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Lynn Deering
ACNW Staff Scientist
US Nuclear Regulatory Commission
Advisory Committee on Nuclear Waste
Washington, DC 20555

Dear Ms. Deering,

Enclosed is my trip report for the DOE/NRC technical exchange on ground-water hydrology held in Denver, Colorado November 29- December 1, 1994. As you recall I was only scheduled to attend the final day, December 1st, which focused on ground-water travel time (GWTT). However, I arrived early enough on November 30th to attend the end of the session on DOE's assessments of the extent and nature of the disturbed zone. In addition, I received a copy of Jeff Pohle's presentation on regulatory guidance to be followed in assessing the extent of the disturbed zone and had a chance to talk with Jeff on this subject. Therefore, my trip report covers not only the GWTT issues discussed on December 1st but also includes my notes on those aspects of the disturbed zone presentations that I received information on.

I wish to thank for the opportunity to participate in this technical exchange and if you have any questions or concerns about this report please contact me at 505-848-0754.

Sincerely,

Paul A. Davis

Paul A. Davis

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ACNW Consultant's Trip Report on the DOE/NRC Technical Exchange on Ground Water Hydrology

by Paul A. Davis

Estimation of the Nature and Extent of the Disturbed Zone

DOE Presentations

The only parts of the presentation I was present for were on thermal and geochemical modeling of the repository region in attempts to assess the extent and nature of a potential disturbed zone around a repository at Yucca Mountain and, in the case of the thermal modeling, assessing whether or not drilling the ESF will adversely effect site characterization. Both modeling exercises were based on very little data therefore it is difficult to draw any firm conclusions regarding this work. However, a couple of salient points on these efforts can be made.

On the Usefulness of Models based on Preliminary Data

One overall comment I would like to make is on the use of modeling results that are based on preliminary site characterization data. The modeling for the Yucca Mountain Program (YMP) is following an iterative approach that can generally be described by the following steps: 1) begin with the available sparse data set; 2) develop a single or very limited set of conceptual models based on this data; 3) perform simulations that by definition are poorly conditioned or calibrated; 4) draw conclusions about the performance of a given system or subsystem; 5) make recommendations about future data that should be collected in support of the modeling effort and; 6) update the models when new site characterization data are available. This general approach is sensible and may appear to be the only way to proceed at this time. However, I believe great caution should be exercised when judging the conclusions and recommendations and I believe there are alternative modeling approaches that could lead to more reliable conclusions and recommendations.

First I would like to address the use of conclusions that are drawn from the modeling. Conclusions in this case ranged from statements to the effect that the drilling of the ESF will have minimal effect on site characterization, in the case of the thermal modeling, to statements about the potential reduction in ground-water flow and transport rates due to precipitation of minerals along fracture walls. These are very important conclusions if they can be supported. In my opinion, whether or not they can be supported depends as much on the modeling approach as the amount of data supporting the models. Perhaps the best way to explain this view is to start with a simple statement that can be made about the modeling. That is, these conclusions are valid given that the assumptions and data used are valid. I am in the same school of belief as Breedeholf and Konikow (1992?) on validation. That is, validation of these types of models (where the term model is defined as the combination of assumptions and data) is not possible. However, I personally believe validation is not necessary. In this sense, I agree with G. Box - "all models are wrong, some are useful." Following this approach another simple but slightly different statement could me made, that is -- these conclusions are valid given that the uncertainty in the assumptions and data have been accounted for in a manner consistent with the purpose of the modeling. For example, the statement that the ESF will have minimal effect on site characterization would be supportable if the modeling would have been formulated in such a way that alternative credible assumptions and/or data would not lead to a different conclusion. In other words, if all credible alternative assumptions and data indicated that the ESF would have less of an effect on site characterization than the original assumptions and data, then the conclusion would be valid. In the case of the thermal and geochemical modeling that DOE presented, a systematic treatment of uncertainty in conceptual models and data was not apparent. Therefore, I find it difficult to lend any credence to the conclusions. Put in an other manner, credible alternative conceptual models (for example, alternative models of fracture geometries and properties) may indicate that the ESF would have a serious impact on site characterization.

