Department of Energy
Carlsbad Field Office
P. O. Box 3090
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SEP 29 2004

Ms. Elizabeth Cotsworth, Director
Office of Radiation and Indoor Air
U. S. Environmental Protection Agency
Washington D.C., 20460

Subject: Response to EPA May 20, 2004 Letter on CRA

Dear Ms. Cotsworth:

In response to the Environmental Protection Agency's (EPA's) letter of May 20, 2004, and the request for information received during the EPA Run Control Inspection the Week of August 9, 2004, the U.S. Department of Energy (DOE) is providing information to answer the questions included in the enclosure to that letter and answer the inspection information request.

This letter is the third and final DOE response to the EPA's May 20, 2004 letter. Additional information was previously provided in Detwiler to Cotsworth letters dated July 15, 2004 and August 16, 2004.

This submittal includes two enclosures. Enclosure 1 is a hard copy of the responses. Enclosure 2 (on compact disc) provides the references for documents identified in Enclosure 1.

If you have any questions, please contact Mr. Russ Patterson at (505) 234-7457.

Sincerely,

R. Paul Detwiler
Acting Manager

Enclosure

cc: w/enclosure
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CBFO:AMO:RP:VW:04-1725:UFC:5400

EPA Comment
G-4 Plan for MgO Emplacement

When we approved disposal of super compacted waste at WIPP in our letter dated March 26, 2004, we imposed the condition that DOE maintain a 1.67 MgO safety factor (Docket Number: A-98-49, II-B3-68). DOE must provide its plan for implementing this condition and emplacing the necessary MgO to maintain the safety factor.

DOE Response

DOE will take necessary measures to ensure, per 40 CFR 191.14 and EPA's certification of WIPP, that sufficient amounts of magnesium oxide (MgO), an engineered barrier, are emplaced within the repository.

Specific plans to meet present requirements are being developed by the Carlsbad Field Office (CBFO) and will be provided to EPA via separate cover letter.

EPA Comment
G-5 Part 3

In item G-8-2 of Cotsworth (2004), the EPA proposed the following: *PA Computer codes - SANTOS, NUMBERS and DRSPALL*
We stated in our preliminary PA code review, completed in June 2003 (Docket Number: A-98-49, ILB3-70):
"After completing the Agency's review, the EPA has concluded that 36 (of the 39) computer codes and three libraries migrated to the Compaq ES45 and 8400 with OpenVMS 7.3-1 are approved for use in compliance calculations for the WIPP performance assessment. Final technical review of the remaining three codes (e.g., NUMBERS, SANTOS, DRSPALL) will be conducted separately as part of the Agency's review and evaluation of the CRA. Specifically, the EPA will ***ensure that****:*

1. *DRSPALL, 1.0 is regression tested on the Compaq ES45 and 8400;*
2. *NUMBERS meets the QAP 19-1 requirements; and*
3. ***SANTOS is properly evaluated for accuracy."***

DOE Response

Emphasis is added to indicate that this memorandum specifically addresses the questions of SANTOS' **"accuracy".**

The SANTOS code was qualified and validated as required by SNL QA procedures. Documentation of the functionality and test problems is available in the Sandia Carlsbad Records Center: WIPP PA (Performance Assessment) Department, 2003. WIPP PA Verification and Validation Plan and Validation Document for SANTOS Version 2.1.7 Document Version 1.20, ERMS #530091. Sandia National Laboratories, Carlsbad, New Mexico.

Based on rigorous implementation of SNL QA procedures, accuracy of test problems, and documentation, we believe SANTOS to be an "accurate" and viable finite element code. SANTOS first replicated results from Stone (1997), which provided the porosity surfaces used in the original compliance certification, before it was applied to re-certification activities. Therefore, based on Quality Assurance requirements, functionality testing, and replication of previous results supporting the certification, SANTOS execution is free from error, i.e., "accurate".

However, another issue with respect to SANTOS modeling was addressed in the response to EPA request G-8-2, which pertains to the accuracy of stresses within the waste itself. In this context, "accuracy" is the degree of conformity to a true value. Stresses modeled within the waste are functions of many factors, but they depend primarily on the waste constitutive model. To determine accuracy, one would need to validate model prediction with its degree of conformity to a true value. We do not have the benefit of direct measurement of the state of stress in a waste room after centuries of compaction by salt creep, but analogous situations such as back-filled rooms in operating mines suggest that a uniform state of stress would evolve in a compliant material. A degraded, compliant waste would likely be compressed to a highly compacted lithostatic state of stress. As it turns out for the waste model used in the CCA, the stresses from the calculations are generally less than lithostatic and non-uniform. Therefore, the EPA questioned the accuracy of SANTOS and an important aspect of the accuracy determination resides within the waste constitutive model itself.

