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Dr. Roy Williams
Williams and Associates
PO Box 48
Viola Idaho 83872

Dear Dr. Williams:

Re : "Procedures for Predicting Groundwater Travel Time", by Williams and Associates, Dated August 14, 1986

I found the subject paper to be very interesting and thought provoking. One of the unavoidable shortcomings of the paper however is its lack of substantiation for several of the premises on the worthiness of large scale tests, small-scale tests (such as slug tests), deterministic models and stochastic models. I will first make my detailed review comments on the report, and follow up with a proposal which I think might lead to a substantial improvement in our ability to interpret field experiments for the purpose of determining groundwater travel time. Most of my comments are not criticisms, but are rather questions which crossed my mind during the review. I believe we should discuss the comments in person or by phone before any changes to the text would be warranted.

Review Comments

1. General - The underlying emphasis of the report is that large scale tests coupled with deterministic models are inherently better than stochastic models coupled with field measurements which stress tests of limited influence (e.g., slug tests). This assertion is based on your expert judgement, but I feel has not been demonstrated in your report, nor do I feel that it could be proven given the lack of field measurements to determine groundwater travel time. Furthermore, it is unlikely that we will have the field data and models to test your premises anytime soon.

2. page 3, second paragraph - I think that the restriction on steady state flow for groundwater travel time calculations is not necessary, especially for cases such as unsaturated flow. It may be the general practice, but need not be the rule. I believe we should leave open the possibility that transient analyses might be needed.

3. page 14, top of page - I don't understand how the deterministic solution requires large scale tests. I agree that large scale tests are needed to verify aspects of the chosen conceptual model, such as the continuity of the hydrogeologic units. The large scale test gives integrated properties for flow paths within the influence of the test however, but these are not

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necessarily the properties or paths needed for the determination of groundwater travel time under natural conditions. For example, streamlines of the natural gradient might be parallel and straight. A large pump test however would induce radial movement to the well. I don't know if it has been proven that the distorted flow paths would lead to accurate measurements which relate back to naturally-occuring gradients. Furthermore, will high pumping rates necessitated by economic and time constraints affect the medium nonlinearly; i.e., would you interpret the same constitutive relationships from you tests at a lower pumping rate , given that you had the time to spend?

Furthermore, I am not convinced that stochastic models, with their dependence on small-scale tests, are unable to simulate hydraulic continuity or lack thereof. Neither case would be excluded if the simulation were performed correctly. There would probably be some realizations of the stochastic data fields which would have hydrologic barriers and other cases which would have high continuity. I believe that this was true in Clifton's paper on stochastic modeling of groundwater travel time for BWIP. Some of Clifton's realizations showed marked structure which forced the pathways to be very tortuous. At any rate, known hydrogeologic structure could be incorporated into the realizations by means of conditioning of the random data fields.

4. page 15, 6 lines from bottom - Your arguments that data from large-scale and small-scale tests should not be combined are not compelling. I don't see why both sets of data could not be used in an intelligently derived framework to define a data field. For example, if a transient mathematical model was employed, the data field could be adjusted manually or by an inverse procedure until the hydrogeologic parameters matched the acquired data, whether it was from small or large scale tests. I agree that parameters derived directly from pump tests by procedures such as the Theis equation might not be compatible.

5. page 17, first paragraph - You give an example of how geologic structure can be incorporated into a stochastic model. I agree with your description, but it seems to contradict statements you make elsewhere (e.g., p 19, bottom of page) that hydraulic continuity is a prerequisite for stochastic modeling.

6. page 20, top of page - Why does the purely deterministic approach assume that the equivalent porous media approach must be used? This does not seem to be necessary.

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7. page 23, top of page - It might be useful to include a discussion about the differences between diffusive and nondiffusive tracers in connection with the determination of effective porosity and the determination of groundwater travel time as defined in the NRC Generic Technical Position.

8. page 26, top of page - I don't understand why the stochastic modeling approach must assume that flow paths are continuous in any direction proceeding away from the repository. Please clarify.

9. page 28, §6.2, first paragraph - I don't understand the meaning of "linear combination" in the context of this section. Please clarify.