Recommendations from these modeling efforts were almost exclusively in terms of required additional site characterization. In my mind, the use of these recommendations is even more questionable that the use of the conclusions. On the surface everyone seems to agree in general terms to the need for additional site characterization data. However, the rational for such a statement does not arise directly from the modeling effort. What does arise from the modeling is what specific data are thought to be needed. Other questions such as how much data and the priorities for data collection remain unanswered. Therefore the question to be posed in the context of this modeling is: are the right data being identified for collection? I don't think this question can be answered with regard to either the thermal or chemical modeling efforts because neither of the efforts accounted for uncertainty in data or conceptual models. Note that only treating one type of uncertainty would not yield supportable recommendations with regard to future site characterization. In the case of this DOE modeling, there was no apparent systematic treatment of conceptual model or parameter uncertainty. The reason this is important goes back to the supportability of statements that can be made about the modeling. So for example, we could again state that the recommendations are valid if the model assumptions and parameters are valid. However, in this case, that statement leads to the conclusion that no future data should be collected because all necessary data supporting the assumptions and parameters must exist for the model to be valid. Now take the hypothetical example of valid model assumptions and uncertain model parameters. This is the implicit assumption made by both the thermal and geochemical modeling presented by DOE. In this case, if uncertainty in parameters had been addressed, the statement could be made that the recommendations are valid given that the assumptions are valid. However for earth science models, even this statement cannot be supported because the data used to define parameters must, in some cases, be the same data that are used to define the assumptions. For example, assumptions about heterogeneity are based on the spatial variability displayed by parameters. The important point here is that as more data are collected the assumptions about spatial variability may change. Essentially, this means that there are no cases where the validity of the assumptions can be proven while uncertainty in the data still exists. Therefore, recommendations for further site characterization based on this type of modeling are, by definition, misleading.

On the other hand, one could foresee a combined approach to site characterization and modeling that explicitly accounted for conceptual model (i.e., assumptions) and parameter uncertainty. Such an approach would provide for a full elicitation of all credible conceptual models along with their associated parameters and parameter uncertainty. Then to focus such a large effort DOE would have to explicitly define the purpose of the modeling. While this may seem like an obvious first step in modeling, I still don't have a clear picture of the purpose and goal of individual modeling efforts undertaken by DOE are. Generally, it appears to me that the goal of ~~there~~ the modeling is scientific understand that once that understanding has reached some undefined level of acceptance, they would then compare the modeling results to the regulatory criteria. Conversely, one could propose that the goal of the modeling is regulatory compliance and that the modeling should systematically approach that goal. In the first case, site characterization would have to focus on which conceptual model and associated data set was believed to best represent "reality," whereas in the second case the focus would be to investigate only those conceptual models that lead to potential violations of regulatory criteria. Given the inability to validate models, I believe the second approach should be preferred.

Specific concerns on the DOE Modeling

Only one specific issue was of serious enough concern to raise at this time. This issue has to do with the coupled hydrologic and geochemical modeling. As I understand it, all of the simulations were performed using saturated conditions. These simulations indicated that precipitation would occur along fracture walls and that in turn the ground-water flow rates would be reduced due to this new material lining the fractures. First, it is not clear to me that the geochemical process would be the same for unsaturated and saturated conditions but I recommend you pose this question to a geochemist. I am not qualified to answer it. Second, however, unsaturated flow should actually increase if the apertures (i.e., the fractures) get smaller. In fact, for the same amount of water you should be getting closer to saturated conditions and gravity driven flow. Also note, that geochemical processes were said to be affected by the ground-water flow rate. Therefore, the predicted precipitation rates may also be in error.

