May17, 2001

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SUBJECT: U.S. NUCLEAR REGULATORY COMMISSION/U.S. DEPARTMENT OF ENERGY CONFERENCE CALL REGARDING QUALITY ASSURANCE AND PERFORMANCE ASSESSMENT ISSUES

Dear Mr. Brocoum:

As discussed with you in our May 4, 2001**,** conference call, the U.S. Nuclear Regulatory Commission (NRC) staff identified apparent technical errors and/or inconsistencies in the Department of Energy's (DOE) Total System Performance Assessment for Site Recommendation (TDR-WIS-PA-000001 Rev 00 ICN01) and Total System Performance Assessment Model for Site Recommendation (TSPA-SR) (MDL-WIS-PA-000002 Rev 00) documents. The NRC staff specifically identified technical errors and/or inconsistencies between the TSPA-SR documents, the underlying Analysis and Modeling Reports, the associated GoldSim computer code results, and associated hand calculations. The staff informed DOE of these errors in a telephone conference call on May 4, 2001, and DOE agreed to investigate. NRC has asked DOE to determine the scope of these errors to evaluate the implications for the quality and adequacy of DOE's performance assessment and the TSPA-SR documents. Further, the NRC has also asked DOE to indicate how these errors have been addressed through the DOE Quality Assurance Requirements Description document and implementing procedures.

Your preliminary inquiry, as described in our follow up conference call on May 9, 2001, confirmed the existence of these technical errors and/or inconsistencies. Also, during that call DOE indicated it would be preparing a plan of action to respond to the technical errors and/or inconsistencies. DOE needs to document the preliminary results of its follow-up actions, provide formal documentation of the technical errors and/or inconsistencies corrections, and provide its final plans for the continued response to this matter.

Further, as discussed in the May 9, 2001, conference call, these errors and/or inconsistencies may be an indication that certain provisions contained in the DOE Quality Assurance Requirements Description document and its implementing procedures were not adhered to during the preparation of the relevant documents. The NRC staff expects to be updated on the status of your follow-up actions during the June 2001, TSPA technical exchange and during future Quality Assurance breakout sessions associated with the quarterly NRC/DOE management meetings.

/RA/

William Reamer, Chief
High-Level Waste Branch
Division of Waste Management
Office of Nuclear Materials Safety
And Safeguards

Enclosure: As stated

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Summary of Audit Findings on Hand Calculations in the TSPA-SR Model Report

The initial review of Total System Performance Assessment - Site Recommendation (TSPA-SR) raised questions relating to several verification calculations. After these initial findings, U.S. Nuclear Regulatory Commission (NRC) and Center for Nuclear Waste Regulatory Analysis (CNWRA) staff conducted an audit review of a subset of the TSPA-SR model verification calculations described in Section 6.3 "Components of the TSPA Model" of Chapter 6 of the TSPA-SR Model Report (CRWMS, 2000a). NRC and CNWRA staff performed independent verification of the hand calculations documented by the DOE. Based on the calculations reviewed by the NRC, approximately half of the sections entitled "verification" in Chapter 6 of the TSPA-SR Model Report describe hand or spreadsheet calculations that could not be readily verified by the NRC or CNWRA staff. These errors raise questions about the checking that was performed. Listed below by section and by model or sub-model abstraction are specific errors and/or inconsistencies identified by the NRC staff.

1. Section 6.3.4.2 In-Package Chemistry

1.1 Page 265, Table 6-42 (CRWMS, 2000a)

Calculated pH values fell outside the expected range of conditions for which the abstraction was developed. It was observed that the calculated and observed pH ranges fell outside of the calculated pH bound for pH_CDSP during the early time phase, even though DOE had indicated that no abstractions were utilized outside their range on page 559 of the TSPA-SR Model Report.

Given the input parameters and the response surface definitions, the calculated pH bounds (hand calculations) are consistent with an ‘Early’ time period where the GoldSim produced value and the hand calculation are consistent with a ‘Late’ time period. Both sets of values (the pH bounds and the pH values) are computationally correct, but they apply to different time periods. The median value problem GoldSim file was consulted and the observed values listed in the table were verified.

