROB. 3.2: p. 58, You need to explain that you used a pie shaped wedge where the grid was placed over the cross sectional face of the wedge. How was discharge from the well, at the point of the pie, handled? What was the thickness of the wedge? By what fraction did you divide the total pumping rate to simulate flow from only a portion of the radial problem domain.

p. 60, 1st line: Change "common methods" to "other methods"

PROB. 3.3: p. 63, 2nd line under section 3.3.2: medium should be media; change "the given problem" to "problem 3.3".

p. 63, 3rd line under section 3.3.2: Shouldn't "point source" be point "point source/sink"? If the code can't handle a point sink boundary condition, how were you able to use it to solve Prob. 3.2? Presumably you mean that the code can't handle a radial coordinate system as well as anisotropy. But this isn't what you say. Please clarify.

p. 63, under point #1: An aquifer thickness of 1 m needs explanation.

p. 63, equation for "f" at the bottom of the page: Do you mean that this factor is for the y-direction? Is there another factor for the x-direction? Your presentation on Table 3.4 would seem to indicate two factors. p. 63, bottom of page: I think you mean to refer to equation 2.10, not equation 2.11. However, reference to either equation is not enough to justify the derivation of the "f" scale factor. You need more explanation here.

p. 66, Table 3.4: Present the analytical results as well.

PROB. 3.4: There is a typo in eqn. 5.2a in Ross et al. (p. 57). Last term on LHS and the term on the RHS uses T instead of u.

p. 69, Fig. 3.3; Table 3.5, p. 72; Definitions on p. 68 nad 70: The use of the subscripts r,R and m is very confusing. Need to explain and emphasize the differences. In particular, explain what you mean by "the combined medium" on the top of page 70 and on p. 68 when defining Km use the word aquifer instead of rock. Also be consistent when referring to the bedrock. At various times you refer to it as "bedrock", "confining bedrock", "cap rock". Also note that Q on the Fig. and in the equations but is QI in the table. Be consistent.

p. 70, bottom line of equations: Lambda should be tau. The definition of alpha is not consistent with Ross et al. (p. 59). Ross et al. use upper case R for the subscripts.

p. 71, under section 3.4.2: Are any special tricks necessary to take advantage of the symmetry of the problem? Did you need to adjust boundary hydraulic conductivities, as in the USGS3D model?

p. 71, 1st para. under 3.4.3: What do you imply by saying you disregarded the bedrock in the second case simulation? Did you remove those nodes from the grid or did you set relevant parameters to zero?

p. 76, caption to Fig. 3.5: Change "bed rocks" to "bedrock"

PROB. 5.1b: Eqn. 3.6 and 3.7 on p. 79 is inconsistent with eqn. 5.1a and 5.1b in Ross et al. (p. 57).

p. 80, Fig. 3.6: What do the zeroes over the T's signify? A T with a zero over it has not been defined.

p. 81, eqn. 3.10: The notation here is inconsistent with the notation presented on p. 70 of the same report. Why has the new symbols k and k' been introduced into eqn. 3.10?

p. 81, under section 3.5.2, definition of velocity. Ross defines velocity (incorrectly) to be Q/b. Define W in the text to be width of the flow section.

p. 81, under section 3.5.3, end of first para.: Insert "used to evaluate the term du/dx in equation 3.6." after "differencing options". Delete "provided in the code."

p. 84, last line of first para.: Delete "as".

p. 84, 4th line of second para.: insert "probably" after "for this is"

p. 84: 5th line from bottom: change "because of the" to "because of greater"

p. 93: Define 2a in the text.

p. 93: Section 3.4.2 should be 3.6.2

p. 96, end of 1st para.: Why did you select a value of 35.5 for Km? Why not select some non-zero value that is closer to zero?

p. 96, 1st line of 2nd para.: change "mentioned" to "necessary"

p. 96, 2nd para., 5th line: The lambda sub D value for KR=0 is missing.

p. 96, last line of text: omit the word "analytically". Give a source for these equations. Refer to p. 92 of Ross et al. or to p. 123 of the benchmark codes report. Also note an inconsistency between these equations on p. 96 and similar equations on p. 123 of this report. In both cases the

symbol v is used. But on p. 96 v refers to Darcy velocity and on p. 123, v refers to seepage (or average linear) velocity. The issue is further confused because Ross et al. (p. 57) refer to v as the average interstitial velocity when they mean the Darcy velocity.

p. 99, 7th line of text: "unbound" should be "unbounded"

p. 100, Fig. 3.13: Label the two analytical curves with values of lambda sub D.

p. 101, Table 3.15: Give the analytical results as well.

PROB. 8.1: p. 103, 1st para. misleads the reader because it later turns out that PORFLO can't handle decay chains so you don't test for all these great things afterall.

p. 103, eqn. 3.17: A different symbol is used here for dispersivity than was used by Ross et al.

p. 104: piezometric is misspelled. In any case, should use potentiometric instead.

p. 105: Change "relating adsorbtion to concentration" to "which relates the adsorbed concentration to the concentration in solution"

p. 105: inconsistency with Ross et al. in symbol used for effective porosity. Ross et al. use n, phi is used here.

p. 106, eqn. 3.19a and b: give limits for t. $\bar{t} > 0$?

p. 106, after eqn. 3.20, Harada et al. (1981) should be (1980).

p. 106, just above section 3.7.2: Need to define retardation factor.

p. 107, Phi is effective porosity, not porosity.

p. 111, end of 2nd para.: Change "for cases 1 through 4" to "for inventory 1 (cases 1 through 4)" and change "for cases 5 through 8" to "for inventory 2 (cases 5 through 8).

p. 114, 4th line of text: Should refer to Figures 3.15 and 3.16 instead of 3.10 and 3.11. Do the breakthrough curves in figs. 3.15 and 3.16 represent data computed by PORFLO or are they taken from the INTRACOIN study?