NRC Presentation on Guidelines for Assessing the Disturbed Zone

Although I was not present for this presentation, I received the viewgraphs and had a chance to talk to Jeff Pohle (the author) on this subject. I believe Jeff has a simple and defensible approach to defining the disturbed zone which is to assess ground-water travel times for both pre- and post-closure conditions. This provides for a direct assessment of the effect of the disturbed zone and the comparison of the two allows for a meaningful determination of the pre-waste GWTT.

Ground-Water Travel Time (GWTT) Presentations

DOE Presentations on Ground-Water Travel Time

Lester Berkowitz - GWTT Interpretation of Applicable Guidelines and Regulations

This talk presented DOE's GWTT criteria for site selection and compared it to the NRC 10CFR60 GWTT rule. One major area of agreement was the inference that the word "likely" in both the DOE and the NRC requirements implies that uncertainty must be addressed in calculations of GWTT. While this is a very positive point of agreement, I was not clear whether DOE thought that conceptual model uncertainty as well as parameter uncertainty was to be addressed. In all examples presented, only parameter uncertainty was addressed.

The most significant difference between the DOE and NRC regulations was the inclusion of the words "pathway of ... significant ... travel" in the DOE regulation and the interpretation of these words with respect to the implementation of the DOE regulation. Namely what DOE has done is state that they would evaluate all potential pathways and determine if a given pathway is "significant" by looking at it's effect on the total system performance. Actually they said that would only look at total system performance when the calculated travel times are less than 1,000 years, the regulatory limit. As I understand it, the NRC on the other hand has stated that any "likely" path is "significant." At first glance, the DOE approach appears reasonable but upon inspection I believe it is inconsistent with NRC's intent behind their multiple barrier philosophy. To illustrate this point consider the following scenario. Suppose that the ground-water travel time analysis showed that the travel time along all pathways to be less than 1,000 years. This situation would lead DOE to evaluating the significance of all pathways. Further suppose that DOE's total system performance demonstrated that there was NO release from the repository over the regulatory time frame of interest - 10,000 years. This could be the result for example if the canisters were expected to have very long lifetimes. In conclusion then, DOE would state that none of the ground-water pathways are "significant". I believe this situation would be a clear violation of the multiple barrier concept.

Finally, one statement that this speaker (and other DOE speakers) made several time causes some programmatic concern. The statement was "preliminary analyses show". My concern is after more than ten years of work at Yucca Mountain when will we begin to see something that is not preliminary?

James Duguid - Calculational Approach to the Definition of the Disturbed Rock Zone

Mr. Duguid gave an overview of the DOE approach to assessing the extent and nature of the DRZ with respect to calculating GWTT. Actually DOE's approach seem less well defined than the NRC's in that DOE did not specify the actual criteria they would apply in their assessment of the DRZ. More importantly, however, this speaker said he agreed with the NRC approach to assessing the effects of the disturbed zone. Hopefully, this agreement between DOE and NRC will be formalized so that this one very important aspect of the GWTT issue can be resolved.

James Duguid - Calculational Approach to Ground-Water Travel Time

In this presentation, DOE presented their approach to calculating GWTT in an attempt to define the relationship between several modeling efforts including: 1) the assessment of the DRZ; 2) the saturated and unsaturated zone modeling; 3) the deterministic and stochastic modeling and; 4) the use of total systems performance in assessing "significance" of GWTTs that are less than 1,000 years. I will not address the assessment of the DRZ since DOE indicated they will follow the NRC guidance given at this meeting. Also the coupling of the unsaturated zone and the saturated zone appears to be a straight forward addition of travel times and that appears to be appropriate if recharge fluxes are demonstrated to be as low as currently assumed. Otherwise, the effect of recharge on the water table elevation and hydraulic gradient would have to be assessed.