If the constitutive model for the waste is wrong or does not capture certain physical elements of response, then the results such as stress and strain would not conform to a true value. The waste constitutive model was developed from compaction tests on typical 55-gallon drums (Butcher and Mendenhall, 1993). The Soil and Crushable Foam (also called Crushable Foam or CF) model employed in SANTOS as a constitutive model for the waste was examined in detail by Callahan, 2004. He determined that the response model could be improved, particularly when the finite element model involves two-dimensional plane-strain analyses. Callahan determined that the stresses can be modeled (perhaps) slightly better than previously calculated by SANTOS and that trends and magnitudes yielded by SANTOS compare favorably with independent corroborating calculations using an independent code.

There are many sources for differences in finite-element calculations such as gridding, discretization, aspect ratios, initial conditions, boundary conditions, solution techniques, iteration methods, number of iterations, and convergence tolerances. One means to evaluate the accuracy of SANTOS—above and beyond the QA pedigree—is to perform corroborative calculations using an independent code, which in this case is SPECTROM-32 (Callahan, 2004). The most important "bottom-line" calculation with respect to performance assessment is a comparison of the resulting porosity surfaces.

Comparisons of room porosity and stress distribution are used to compare between SANTOS and SPECTROM. These outputs—as displayed in the following set of figures—show that for all the important room closure calculations as now implemented in performance assessment are reasonably replicated between these two completely independent finite-element codes. These calculations corroborate the stress results from the SANTOS calculations. After significant re-examination of the constitutive model for the waste, the state of stress in the waste, as calculated by SANTOS, was found to be accurate. Improvement of the constitutive model is possible, but perhaps not warranted because the mechanical response of the waste is of minor importance when gas is generated.

To compare with SANTOS, selected results are taken from recent calculations by Callahan, 2004. Callahan, 2004 conducted a study of WIPP disposal rooms with alternative TRU waste models. The purpose of the study was to investigate the influence of the TRU waste material model on the WIPP disposal room results. The study included scoping investigations and corroborative analyses to support existing calculations and was not intended for use directly in performance assessment of the WIPP. The main objectives of the study were to examine the effect of TRU waste constitutive models and to gain an understanding of the generation of the out-of-plane tensile stresses including their effect on room porosity. Therefore, TRU waste models with different elastic and inelastic attributes were selected for investigation. By significant re-examination of the constitutive model for the waste, the stresses can be modeled perhaps slightly more realistically than previously calculated by SANTOS, but the trends and magnitudes yielded by SANTOS are correct.

Figure 1 compares the average room porosity results obtained from SPECTROM-32 and SANTOS for three different problems. Figure 1 uses the following abbreviations:

1. **CF/*p*** – Elastic-plastic crushable foam material with Poisson's ratio equal to ***p***.

   NE/*n* – Nonlinear elastic material with Poisson's ratio equal to *n*.

3. *f* – *f* is a multiplier used to scale the gas generation rate. A value of $f = 1$, corresponds to the reference gas generation potential; whereas, a value of $f = 0$ corresponds to no gas generation, and $f = 0.4$ corresponds to 40 percent of the reference gas generation potential.