Tables 3.18 and 3.19: According to Ross et al. there is an analytical solution for this problem. No reference is made here to the analytical solution. Why not? Should present a comparison with the analytical solution.

PROB. 8.2: p. 121, Eqn. 3.16 should be labeled eqn. 3.21. This equation is inconsistent with Ross et al., where upper case c's are used.

p. 123, below eqn. 3.22b: Should reference eqn. 3.20, not 3.19.

p. 123, 3rd line from bottom: Reference to "the mentioned limitation" is too vague. Be specific.

p. 125, top of page: change "zero normal concentration gradient was used on the" to " a concentration gradient equal to zero was assumed normal to the"

p. 125, 6th line of section 3.8.3: the lambda is missing from the power of e. Also, Section 3.5.2 should be 3.7.2.

p. 126, 4th line from the bottom: "reasonable" should be "reasonably"

p. 130, Table heading; "Azis" should be "Axis". Give units for flux.

p. 131: typo on label for horizontal axis: i per cubic meter should be ci per cubic meter. p. 132: Why was the value for y=0 omitted?

PROB. 8.3: p. 135, 3rd line from top: Section 3.5.2 should be 3.7.2.

p. 135, 2nd line from bottom: Give a page number for the INTRACOIN report or better still reproduce the curves in the present report.

p. 136, top line of table: V should be lower case v; porosity should be called "effective porosity"

There are typos in eqn 8.1 of the Ross et al. report (p. 88). All the differential signs were omitted from the equation.

PROB. 9.1: The notation used in eqn. 3.24, 3.25 and 3.26 is inconsistent with notation used by Ross et al. (p. 99-100). Moreover, the equations themselves are different because the present report presents a more general form of the equation.

p. 141, definitions under eqn. 3.24: Use a lower case v for seepage velocity.

p. 143, eqn 3.27a: Use a lower case v for velocity.

p. 144, eqn. 3.28a and b: Give limits for t -- t>0 ?

p. 144, definitions under eqn. 3.28b: Is fracture "porosity" the correct term? It seems to me that fracture density would be better. The porosity of a fracture is always one or 100 percent.

p. 3.27, 2nd line of table: Use lower case v for velocity.

p. 146, 4th line: insert "as explained in section 3.7.2" at the end of the sentence which ends in the middle of the 4th line.

p. 146, last line: "the PROFLO code" should be "the PORFLO code". Furthermore what exactly is meant by the statement: "The PORFLOW code did not couple the contribution of the fracture domain correctly into the solution of the system of finite difference equations"? --"couple the contribution of the fracture domain"????????

p. 147, Fig. 3.24: What is the meaning of the symbol following the word "FRACTURE"?

p. 147, insert "(Run 1)" at the end of the table heading.

CHAPTER 4
BENCHMARKING OF SWIFT (POROUS MEDIUM PROBLEMS)

GENERAL COMMENTS: In Chapters 4 and 5, both on SWIFT, and in Chapter 7 on DWFT/DVM and in Chap. 9 on CCC, a different convention is used in labelling figures and tables. In the rest of the report figures and tables are labelled, 2.1,2.2,2.3 ..., for example, but in Chap. 4, 5, 7, and 9 they are labelled, 4.1-1, 4.1-2...4.2-1, 4.2-2, 4.2-3...

PROB. 3.2: p. 154, 2nd line: change "analogous to the specified parameters" to "consistent with the parameters for problem 3.2 specified by Ross et al. (1982)".

p. 154, near eqn. 4.2-2b: define re to equal aquifer simulation radius. Also, what is the Carter-Tracy boundary option? Explain and give a reference. Define "exterior system" explicitly.

p. 154, last para., 1st line: insert "vertically-oriented" after "one-dimensional".

p. 158, Change heading to "Distance to Block Center from the Origin"

p. 159, 2nd para., change beginning of 3rd line to: "problem determined by the time of travel...." Then delete "was used in this consideration." from the 4th and 5th lines.

p. 159, last para., reference Table 4.2-5 and comment on the discrepancy evident in Fig. 4.2-2 at early times.

p. 160, footnote says node 1 is at the "outer extremity of the aquitard" yet Fig. 4.2-1 shows the node well within the aquitard. Footnote says node 20 "attaches to a global block" yet Fig. 4.2-1 doesn't show this.

PROB. 3.4: 1st para. under 4.3.3. It is said that storage coefficients for the river bed nodes are given in Table 4.3-1. They are not listed in this table.

p. 164, 1st para. under 4.3.3: "This is of no consequence" What is of no consequence? If the storage coefficients for the riverbed are of no consequence, then why was it necessary to add them to the model?

p. 166: Define symbols for wells on Fig. 4.3-1b.

p. 167: Change heading to "Block Number"

p. 168: end of 1st para.: Define pore volume--see p. 193 where it is finally defined.

p. 168, 2nd para: reference Fig. 4.3-1 instead of Fig. 2.10.

p. 169: Change heading to "Distance from the bottom of the river*" You need to add a figure--perhaps an inset to the table-- to show these grids and how they attach to the main aquifer.