Also, I have already commented on the use of performance assessment in determining "significance" and there is only one point Mr. Duguid made that I would like to add to that discussion. That is, he stated that they would not know how to use the total system's performance assessment results to address significance until they did the calculations. The reason I bring this up is to illustrate a general point about the DOE process of calculating GWTTs. Namely, it is very difficult to assess the process unless DOE defines the specific criteria and logic to be used at decision points. I have included the DOE flow chart that Mr. Duguid included for illustration (see figure 1). Please note that this flow diagram does not include any decision diamonds, let alone any criteria that will be used to make decisions. Perhaps one of the more important points that is left out of the DOE logic diagram the decision logic needed to determine when will enough data have been collected for either the site suitability decision or the final compliance decision. While the required quantity of data needed cannot be identified at this time, the DOE should be able to spell out the decision process and criteria.

The other point I would like to make is with regard to DOE's modeling process. Referring to Figure 1 note that the DOE process involves data collection (site characterization) followed by parallel paths of saturated and unsaturated modeling and another parallel path containing the analysis of the DRZ followed by total system performance. For this discuss the focus is on the site characterization - ground-water modeling paths. In each case, the process involves site characterization followed by model selection, followed by deterministic flow modeling with sensitivity analysis, which is, in turn, followed by stochastic analysis that generates a variety of flow paths and travel times. The point I would like to make is simple to state but more difficult to explain. That is, the sequence of deterministic/stochastic modeling renders the stochastic analysis questionable at the least, and more likely, meaningless. Since the deterministic analysis does not address uncertainty, it is not of value in assessing regulatory compliance. The fundamental reason for these conclusions is the uncertainty caused by spatial variability of hydraulic properties and the treatment of that uncertainty. First it is important to point out that spatial variability is not an uncertainty in and of itself but our lack of knowledge of spatial variability is the uncertainty. In efforts to quantify this uncertainty, hydrologist have developed approaches based on stochastic analyses of the spatial variation of hydraulic properties. Briefly, these approaches estimate both the value of hydraulic parameters and their associated variance at various points in space (usually taken to be nodal points of associated ground-water flow models. Then, the effect of this spatial variance is quantified by Monte Carlo methods, which sample values of the hydraulic parameters based on their estimated values and associated variances and perform multiple ground-water flow simulations based on the sampled values. A key feature of such an analysis is that the ground-water flow path changes which each sample. This is a simple result the spatial variability of the hydraulic parameters changing with each sample and then the water finding the path of least resistance for each simulation. By preceding the stochastic modeling with deterministic modeling the DOE is not only constraining the effects of spatial variability to the domain of the stochastic model, they are doing so in a way that makes the stochastic modeling non-conservative. To illustrate this point consider the following. The DOE (at LBL) is doing "detailed" deterministic modeling in three dimensions. This next step in the DOE modeling sequence is stochastic modeling (at SNL) and is two dimensional. This two-dimensional modeling by definition can only represent one "slice" through the three-dimensional model. The choice of which slice is assumed to come from the sensitivity analysis of the three-dimensional model. Now comes the problem. The stochastic modeling can only represent spatial variability in two dimensions and only in the X-Z plane. The result is two fold. First, the full characterization of spatial variability in three dimensions would yield tortuous flow paths that essentially would come into and out of the plane of the three-dimensional model. On first glance approximating this behavior in two dimensions may appear conservative because the apparent travel path in two dimensions is shorter that the travel path in three dimensions. However, the reason that the path is longer in three dimensions is that the water is following the path of least resistance (that is, following the zones of highest unsaturated hydraulic conductivity). By forcing all of the flow into the two dimensions of the stochastic model, the water is also being forced to travel through zones of lower permeability which, in turn, leads to longer travel times. These problems could be avoided if the uncertainty associated with spatial variability was treated in the domain it exists -- in the three-dimensional domain. My understanding of DOE's reason for not doing so is a concern about the computer costs associated with stochastic simulations of total system behavior in three dimensions. First, I find it difficult to imagine that computer costs would ever be significant relative to the total cost of this program and second, and more important, costs cannot be an excuse for introducing errors into the process.

