MAY 22 1990

Dr. Evaristo J. Bonano, Supervisor
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Division 6416
Sandia National Laboratories
Albuquerque, NM 87185

Dear Dr. Bonano:

Enclosed are NRC staff comments on the draft report prepared under Subtask 2.6d - Comparison of Uncertainty and Sensitivity Analysis Techniques. The title of the report is, "A Comparison of Parametric Estimation and Sensitivity Analysis Techniques for Ground Water Flow Models and Their Impact on the Uncertainty in Model Performance Predictions." These comments were prepared by Dr. Richard Codell of the Geosciences and Systems Performance Branch in the Division of High-Level Waste Management. Comments are directed toward needed corrections, qualifications, revisions and clarifications.

The report compares uncertainty and sensitivity analysis techniques for groundwater flow and transport models using data from the Avra Valley in southeastern Arizona. However, available state-of-the-art techniques were not used for parameter identification and uncertainty and several more sophisticated sensitivity techniques were not used. For the report to be more effective in transferring performance assessment technical assistance contract work to the Center for Nuclear Waste Regulatory Analysis and the NRC staff, a brief statement should be included to say why the more advanced techniques were not used.

The action taken by this letter to considered to be within the scope of the current contract (FIN A-1165). Please notify me immediately if you believe this letter would result in a change to cost or delivery of contracted products.

Sincerely
/s/
Pauline Brooks
Technical Monitor, FIN A-1165
Division of High-Level Waste Management, NMSS

Enclosure:
As stated

cc: P. Davis, SNL, Div. 6416
L. Price, SNL, Div. 6416
D. Tiktinsky, NMSS/PI

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Review of "Comparison of Parametric Estimation and Sensitivity Analysis Techniques for Ground-Water Models and Their Impact on the Uncertainty on Model Performance Predictions" by D.A. Zimmerman, R.T. Hanson and Paul Davis, SNL Draft Report for Subtask 2.6d.

GENERAL COMMENTS

1. The report should explain why available, more advanced techniques for uncertainty and sensitivity analysis were not used. The following paragraphs give some of the concerns that might be addressed briefly in appropriate part(s) of the report. In light of currently available time and funds, no major revision is expected.

   a. Parameter Identification and Uncertainty. Since the investigators are familiar with the previous studies at Avra Valley, it is not clear why they approached this problem in a new, but seemingly less-advanced method than previous studies. For the last decade at least, there have been numerous papers and dissertations from the University of Arizona under the direction of S.P. Neuman that explored parameter identification on this site. The present report hardly acknowledges these studies, nor does it employ any of the sophisticated techniques for parameter identification already developed and codified into computer programs specifically for this purpose. Instead, mainly simple techniques have been employed for this study, much less sophisticated than those techniques already published for exactly the same problem. When a state-of-the-art method of parameter identification (GEOINVS) was used, the code did not work properly because of computational problems. A nonlinear regression technique was also tried without success.

      The work in this report might have followed the lead of the University of Arizona theses, particularly the work done by Clifton and Neuman ("Effects of kriging and inverse modeling on conditional simulations of the Avra Valley aquifer in Southern Nevada", WRR Vol 18, no 4, August 1982, pp. 1215-1234). In this paper, the authors explored inverse modeling, kriging, conditional simulation on the steady state hydraulic heads. This technique worked well in reducing the variance of the steady-state hydraulic heads. Although the authors cite Clifton's master's thesis, it is not clear why they did not adopt his methods or acquire his computer codes, especially since they appeared to work so well for heads.

   b. Sensitivity. Rather than use more time to get several of the sensitivity techniques such as adjoint or GRESS working, the authors used the relatively crude approach of varying one input variable at a time in order to generate partial derivatives of response (e.g., groundwater travel time) to the value of each variable. It is unfortunate that only the least sophisticated techniques were tried. The concern at hand is less with the example of Avra Valley than with the methodology that can be applied to other more germane problems. The approach used here seems to have been done for expediency. For example, the methods employed by Doctor ("A Comparison of Uncertainty Analysis Methods Using a Groundwater Flow Model," P.G. Doctor, PNL 5649, 1988) for exactly the same site might have been followed.