PROB. 3.5: p. 175, last para, 2nd line: "the and" should be "and the". Also what is meant by a mass balance of unity? Is this 1% or 100%?

p. 176: The explanation of the flow pattern seems to differ from that presented on in Chapter 2 for the USGS3D simulation. Furthermore, the explanation here seem more correct but is a bit garbled. Change "from the crushed and coarse-sediment zones" to "from the presence of the crushed and coarse-sediment zones"--11th line from bottom of page.

p. 176 and throughout the discussion of this problem in Chap. 4 reference is made to the basalt by which is meant the aquitard in Chap. 2. Use consistent terminology or define the aquitard to be composed of basalt.

p. 181-182: These figures are extremely confusing. Fig. 4.4-3 is not too bad when you realize that the "BASALT" in AQUIFER1/BASALT refers to when the contaminant moves vertically through the aquitard. You should note this fact in the caption and should label the recharge area as AQUIFER 2. However, Fig. 4.4-4 is really misleading. What you mean to convey by "BASALT/CRUSHED ZONE" is not at all clear. You must replace this figure by a three-dimensional representation. Or else delete the figure altogether. One's first impression upon viewing the present figure is that it doesn't make sense that the flow lines are deflected upon hitting AQUIFER 1, which is more permeable than the aquitard (the basalt). If you do replace it (the figure) by a 3D picture, be sure to give the orientation and location of the figure within the problem domain. No location is given for the cross section depicted in the present figure.

PROB. 3.6: p. 184, end of 4th line of last para: Change to "In those problems, it is further supposed that the repository"

p. 184, 3rd line from bottom: Change "as also shown in Figure 4.5-1" to ", shown as a rubble zone in Figure 4.5-1".

p. 186: The size of the nodal increments is not given. There is no scale on Fig. 4.5-2.

p. 188: Change heading to "Hydraulic Conductivity"

p. 189: Change "well" to "sink" and note that a sink of constant discharge was used to represent the river.

PROB. 4.6:p. 191, after 4.6.2: Reference to Table 3.7 should be Table 3.13 and Fig. 3.6 should be 3.11.

p. 193, after eqn. 4.6-2: "to completely specify" is a split infinitive.

p. 193, after eqn. 4.6-3: "transmissibilities" should be "transmissivities"

p. 193: Need to define "extensive" parameters explicitly as those parameters that depend on block geometries. The present phrasing is unclear. Same with "intensive" parameters.

p. 203: Footnote: Change "adjacent to" to "surrounding the"

p. 206, 2nd line at top of page--typo "Dimensionaless". Also give the analytical solutions as well.

PROB. 4.7: p. 207, 1st para: Refer to Section 2.5 (not 2.4) and to Figures 2.16 through 2.16 (not 2.14-2.16).

p. 208: Show the boundaries of the various geologic units on this figure.

p. 209, Figure is misleading: The dense basalts appear to be the same thickness. On p. 216 it is implied that the upper dense basalt is 500 m thick while the lower dense basalt is 1000 m thick. Give thickness of all units on this figure and draw to scale.

p. 213: end of 1st para. and Fig. 4.7-3: The boundary conditions are not given in the figure. The boundary conditions for this problem need to to specified on four sides and should be specified for flow as well as temperature. The Fig. gives values of "P" in meters on only two sides. Presumably "P" should be head? Units are not correct for pressure.

p. 213: 1st para of section 4.7.3, 4th line: What is the 140 m strata? 5th line: "thermally" should be "thermal". End of para: last sentence doesn't make sense. The reference to Table 4.7-5 is inappropriate; none of the figures show that the underburden continues to transport head after 1000 years.

p. 213: 2nd para. of section 4.7.3, 2nd line: Change to "conduction as would be expected from"

p. 213, last line: change to "all positions have water flowing"

p. 214: This Figure is a drawn incorrectly. The boundaries of the units should match those shown on p. 45 (Fig. 2.18). It certainly doesn't make sense to have a recharge zone sandwiched in between two aquifers in a cross section. Figure should be re-drawn. Boundary conditions for flow and temperature should be indicated on all four sides of the figure. The reference to "Constant Head Boundaries" in the caption should be changed to "Specified Head Boundaries" because the heads are not constant in space. A scale should be provided.

p. 218 - 219: The lines indicating boundaries of geologic units are incorrectly placed. Figures should be re-drawn and geologic units should be labelled. A scale should be provided.

p. 220: The lines on this figure are drawn differently from the lines on the figures on p. 218-219. But these lines also are incorrect.

p. 221: What happens to velocity at point D? This is not clear from the figure. Also the line labelled with A and C should be labelled A and B.

p. 222, 2nd line: "three-dimension" should be "three-dimensional"

p. 222, 2nd para: Change to "...the response is lagged because compressions retards the pressure pulse and time is required to transport the heat." Also change "slow down to some degree" to "decrease".

p. 222, last sentence of 2nd para: add "as a result of high temperatures (see Table 4.7-3)" at end of sentence.

p. 222, last para: Change to: "transport away from the repository is predicted to be on the order of millimeters..."