10. page 29, middle of page - I think that there is some confusion with the use of the term "zero geostatistical range of influence." To me, this would mean "totally random." If the medium is hydrogeologically uniform, then it is perfectly correlated spatially. I believe that you would call this property an "infinite range of influence".

11. page 30, under Method 1 - The third sentence isn't supported by the first two. If the sampled values were uniform for each pass, then the medium would be "homogeneous" rather than "statistically homogeneous". This also applies th the use of the term "statistically homogeneous" under Method 2.

12. page 31, first sentence - I believe that the "estimated value" is the same throughout a particular subregion rather than "estimated distribution."

13. page 33, bottom of page - I cannot agree with your appraisal that the distribution of simulated values can never be proven to include the real groundwater travel time. I think that the gap between stochastic modeling and deterministic modeling gets narrower with the addition of more data.

Recomendations for Testing the Strategies Put Forth in Paper

Since it is unlikely that we will have the direct experience or data to test the theories of this paper, I make a modest proposal that I feel can partially alleviate this need. This is just an outline which can be modified and embellished later. I believe that it should start off simple, however, since there will be ample opportunities for pitfalls even at the most modest stage. The idea is basically to generate a synthetic surrogate of a realistic data field that can be modeled on a digital computer, and then employ various hydrogeologic testing strategies to derive data from the model to use in procedures to calculate the GWTT.

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Statement of Problem

Sites for the geologic disposal of high level radioactive wastes will be purposefully chosen to be in media which are inherently of poor potential for water yield and mineral resources. As a consequence, hydrogeologic data necessary for site characterization will not be widely available unless gathered for that purpose. Collection of data will be costly and difficult. No current site has been adequately characterized to date. The site characterization activities planned for the sites includes large and small scale tests. It has not been conclusively demonstrated however that such tests can adequately characterize the site.

To partially alleviate this problem, a experiment could be devised in which a synthetic but realistic data base would be generated, and then tested with the alternative strategies. Hufschmied (1986), who proposes a similar experiment for transport of radionuclides, points to several advantages of a synthetic experiment over "real world" experiments:

"(1) The physico-chemical processes involved in the synthetic experiment are well defined. Thus, there is no final information uncertainty when interpreting and comparing the results of conceptually different geosphere performance assessment codes.

"(2) A synthetic migration experiment is non-destructive: it allows to explore (sic) different testing procedures on the same piece of computerized geosphere. e.g., prior to real world experiment. Such a project could be key to an improved collaboration between modellers and "real world" experimentalists.

"(3) A synthetic migration experiment could serve as a research tool aiming at the development of scientifically sound validation strategies."

The scope of the synthetic experiments which I had in mind would be limited initially to hydrogeologic testing strategies for determining the groundwater travel time. The procedures one would follow are outlined below:

A. Generate a large detailed, synthetic data array representing a hydrogeologic setting, e.g., hydraulic conductivity and effective thickness. The synthetic data field will be very detailed, perhaps with a resolution on the order of several meters. The scale of the data field would be several to several tens of kilometers, containing up to a million data points.

   The data field would be generated one time only, by means of a multivariate random number generator, or using a technique such as "turning bands" (Journal, 1978). It would be spatially correlated to some typical length scale for a realistic geologic repository environment. At the initial stages of this project, we would restrict ourselves to simple concepts, say a single layer, two-dimensional field, with equivalent porous media flow, and no marked geologic structure. Later data fields could include fracture flow, dual porosity structure and multilayer phenomena, but I wouldn't want to make it too complicated at the early stage. I am currently in possession of a working conditional simulation program which will generate up to six cross-correlated, conditioned, spatially varying random fields (Carr, 1984).

B. Using the synthetic data field, simulate a realistic large-scale pumping test using a mathematical model to calculate drawdown and possibly the movement of tracer from test points. The pumping rate of the drawdown well(s) and the locations and number of the monitoring wells would be picked on the basis of realistic field practices and assumed economic and time constraints. It might not be necessary to use the finest resolution of the synthetic data array for the large scale drawdown test; a coarser grid could be used based on averages of the fine scale grid if it can be demonstrated that it doesn't make much difference to the results. This might be necessary for computational expediency, since the fine scale grid of data might contain up to a million points. It would be necessary to add some sort of "noise" to the data to simulate the kinds of errors likely to be encountered in the field. Expert judgement would apply here.