On a separate note, Mr. Duguid's presentation pointed out that DOE intends to include the effects of matrix diffusion and dispersion in the GWTT analysis. First of all, these are generally considered transport phenomena and therefore not appropriate for inclusion in a GWTT analysis. Second, this appears to be an undo complication of what was meant to be a relatively simple analysis. And finally, I'm not sure I understand what the analysis would actual consist of. I believe the history of the development of the GWTT rule is quite clear that transport phenomena where not to be included. As I recall, the belief at the time was that the transport phenomena were too poorly known to allow the development of a radionuclide transport time. Also, if NRC would have included transport in the definition of the regulatory criteria, the number would not have been 1,000 years but much longer. Referring to the second point, the work in support of the GWTT rule is based on assessing compliance with the travel time through a simple use of the advective term in the transport equation FOR THE SAME MODELS THAT ARE USED FOR ASSESSING TOTAL SYSTEM PERFORMANCE. This point appears to have been lost in recent NRC and DOE discussions of the matter. With respect to the final point, I am not clear on what type of analysis DOE is proposing. For example, I don't understand how matrix diffusion can effect the ground-water travel time unless: 1) DOE is proposing to transport something other than water in doing the GWTT analysis; 2) DOE is proposing to transport water through the fractures that is of a different chemical composition than water in the rock matrix (note: this would be water of a hypothetical composition because in situ sampling only samples matrix water) or; 3) DOE is intending to include Brownian motion in the calculation. With regard to the use of dispersion in the analysis, I am equally confused. One way to think about dispersion in this context is that it is a transport phenomena that results from variation in the velocity field (which occur due to variations in hydraulic conductivity) occurring at scales smaller than a model grid block in the stochastic model. That is, hydraulic properties and driving forces are assumed to be constant over each grid block. For transport analysis, dispersion is then used to account for variations in hydraulic properties that occur at scales smaller than the grid block. In this case, it is conceivable that variations in velocity cause variations in the GWTT — if the volume of ground water that NRC wishes to regulate is smaller than the grid block size. The problem as I see it here is not one of GWTT at all. The problem is what scale of spatial variability should be accounted for in ALL Yucca Mountain analysis, the total system analysis as well as the analysis? Once this question is answered, the conditions are set for both analyses.

Bodvarsson - Site-Scale Unsaturated Zone Model

This presentation for the most part was the same one given at an earlier ACNW meeting. Therefore, most of the same comments apply. A few of the major points deserve reiteration, however. First, in contrast to the flow chart shown by Mr. Duguid, this modeling iterates with site characterization before passing on the results to the stochastic models. In fact it is this iterative loop of "calibrating against all data" and "predicting parameter values at all new wells" that cuts it off from the overall purpose of the Yucca Mountain program, i.e., regulatory compliance. Without a direct tie to compliance, the iterative loop with site characterization has a never ending potential.

This modeling effort and its relation to the stochastic modeling points to the need for the NRC to be very careful in tracking the treatment of spatial variability. Key issues include: 1) what is the assumed correlation length caused by the gridding schemes - noting that the grid blocks are larger for the site-scale model than they are the stochastic model; 2) how does the minimum correlation length relate to either grid block sizes and; 3) how do the data locations, the spatial correlation length and the location of the 2-D stochastic model relate?

Raleigh Bernard - "Fast" Path Modeling and Saturated Zone Modeling

Dr. Bernard presented the stochastic analysis of ground-water travel times using a two-dimensional equivalent porous media ground-water flow modeling that employed Monte Carlo techniques (LHS) for the propagation of parameter uncertainty. The overall DOE calculational approach shows this model linked to the site-scale model but at this time they are unrelated efforts.

Perhaps the most important lesson of this modeling was in the meaning of "conservative". The author stated several times during the presentation that he believed the model input and assumptions to be "extremely conservative". This is very interesting in light of the fact that this modeling produced much longer ground-water travel times than those indicated by the isotopic data. Given the scarcity of site data, current statements of "conservatism" are merely expressions of personal belief with little relation to "reality".