p. 227: Fig. 4.8-3 is cited before 4.8-2. Need to switch the figures.

p. 227, 11th line from bottom: delete "though"

p. 233: 3rd and 4th lines from top: Change to: "The U-shape of the flow field is maintained throughout the transient response to the change in temperature and is basically the same as that shown in Fig. 4.8-1."

p. 233, last sentence of 1st para: Change to: "The velocity at point E is increased as a result of the heat, sometimes by as much as a factor of two."

p. 233, 2nd para, 2nd sentence: Change to: "In contrast to the undisturbed system, there is approximately 30 percent less salt available for dissolution ..."

p. 233: The discussion about dissolution rate is unclear. You first say the dissolution rate is 21.3 percent less. Then in the next sentence you say the rate is higher.

p. 233, last sentence: "to slowly return" is a split infinitive.

p. 235, figure caption: Change "at the River at" to "at the River as"

PROB. 8.2: p. 238, above eqn. 4.9-3: Change "analytic pressures" to "pressures determined analytically". Also give a source for the analytic solution.

p. 238, definitions below eqn 4.9-3: Change "flow rate" to "flow rate of well"

p. 244, below definitions for eqn: Give more information about the centered-in-space criterion. What is the criterion? Are you referring to the Peclet number?

p. 244, 10th line from bottom: delete "then"

p. 247, 3rd para: "occured" should be "occurred"

p. 250: Why is the label C-MAX used for both concentration (ci/cu.m) and for flux (ci/yr)? This occurs throughout the report and is extremely irritating and confusing.

p. 257: the horizontal axis is not labelled.

PROB. 4.10: p. 264, 2nd para: "As discussed in Section 4.7" This matter is not exactly discussed in Section 4.7. Section 4.7 only deals with times less than 10,000 years, not up to 725,000 years.

p. 264, last line of section 4.10.1: "specie" should be "species"

p. 264, last line: Refer to Fig. 4.4-3 and 4.4-4 not 4.4-5. Change to "The magnitude of several multidimensional effects were then evaluated relative to"

p. 267, 3rd line: change to "were evaluated along all five streamlines." 6-7th lines: What do you mean by "an approximate theoretical fasion"? Be specific. 8th line: Change to "breakthrough, there was concern that material would be dispersed laterally" 9th line: "streamline" should be "a streamline". 10th line: You need to make some conclusion about your second point before you go on to point #3. Presumably the point you want to make is that lateral dispersion was negligible. Last line: "base" should be "basic".

p. 267, 2nd line of 2nd para: You say there are 9 separate legs--one for each hydrologic unit. But there are only 4 geologic units--Aquifer 1, Basalt,crushed zone and ancient river bed. What do you mean by a "hydrologic unit"?

p. 267 and Fig. on p. 268: You say that the river is a "pressure boundary condition". On p. 189 the river was simulated as a sink. Comment on this switch from specified flow to specified pressure.

p. 270: The "2" superscript should be placed after "Velocity" not after "Darcy".

p. 272: Last two columns should be labelled as + and - values of TMAX not T.

p. 274: Indicate that tabulations are at a point representing the river.

p. 274: Should provide graphs showing these results as well as tables.

CHAPTER 5
BENCHMARKING OF SWIFT (FRACTURED MEDIUM PROBLEMS)

PROB. 6.1: Notation in equations 5.2-1a & b is different from Ross et al.

p. 278: What is a "singly porous media"? A single porosity medium??

p. 278, last line: change to: "single porosity characterized by a storativity S1+S2."

p. 281, 4th and 5th lines in section 5.2.3: reference Fig. 5.2-2 amd 5.2-3.

p. 281 and 283: Seems to me that the "pseudo-steady state case" should be called the "single porosity case" and the "dual-continuum case"should be called the "dual-porosity case". I don't understand the rationale for your terminology.

p. 282, Fig. 5.2-4(b): the arrow supposedly showing the limits if d and a can't be correct.

p. 283: 1st full para, 3rd line: "transmissibilities" should be "transmissivities".

p. 283, line above eqn. 5.2-10: Change "providing" to "provided"

p. 283: Seems to me that eqn. 5.2-11 is incorrect. Should be

$$B_1^2 = \Delta z_1 (\Delta z_1 + \Delta z_2) K_1 / 2 K_2 S_2$$

p. 283, 4th line from bottom: What do you mean to convey by the statement that "all of the fractures were treated simultaneously"?

p. 283, 2nd line from bottom: 5.2-4b should be 5.2-5b.

p. 285: Change headings to "Distance to Block Center (m) from r = 0"

p. 287: What do the 6 dots on this figure represent? It is not at all clear how the "global blocks" fit into this discretization scheme. You need a paragraph of text to explain how global blocks work. label this figure as "(a)". Correct typo in last line of caption.

p. 289, 2nd line after eqn. 5.2-12, the values of parameter "a" are not given in Table 5.2-4.

p. 289, last para: What is the Carter-Tracy boundary-conditon option?

p. 290: Is B on this table supposed to be the same as B1? Same applies to tables on p. 293-294.

p. 291: The footnote is not clear because the way the global blocks work has not been made clear. Node 1 is at the "outer edge" of what? Node 11 is attached to "a specific grid block"--what does this mean? Are there vertical nodes, grid blocks and global blocks as well? ---3 types of gridding, or only 2? IT WOULD BE HELPFUL TO EXPLAIN THE MYSTERIES OF SWIFT GRIDDING IN SOME DETAIL IN A SEPARATE SECTION AT THE BEGINNING OF CHAPTER 4.

p. 292, 2nd para.: What does the fact that the rock matrix was described in more detail in the dual-porosity simulation, have to do with the differences in the curves? Need somemore explanation here. Surely the difference is related to a fundamental difference in viewpoint between the two approaches and presumably the analytical solution takes the single-porosity (pseudo-steady state) viewpoint.