Once the hydrogeologic data have been collected from the simulated experiment to the satisfaction of the investigator and with the assumed economic and other constraints imposed on the test, the data would be interpreted to yield hydrogeologic parameters necessary to run a computer model to calculate groundwater travel time. The groundwater travel time would be determined from a point representing the disturbed zone to the accessible environment using a deterministic model. In this way, the groundwater travel time would be a single value rather than a distribution.

Several subsets of this step might include the exploration of alternative conceptual models for the hydrogeologic setting, in order to interpret the well testing data and to calculate the groundwater travel time. Errors caused by the long recovery time of low permeability media could be simulated realistically in this step.

C. Again using the synthetic data base, perform simulated small-scale tests such as slug tests to determine the hydrologic data at numerous points. For these simulations it would be necessary to use the finest resolution of the synthetic data field, but because of the small radius of influence of the simulated tests, it would be necessary to include only a small part of the data field in each run, so a reasonably small number of data points could be used. Expert opinion would again be used to add a reasonable level of experimental error to the "data" collected from the simulations.

The "data" collected from the small-scale simulated tests would be interpreted using standard techniques (e.g., Theis equation) Probability distributions of parameter values would be generated from the data. Variograms would be used to determine the correlation scales of the parameters. The distributions and correlation scales would then be used in a stochastic, possibly conditional modeling approach to generate a groundwater travel time distribution. As with step B, alternative conceptual models could be proposed to interpret the data and calculate the groundwater travel time. We would also be able to compare the various types of stochastic models you discuss in Section 6, and approaches based on sensitivity techniques such as the adjoint method.

D. Since we actually know the synthetic data base exactly, we can use it to calculate a steady-state flow field and directly simulate a groundwater travel time. This would represent the "true" groundwater travel time, and would be used to compare the results of steps B and C above. This would then constitute a test of the stochastic and deterministic modeling approaches and their data collection strategies.

E. Once we are satisfied with the simple cases, we could then move on to more complicated analyses. I think the next logical step would be to look at the effect of geologic structure on the results, since these are likely to demonstrate the difficulties of small scale pumping tests to identify the hydraulic continuity of the site. It would also be interesting to examine the pitfalls of large scale tests for situations where they are most likely to give erroneous results. For example, a dual porosity mathematical model could demonstrate conditions for which a high pumping rate might give erroneous values of effective porosity from the movement of dissolved tracers. The differences in the movement of diffusive and non-diffusive tracers could also be explored. The movement of water in layered, leaky aquifers induced by large scale tests would be a test involving three dimensional models.

Conclusion

The procedure outlined above for testing modeling and data collection strategies are not necessarily original. I know of at least two studies which employ similar ideas. Dr. Lynn Gelhar is generating a spatially correlated,

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three-dimensional random field of about a million points in order to test an analytical unsaturated flow and transport theory against a numerical simulation (Ababou, 1985). The simulation is expected to take several hours on a Cray computer. The other study has been proposed by Hufschmied (1986) for the upcoming INTRAVAL study. These two studies are somewhat more ambitious than the one I have outlined, however. I enclose a copy of Hufschmied's proposal for your interest.

I hope that the above discussion will stimulate enough interest that we (NRC, Williams and Associates and Nuclear Waste Consultants) can plan to go forward with such a study. I would also like you to consider the usefulness of the Hufschmied proposal to NRC, and our possible involvement with INTRAVAL. The workshop which Jeff Pohle mentioned in his letter of August 26, 1986 would be an ideal forum to discuss the merits of my proposal.

Sincerely,

ORIGINAL SIGNED BY

Richard B. Codell
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Division of Waste Management
Office of Nuclear Material Safety
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Enclosure:
INTRAVAL proposal by P. Huffschmied

References

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P. Hufschmied, J. Hadermann, F. Herzog (1986) "Proposal for a synthetic migration experiment with the purpose of studying validation strategies for geosphere performance assessment models", INTRAVAL ad hoc group meeting, April 17 and 18, 1986, Stockholm

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