The errors in the table led the reviewers to conclude there is a potential error in the TSPA conceptual model abstraction for in-package chemistry. The ‘Early’ chemistry conditions should apply to all waste packages. As the packages fail over time, all of the packages in a bin will experience the ‘Early’ chemistry for the first X years (currently 1,000) conditional with their failure time. A package failing at 100,000 years will have 1,000 years of early chemistry conditions just as a package failing at 43,000 years would. The implications are that there won’t be the very long unzipping times currently in the model. The peak mean dose at 100,000 years is likely underestimated.

1.2 Page 266, Table 6-43 (CRWMS, 2000a)

The Total Carbonate Concentrations in Table 6-43 (hand and model produced) are identical but can not be obtained by using the appropriate equation in Table 6-38 and the appropriate input conditions.

The DOE median-value file was reviewed and it was determined that the values listed in Table 6-43 of the document are produced in the model. It was observed that the median-value file, the base-case file for 1,000,000 years, and the hand calculation spreadsheet all used the wrong equation. The equation listed in Table 6-38 is correct based on a review of the input AMR. This error makes all of the TSPA-SR results incorrect; however, the impact to risk is unknown.

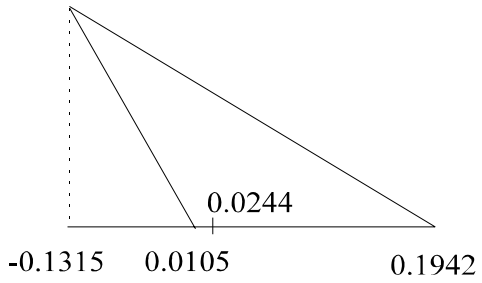
2. Section 6.3.4.3 Cladding Degradation Model (CRWMS, 2000a)

The last paragraph on page 285 states, "Table 6-45 (linearly interpolated between points) is used to define the creep failure distribution (triangular) with the minimum equal to 0.0105, the mean equal to 0.0244, and the maximum equal to 0.1942." However, the triangular distribution in GoldSim uses the minimum value, maximum value, and most likely value, not the mean. It is not clear whether this problem represents a numerical problem, or if there are errors in the documentation and the checking of the documentation.

The information in the TSPA-SR Model Report appears to be incorrect. If the documentation is accurate with the description of the distributions by the minimum value, maximum value, and mean, then there may be a numerical error as discussed below.

If the mean is 0.0244, the peak of the distribution is at -0.1315. As shown in figure 1, the peak lies outside the range represented by the minimum and the maximum values. When parameters are sampled from such a distribution, values outside the range will have two probabilities of occurrence. One value cannot have two different probabilities of occurrence from any distribution function.

Similar arguments can be made to show that the peak for the triangular distribution presented on page 288 (*Unzip_uncer*t, is defined as a triangular distribution with a minimum equal to 1, a mean equal to 40, and a maximum equal to 240) has a peak that lies outside the range (i.e., peak is at -121).



3. Section 6.3.4.4 Dissolution Rate Model

Page 301, Table 6-54 (CRWMS, 2000a)

The calculated values for High-Level Waste glass dissolution rate were not identical to the observed values. Differences in the precision of the values in the document are explained by DOE as being attributable to round-off error. In order to check the calculation, the staff put the appropriate values and equations,into a spreadsheet; however, the differences could not be explained with round-off error. Similar problems are possible for the solubility limits calculations presented in Table 6-60 on page 316.

4. Section 6.3.4.5 Dissolved Concentration Limits (CRWMS, 2000a)

4.1 The calculated values for dissolved concentration limits were not identical to the observed values. The hand calculations were requested and reviewed. The hand calculations provided by DOE had different inputs (i.e., environmental conditions) than those provided in the document. The reason that the provided hand calculations differ from the documented verification calculations is uncertain. The source of the imprecision in the calculations — the reason that the calculations were examined in greater detail — could not be determined. The degree of precision that is required by DOE QA procedures during model component verification calculations is unknown to the NRC.

4.2 Page 316, Table 6-60 (CRWMS, 2000a)

Hand calculations for the TSPA-SR Model Solubility Limit Calculations for U, Am, and Np could not be verified.