Doctor applied three different methods for uncertainty analyses to the Avra Valley example.

2. Referencing is inadequate throughout the document. For example, page 1-5, line 16 states that "this site was chosen because it had been studied numerous times in the past...", but fails to give any references. Page 2-13, first paragraph, refers to nonlinear regression techniques available, but again does not cite any references.

3. Terms, unfamiliar to the reader who is not familiar with the topic, should be defined when they are first introduced. See specific comments 2 and 4 for examples.

SPECIFIC COMMENTS

1. Page 1-2, lines 8 and 9. The term "groundwater travel time" must be used carefully in a document relating to NRC regulations. Groundwater travel time is a regulatory term from 10CFR60, and has not been actually defined by a technical position. Therefore, what is meant by groundwater travel time in the context of this report should be stated carefully. Perhaps it could be called something like "arrival time distribution for conservative tracer."

2. Page 1-4, line 1. What is meant by "first order approach" at the top of page 1-4? This paragraph conveys very little to the reader and should be explained better.

3. Pages 2-1 through 2-21. Much of the discussion on uncertainties and errors in the Avra Valley site data in Chapter 2 is very useful and generally clear.

4. Page 2-21, lines 12 and 13. The non-specialist would not be able to understand the unexplained jargon, e.g., "a 5-spot vs. 9-spot for finite difference models."

5. Page 4-2, lines 2-4. Explain why it is acceptable to take prescribed head boundary values from the USGS calibrated model of pre-development conditions in the Avra valley. What assurances can you give that these boundaries also apply to post-development conditions?

6. Page 4-2. Alternate Conceptual Model. In this section, using the same transmissivity field as the original calibrated model is mentioned. In the next section, Monte Carlo sampling of transmissivity at points or in zones is discussed. This is confusing.

7. Page 4-16, end of page. The use of a single value of porosity seems very unlikely. Couldn't it have been treated as an uncertain spatially varying quantity? The importance of this variable seems inconspicuously buried.

8. Pages 5-13 and 4-14. In the first paragraph on page 4-14 it is said that there is no correlation other than drift in the transmissivity data. In the section starting on page 5-13; however, a correlation scale of about 40,000 ft. is used. Also a correlation length of 50,000 ft. is used on page 5-36, line 18. Please explain the discrepancy.

9. Page 5-24, lines 15-16. There are cokriging algorithms that allow incomplete sampling, where there are not observations of all variables at all points.

10. Page 5-32, lines 15-16. The reason for choosing a zero nugget seems weak. Furthermore, the nugget is not an expression of uncertainty. One can have certain data and still get a nugget from the variogram analysis.

11. Page 5-39, Nonlinear Regression. Cooley's method apparently works best for a smaller number of regressed parameters than chosen here. It is evident that having 215 parameter zones and only 100 observations would have been unacceptable. The better alternative to supplementing the data would be to reduce the number of parameters greatly, e.g., only 20 or 30 parameter zones. Appendix D is missing, so your experiences with using the method could not be followed.

12. Page 5-45, line 26. Explain why the hydraulic head information can't be used in the generalized covariance kriging procedure.

13. Page 5-47, Table 5-3. Note that all of these errors are with respect to heads, not the object of this exercise, i.e., "groundwater travel time."

14. Page 5-48. This and many other figures need better captions. It is very difficult to tell which label applies to which curve.

15. Page 6-12, Figure 6-5. This figure suggests that the wrong flux boundary conditions for your modeling with the fixed flux were chosen. The fixed flux line should go through the alternate conceptual model curve.

16. Page 8-1, end of page and top of page 8-2. It should be clearly stated that the GEOINVS runs were only partially successful and apparently were not used for any "groundwater travel time" predictions.

17. Page 8-13, lines 2-19. There is little if any technical support in the text for the proposal to account for the existence of multiple minimums in the inverse problem and perform uncertainty and sensitivity analyses simultaneously. Either support the proposal with technical detail and references or delete.