G. Zyvoloski - FEHM Code

This speaker presented an overview of the FEHM code that, as I understand it, was designed to simulate flow and transport along discrete fractures. This code has the advantage of dynamic grid generation which allows for the easy assessment of numerical stability as a function of descretization. The intended use of the code is to simulate flow through discrete fractures. It was not evident to me how this code fits in with the site-scale model or the stochastic model. To the contrary, this speaker stated that this code would take its input from another code- FRACMAN- which is designed to generate possible discrete fracture networks. From a geologist point of view, it is difficult to imagine ever collecting enough data on the geometries of fractures let alone the properties of those fractures to support such a model.

NRC Presentation on Guidelines for Assessing Ground-Water Travel Time

Jeff Pohle presented a straw-man approach to assessing ground-water travel times that was clearly stated to not be the final NRC guidance on the issue. His approach involved performing stochastic ground-water flow analysis via Monte Carlo sampling of hydraulic parameters. Then for each sample, multiple GWTTs would be calculated based on assessing the travel time from multiple release points within the repository. This, in turn, results in multiple distributions of GWTTs because of the multiple samples and the multiple potential pathways for each sample. Mr. Pohle went on to propose that the fastest travel path for each sample be accumulated into a distribution of the fastest paths and that the mean of that distributions be used to compare with the 1,000 year GWTT limit.

DOE interpreted this approach to be a "worst case" analysis which, in turn, would result in a disqualification of the site. It's a bit premature to believe that this approach would lead to disqualification of the site and it's also premature to label this approach as worse case. There is no apparent reason to believe this would lead to a worse case analysis. Instead, any conservatism in the DOE answers will be more related to their model assumptions and input distributions than to this approach. If DOE invokes worst case assumptions and probability distribution functions (pdfs) that extend beyond the measured or inferred data then the answer will be worse case. On the other hand, if the DOE uses assumptions that are supported by the data and confines their pdfs to ranges supported by the data then the answer represents the fastest path of likely ground-water travel.

One misstatement that was made by several DOE commenters deserves clarification. Namely, several commenters stated that samples taken from the tails of probability distributions are less likely than samples from other parts of the distribution. However, the DOE stochastic modeling is using the Latin Hypercube Sampling (LHS) method which insures that each sample is equally likely. Also note that as the number of samples taken goes to infinity, the likelihood or probability of each individual sample goes to zero.

Perhaps the next time the DOE and NRC have a technical exchange on this subject they could focus more on the sources of uncertainty, their quantification, and their propagation through the analyses. I believe this type of a discussion would lead toward a clearer understanding of which analyses are worst case and which are not. It may also lead to the recognition that neither NRC or DOE has quantitatively addressed potentially the largest source of uncertainty, the uncertainty associated with conceptual models of site performance.

CONCLUDING REMARKS ON GWTT AND THE MULTIPLE BARRIER CONCEPT

As I understand it, the multiple barrier concept is NRC's "defense in depth" strategy, wherein if there are errors or unaccounted for uncertainties in the total system's assessment, meeting the sub-system requirements will assure that public health and safety are protected. If this is a correct assessment of NRC's desire to have sub-system requirements, then it would be inappropriate for DOE to use total system performance assessment to weight the results of their GWTT analysis. Otherwise errors in the total system performance would propagate as errors in the GWTT analysis.

On the other hand, it is not clear that any errors or unaccounted for uncertainties in the total system performance are not inherent in the GWTT analysis anyway. For example, if the unaccounted for uncertainties are a result of a poor understanding of the site geology or hydrology, then neither the total system performance nor the GWTT analysis are credible. If the NRC concern is errors in the total system performance assessment, then the problem would appear to be inadequate quality assurance which would also affect the GWTT analysis.