The text indicates that the time (t=100,000 years) was randomly selected. Figure 6-99 shows that the pH of the CSNF waste package in bin 4 is approximately 6.75 (or equal to the pH listed in Table 6-60. The following discussion applies to the hand calculations for uranium solubility within the bin where the environment is always dripping. The hand calculation uses a pH of 3.4454, which is quite different than what is listed in Table 6-60; the pH for the CDSP is different than what is listed in table 6-60, but is close. The temperatures for the hand calculations of both the CSNF and CDSP are different than what is shown in Table 6-60. The pH used in the hand calculation for the CSNF is outside of the abstracted solubility relationship for U on page 314; 3.4454 was used in the hand calculation, but the stated range of the relationship was between 5 and 9 (see page 314). The calculated solubility in the hand calculation is 8894 mg/L for CSNF, compared to 2.4630 mg/L in Table 6-60. The hand calculated value for CSNF is approximately 2 orders of magnitude larger than the largest solubility limit for uranium displayed for the median value calculation.

5. Section 6.3.9.1 Volcanic Release

Page 472, Table 6-133 (CRWMS, 2000a)

Hand calculations relating to Table 6-133 “Dose from Direct Volcanic Release at 500 Years” (probability weighted) could not be verified.

The hand calculations appeared correct, but differ from Table 6-133 by five orders of magnitude. In the electronic mail message from DOE providing the hand calculations, this difference was attributed to a known ‘bug’ in GoldSim 6.04, which is purported to have a five order-of-magnitude difference between numbers displayed in table form (wrong values) and chart form. Don Kalinich, DOE, surmised that during one of the draft revisions of the report, the GoldSim table values were put into both columns of Table 6-133. The values in table 6-133 are inconsistent with the values expected, given the values in Table 6-132 (not probability weighted), which shows dose values approximately 12 orders-of-magnitude different than those in Table 6-133 (probability weighted for a volcanic event with a probability of 8.80×10^{-9}). Tim McCartin, NRC, raised the error in Table 6-133 to Peter Swift, DOE, in January 2001. The request for a copy of the hand calculations was made on April 4, 2001. The statistics on the Excel spreadsheet indicate that the file was created on April 10, 2001.

6. GoldSim Error Messages

The GoldSim Run Log file contains a list of numerous error messages created during execution of the median-value calculation that need to be addressed for potential significance. It is believed that error messages are likely produced in the execution of stochastic GoldSim calculations, based on their presence in the median-value calculation GoldSim Run Log file. The error messages do not appear to be addressed in the TSPA-SR documentation. It is unclear whether the error messages were addressed during verification efforts necessary to determine that the TSPA-SR model is producing expected results. The significance of the error messages with respect to the calculated result is unclear.

7. Use of Conditions Outside of Intended Ranges (CRWMS, 2000a)

The staff were able to identify several instances in which the DOE model was applying abstracted models when the physico-chemical conditions were outside the range of conditions under which the abstractions were developed (see 4.2, above). However, DOE indicates that no abstractions were utilized outside of the intended range on page 559 of the TSPA-SR Model Report.

8. Incorporating Intrusive Event Probability

Pages 4-18 - 4-20 (Section 4.2.1) in TSPA-SR Technical Document (CRWMS, 2000b)

This section of TSPA-SR discusses how event probability is used to calculate the expected annual dose from igneous events, both extrusive and intrusive. The intrusive calculation uses the cumulative probability of an event occurring over the time period of interest to weight the results of the calculation. The TSPA-SR calculations are performed over a 50,000 year time period of interest, so the cumulative probability is calculated as the mean annual probability of occurrence, 1.6×10^{-8}/yr, times the 50,000 years. However, the result of this multiplication is reported in TSPA-SR as 8×10^{-3}, not the correct result of 8×10^{-4}. It is not clear whether this is simply a typographical error, or if this probability was actually used to calculate the results for

the intrusive scenario. The 8×10^{-3} value is, however, repeated later in the section. Questions were raised about the intrusive volcanism calculation during the June, 2000, TSPA Technical Exchange.

References:

CRWMS 2000a. Total System Performance Assessment (TSPA) Model for Site Recommendation. MDL-WIS-PA-000002 REV. 00. Las Vegas, Nevada.

CRWMS 2000b. Total System Performance Assessment for the Site Recommendation. TDR-WIS-PA-000001 REV. 00 ICN 01. Las Vegas, Nevada.