PROB. 9.1: p. 295, end of 1st para: What do you mean by "one-dimensional prismatic units"? A figure might help.

p. 295, eqn. 5.3-1a and b: The notation and the equations themselves are different from those in Ross et al.

p. 296: What do the 5 dots represent?

p. 297, eqn. 5.3-1c: Notation here is completely different from Ross et al.

p. 297, definition of symbols--u and v: In other sections of the report v is called the seepage velocity or the Darcy velocity. Here it is the interstitial velocity. First of all, the use of intersitital is inappropriate for a fracture which doesn't have interstices. Secondly, I do wish you would establish a consistent notation and terminology for this very important parameter. Call u the Darcy flux. Call v the average linear velocity. Please be consistent. I FIND THIS WAVERING IN SYMBOLS AND TERMINOLOGY MADDENING.

p. 298, 5th line: some words are missing here...

p. 298, above eqn. 5.3-5a-- the B1 condition. It is unfortunate that B1 was one of the important symbols in the previous section, where it had a completely different meaning. Can't you call this condition something else?

p. 299: line above eqn 5.3-6, correct typo "sytem"

p. 300: Here again we have "interstitial velocity"

p. 301: Don't use Kv for Retardation. The caption on the table says retardation is represented by the symbol R, which is the standard usage. Surely you don't mean to square the distribution coefficient? Also use an upper case K with a d subscript for distribution coefficient.

p. 304, 2nd para: Show graphs of the breakthrough curves. Few will care to follow your discussion without the graphs.

PROB. 9.2: p. 308, 1st para: Explain what you mean by "spherical units". A figure would help.

p. 311: "interstitial velocity" is used again.

p. 314: Correct typo: "Separtion"

p. 322: "to significantly impact" is a split infinitive.

p. 336: 1st para: Show graphs of the breakthrough curves.

PROB. 9.3:

p. 361: The SWIFT solution is not shown in this figure.

p. 363: The caption for this figure is incomplete. Should indicate that this is Bibby's finite element grid and that the dots represent nodes and the numbers are the node numbers. Why not show the entire gird of 252 nodes and 221 elements?

p. 367: What are the numbers along the outer edge of the figure?

p. 370: 6th line from the bottom: delete "and a time discretizations"

p. 376: The use of * is confusing here because it is part of the symbol for diffusion coefficient, D*, and is also used to indicate a footnote for the symbol 2a. Should use the symbol D', introduced in earlier sections to represent diffusion coefficient. Also should place the * after 0.5 m rather than after 2a.

p. 376, footnote, 1st line and last line: Is "q" a typo? Do you mean "a"? What is Dd? Is it diffusion coefficient, D* (or D')? If so then I am still missing something because diffusion coefficient (1.59 E-6) divided by 0.25 squared does not equal 5.1 E-5.

p. 377: last para, 2nd line: change "adapted" to "modified". 2nd line from bottom of para: "Forth" should be "Fourth". last line of para: What do you mean by the "Wingham data"? Are these the data in Fig.5.5-2? If so reference this figure.

p. 377, footnote: interstitial velocity is used again...

p. 383, 3rd line from bottom: diffusivity does not equal diffusion coefficient. You mean diffusion coefficient.

CHAPTER 6
BENCHMARKING OF NUTRAN

PROB. 8.1: p. 385, bottom of page: Give the formula for the increase of time step and give the initial time step value you fed into the formula for problem 8.1.

p. 387: end of 2nd para: Tell us the numerical value of "NUTRAN's time step of peak release"

p. 388: Evidently the second line represents the analytical results but you don't tell us that and make the reader play detective. Give us a break! Also, what is the footnote supposed to mean? Where is the error in UCB-NE reported? And asterisk is no indication of error.

p. 389: middle of 2nd para.: refer to the page in the Benchmark codes report ("A Summary of Repository Siting Models") by Thomas et al. (1982) where NUTRAN's "correction factor method" is discribed or take some space to discribe it here in the present report.

p. 390: Need to present tables of values as well as figures.

p. 398: 1st para: What was the initial time step for this problem?

p. 398, 3rd para, 3rd line: Change "the figure shows" to "Fig. 6-8 shows" Also change rest of line to "the release has a broad, flat peak and a small change in the numerical results can cause a different part of the crest to be slighly higher than the rest of the crest." Later in same paragraph yos you say that NUTRAN underestimates the radium peak. This implies that you believe the SWIFT results. Even if you suspect NUTRAN to be wrong, why do you imply that the SWIFT results give the exact answer?

p. 402: I went back to the SWIFT chapter and tried to find the numbers cited in this table. I was unsuccessful. I did find the times as stated in this table under the cartesian simulation. However, the rates I found in the SWIFT chapter were different (4.14 instead of 8.29 for U-234, 3.11 instead of 6.23 for Th-230, and 8.99E-6 instead of 1.90E-5 for Ra-226). What's going on? Also I thought the cartesian simulation for SWIFT was less accurate than the curvilinear simulation. Help reader find these numbers in the SWIFT chapter. Also, why not give the PORFLO results too for completeness, although I realize the PORFLO simualtion isn't exactly comparable. But it was used to solve this problem afterall.

PROB. 8.3: p. 403, 1st para. under section 6.4.3, 2nd line: "of as"--delete "of"

p. 403, last para: According to Ross et al. (p. 95) Prob. 8.3 corresponds to INTRACOIN Prob. #2. Now you say that the comparable INTRACOIN problem has different inputs and a comparison is not possible. What's going on? I feel cheated.

p. 403: Should give tables of results as well as graphs.

p. 406: Present PORFLO and NWFT/DVM results too.

PROB. 8.4: p. 407, 3rd para.: Section 4.10 should be 4.10.3. Also the statement "A similar assumption was made for convenience in the steps" doesn't make sense. What steps? What assumption? Convenience for what?

p. 407, 2nd para, end of 3rd line: Change to "a series of nine" p. 409: Give comparisons with the SWIFT results from table 4.10-6.

p. 410: Give tables of values as well.

p. 411, 1st full para.: Th and Ra are different too, not just U-234. Comment.

p. 411, last para.: What is meant by "the code's current versions of deterministic state changes and square-wave leaching". Explain everything clearly and completely or forget it.

CHAPTER 7
BENCHMARKING OF NWFT/DVM

PROB. 8.1: p. 414, 1st para. under section 7.2.3: refer to the page in the Thomas et al. report where the "distributed-velocity method" is described.

p. 414, bottom of page: This business about half-maximum concentrations has been bothering me since I first encountered in Chap. 4. It occurs is several places between Chapter 4 and p. 414 and beyond 414. First you need to define what you mean by half-maximum concentrations. It is not self-evident. Try to help the reader as much as you can. I assume you mean the concentrations that are half of the peak. On a breakthrough curve for a non-continuous release, there are two half-maximum concentrations, one on either side of the peak. Evidently for some logic that escapes me the one which occurs after the peak is indicated by a -50% while the one that occurs before the peak is indicated by a +50%. Seems to me it should be the other way around.

p. 415: Why don't you show us the comparison with the INTRACOIN study? Don't just tell us that the comparison was "quite good". Show us and let us judge for ourselves.

p. 415, 3rd line from bottom: Surely "conservativity" isn't a word. How about "conservatism"?

p. 415: Show graphs of the results as well as tables.

PROB. 8.3: p. 421, 1st line under section 7.3.2: Change "of that section" to "of section 3.9".

p. 421, 1st line under section 7.3.3: Change "The model" to "The model NWFT/DVM". 3rd line: What desired speed and dependability? You mean to say that the model as it was written is not dependable. You need to be more specific here. What sort of "statistical calculations" are you talking about? Why can't the model be run on this problem without retaining the statisical nature of the model?

p. 421, 2nd para. under section 7.3.3: "specie" should be "species". Also define $\bar{R}$ with a bar over it to be an effective retardation factory. I assume you mean "retardation" to imply the usual retardation factor? If so use retardation factor not just "retardation".

p. 422, results: Should present graphs of results as well as tables.

p. 422, 2nd para. under section 7.3.4: Ra is compare low to INTRACOIN? How do you know INTRACOIN is the correct answer? Also define "secular equilibrium" here and elsewhere in the report. I know it occurred in one of the earlier chapters. I asked a friend who is a physical chemist the meaning of secular equilibrium. He didn't know for sure. I think you need to define it. His best guess was that it meant equilibrium throughout the system as opposed to local equilibrium. You can't expect all your readers to be radio-chemists. Please define your terms. Again please refer to "retardation factor" instead of just "retardation".

p. 422, above eqn. 7.3-3: Change to: "However, NWFT/DVM uses an effective retardation factor defined by eqn. 7.3-1.

p. 423: Refer to "retardation factor" not "retardation"

p. 424: Footnote: How were the parameters "suppressed"? Do you mean these parameters are not relevant to NWFT/DVM? I see that L1 is irrelevant. I've forgotten the meaning of the other symbols. How about giving the reader a break and not make him hunt through the report to search for their meaning?

CHAPTER 8
BENCHMARKING OF FEMWATER AND FEMWASTE

p. 426: First reference to 10.1 should be to 4.3.

PROB. 4.1: p. 429, give limits on x and t for the boundary and initial conditions.

p. 435: Give the analytical results too.

PROB. 4.2: p. 437, 1st sentence: Should be "to test the code's". Also the notation used in eqn. 8.4 is inconsistent with Ross et al. and the equation itself is in a different form.

PROB. 4.3: p. 445: Notation in eqn. 8.6 differs from Ross et al.

p. 451, 2nd para, last sentence: Change phrase to: "the referenced time value (t^*)".

p. 460: present the analytical results as well.

PROB. 10.2:, p. 461: Notation in eqn. 8.10 differs from Ross et al. Ross et al. use the non-standard symbol "B" for retardation factor. The standard symbol "R" is used in eqn. 8.10.

p. 464, top line: Should use the standard symbol, alpha, for dispersivity to be consistent with the rest of the report. Unfortunately, Ross et al. use several symbols, including chi, to mean dispersivity.

p. 466, 2nd para, last sentence. Do you mean to imply that the numerical oscillation causes errors to accumulate so that the solution becomes worse through time?

CHAPTER 9
BENCHMARKING OF CCC

PROB. 3.2: 1st line: "overlained" should be "overlain". 3rd line from the bottom: typo--"summalized". Last two lines: You need to explain this business about the "vertical connections". Are these "connections" similar to the nodal connections in SWIFT? Evidently they aren't the same sort of thing. You need to discuss and contrast with SWIFT.

p. 472, 2nd para.: If the 2 equations are solved sequentially without iteration they are NOT coupled. Change sentence to: "The equations are solved alternately by interlacing them in time."

p. 472, end of 2nd para: If the code controls the time steps automatically then the user does not control the time step. You can't have it both ways. What do you mean here? The user has some control evidently by specifying certain criteria which feed into the time step formulat. Specify the criteria.

p.473: Change or delete the last sentence. The reference to one and two dimensional simulations is confusing.

PROB. 5.1a: 3rd para, 6th line: insert "of" after "upper half". 4th line from bottom; "assumption" should be "assumptions". 3rd line from bottom: Give reference for Avdonin solution.

p. 489: 2nd para: 5th line: "taking" should be "taken". last sentence: change to: "We used grid blocks similar in size to those specified for other codes used to solve this problem."

PROB. 5.1b: p. 487, 3rd line of 1st para: Change to "...the first 40 are the smae as those in Table 9.4-2 but with half the spacing and an additional 35 nodal blocks with spacing of 30 m were inserted. For a coarser mesh, we doubled the sizes of the first 22 nodes of Table 9.4-2 to represent the aquifer.

p. 487, 2nd line from bottom; insert "the" after "with"

p. 488: correct typo: "accutrately"

p. 493: Footnote doesn't make sense. What does it mean? p. 495: Footnote doesn't make sense.

p. 499: Delta signs are missing from the key.

PROB. 5.2: The figures and tables are all grouped at the end of this section unlike previous sections in the report where figures were placed within the text. Moreover, throughout the section reference is made to Figures and Tables in section 5.4 when section 9.5 is intended. For example: p. 500 above eqn. 9.5-2, Fig. 5.4-1 should be Fig. 9.5-1. Also, see p. 501, there are three references to Fig. 5.4-2 when 9.5-2 is intended. Also there are two references to Table 5.4-2 when Table 9.5-2 is intended.

p. 500, 2nd line above eqn. 9.5-2: "an the dimensionless" should be "and the dimensionless"

p. 501: middle of 2nd para: the discussion of the 0.03 factor and the use of the 3% injection rate is TOTALLY unclear.

p. 502: one line beneath eqn. 9.5-5: correct typo: "coordiante"

p. 502: 7th line from bottom: Give reference for Gringarten and Sauty.

PROB. 5.3: No information is presented except a note that Problem writeup in preparation".

TECHNICAL STATUS

Tasks 4&5 - Radiological Assessment Codes

During July the program ANSIDECH, a short Fortran program developed by CorSTAR was run for all of the decay heat benchmark problems. Comparisons between ANSIDECH predictions of decay heat levels and predictions made using using the code ORIGEN indicated very good agreement for pressurized water reactors at high fuel exposure and fair agreement for BWR fuel assemblies at high exposure. We believe that the discrepancy between ORIGEN and ANSIDECH predictions for the BWR fuel assemblies are caused by the cross-section library used with ORIGEN. This will be investigated further as additional ORIGEN runs are made with different cross-section libraries.

TECHNICAL STATUS REPORT
ATTACHMENT TO PROGRESS REPORT FOR JULY

Repository Design Codes

Task 4 - Solve Benchmark Problems

Code Procurement

No new codes have been received during the month.

Discussions have been held during the month related to the use of ADINA/ ADINAT. As stated in last month's progress report, the NRC's version is outdated and does not include ADINAT. We recommend that the NRC procure this code for the following reasons:

- ADINA/ADINAT is a widely used two- or three-dimensional general purpose finte-element code supported by its developers. This is the only such code we will be benchmarking. General purpose codes such as these are used for a variety of problems by a large number of engineers and are thus tested through continued use. For this reason, results from a widely used code are likely to be more generally accepted than from a special purpose code.

- ADINA has a failure criteria specifically applicable to geological materials (Drucker-Praeger); whereas, many of the other general purpose codes such as ANSYS do not.

- Although ADINA/ADINAT is widely used, it is not as sophisticated with respect to user friendliness as codes such as Version 4.0 ANSYS. Although this is a slight disadvantage, costs for procurement of ADINA/ADINAT are significantly less than for ANSYS.

- It has been suggested that the NNWSI project will use ADINA/ADINAT (D. Fehringer letter of February 1, 1983). No confirmation of this has been received.

- The procurement of ADINA/ADINAT would result in savings of computer costs as opposed to running the codes on a time/sharing service. Although the cost to the NRC of computer time at Brookhaven is not known, the procurement cost of ADINA/ADINAT could easily be exceeded by usage fees from an outside timesharing service.

The ease of use of ADINA/ADINAT has been questioned by the NRC. The code has a fixed format data entry requirement and relatively simple data generators. Although this is rather cumbersome, with the use of a personal computer for data preparation, it is not difficult. The format is similar to the SAP IV and the DOT formats. It is considered that a working knowledge could be gained in code use in about one week (for someone familiar with finite element theory).

Code Installation

MATLOC and COYOTE have been compiled and absolute versions installed on MFZ. MATLOC required minor modifications to locate certain blocks in the large core memory (LCM). COYOTE was much more difficult in that both a large number of blocks had to be located in the LCM and an overlay structure had to be employed. Although COYOTE was installed for use on MFZ, two problems should be noted:

1. Certain cards from the plotting deck had to be deleted because the package is unavailable at BNL; and

2. The absolute load module (ALM) for the COYOTE program could not successfully be copied to a file for future reference. The problem is due to the overlaying feature used to allow the program to be compiled. Overlaying causes different sections of the program to occupy the same computer core space but at different times. Therefore, the ALM is not a constant but changes dependent upon input data sets. The relocated object nodule was stored instead, requiring a load sequence before each execution of the program.
   These are not considered critical to COYOTE's benchmarking or use at this time.

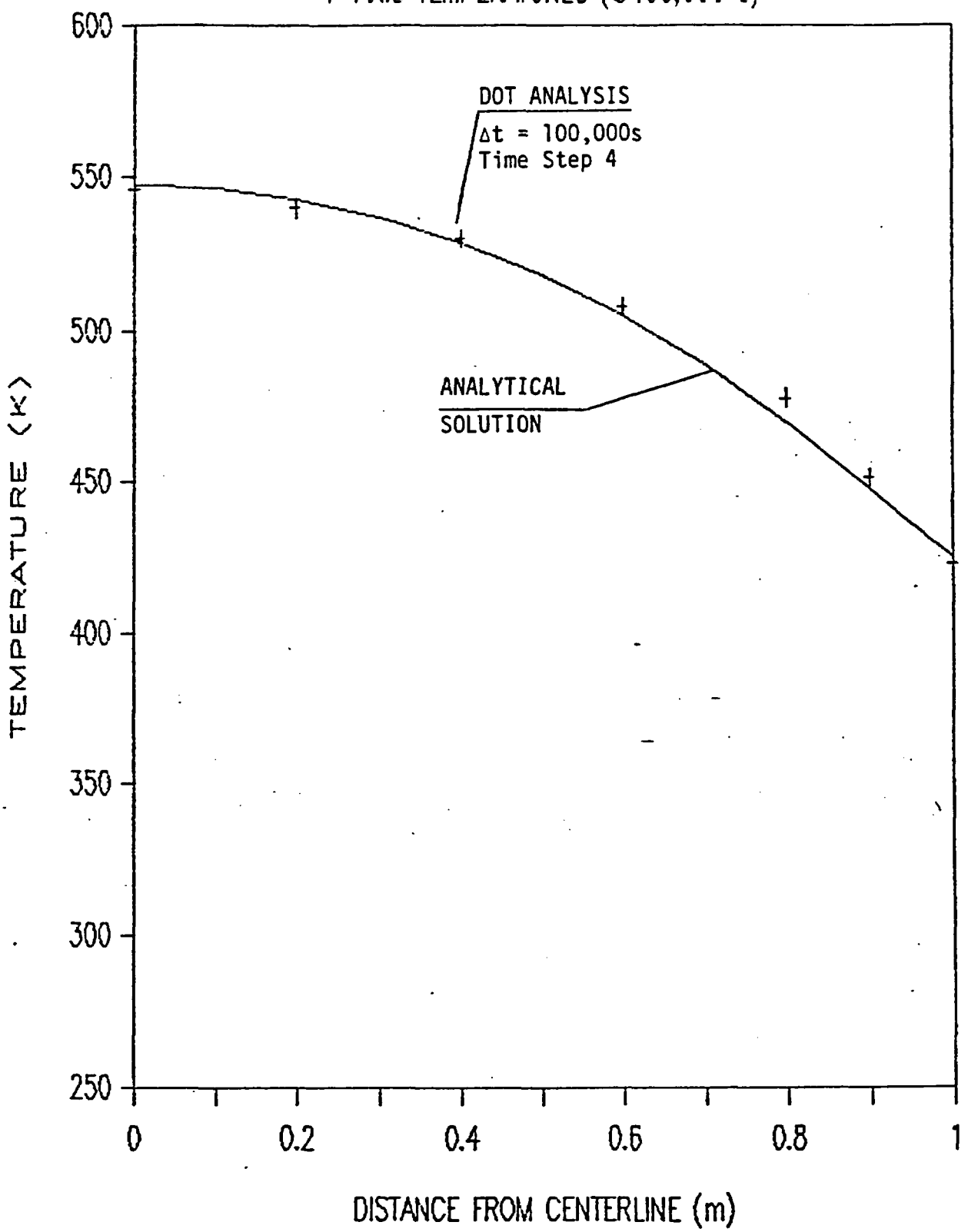
Benchmark Problems

Problems 2.6 and 5.2 (Basalt) have been successfully run with DOT. The results of 2.6 compare favorably with the analytical solution (see comparisons attached).

Problems 2.6, 2.8 and 5.2 have been set up for COYOTE but not run due to delays in compiling COYOTE.

RHC/jld
P6678.250
8/6/84

DOT PROBLEM 2.6



DOT PROBLEM 2.6