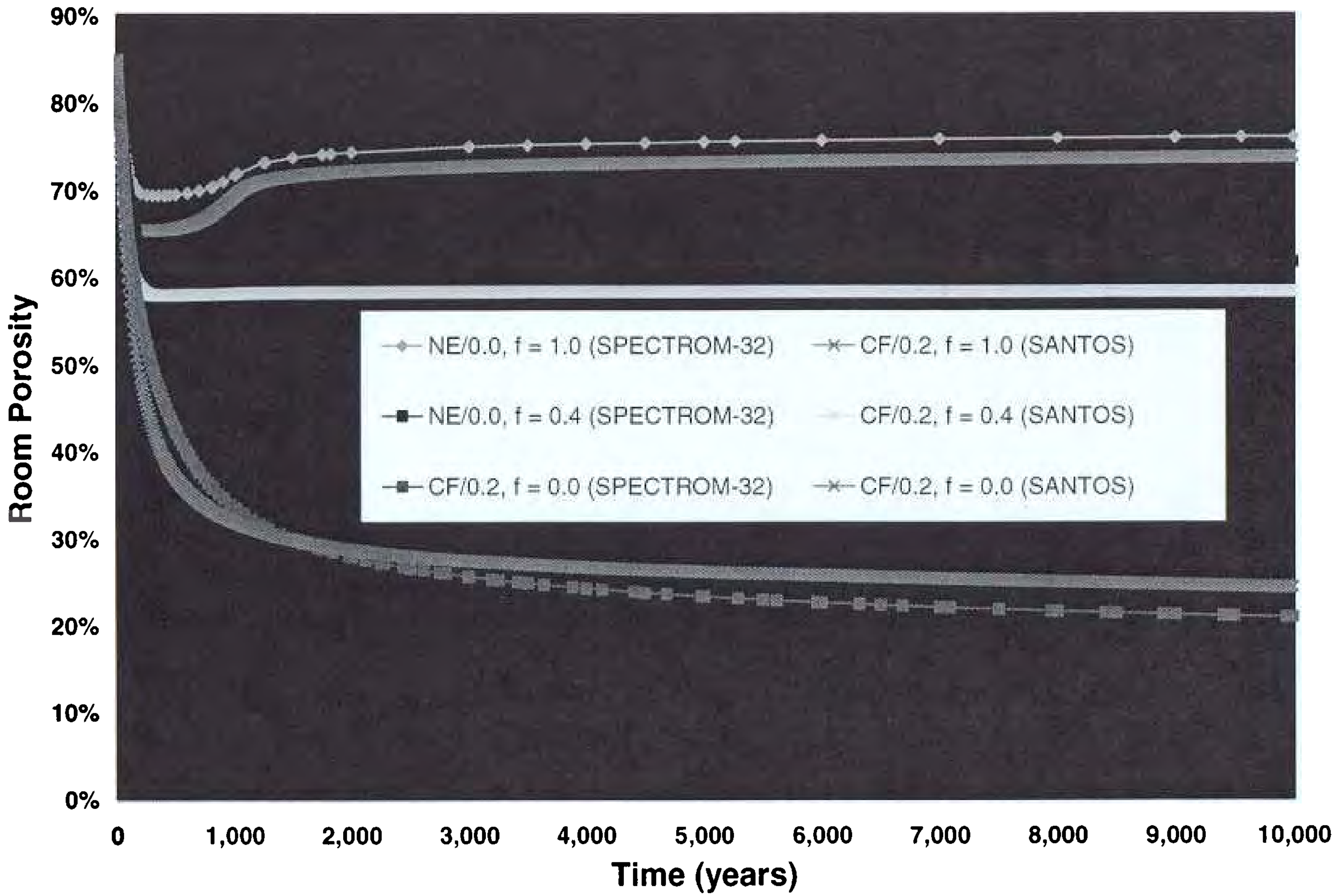

Figure 1. Comparison of SANTOS and SPECTROM-32 Results for Three Different Gas Generation Rates.

Figure 1 compares room porosity results obtained with SPECTROM-32 and SANTOS for gas generation rates (f) of 0, 0.4, and 1. For the case with no gas generation, the SPECTROM-32 porosity results are slightly higher than the SANTOS results earlier in time and slightly lower than the SANTOS results later in time. At 10,000 years, the SPECTROM-32 and SANTOS results differ by about 3.4% room porosity (i.e., 20.9% versus 24.3%). For the gas generation cases ($f = 0.4$ and $f = 1.0$), the SPECTROM-32 results were computed using a nonlinear elastic model for the TRU waste with a Poisson's ratio of zero; whereas, the SANTOS results were generated using the crushable foam model for the TRU waste with a Poisson's ratio of 0.2. Despite these TRU waste model differences, the SPECTROM-32 and SANTOS room porosity results are quite similar with the SPECTROM-32 results being consistently higher than the SANTOS results. At 10,000 years, the SPECTROM-32 ($f = 0.4$ case) result is about 3.4% room porosity higher than the SANTOS result (i.e., 61.7% versus 58.3%). At 10,000 years, the SPECTROM-32 ($f = 1.0$ case) result is about 2.2% room porosity higher than the SANTOS result (i.e., 76.0% versus 73.8%).

Improvement to the TRU waste model can be obtained with the nonlinear elastic model by elimination of the out-of-plane tensile stresses; however, the global response of the waste will not be affected significantly. The uncertainty in the constitutive model for the waste is minor and inconsequential in cases involving moderate gas generation because the presence of the waste is not important when the room is supported by the generated gas pressures. These results show that the TRU waste constitutive model becomes less important with gas generation. In other words, as the magnitude of the deformation in the TRU waste decreases because of gas generation, the mechanical behavior of the waste and its interaction with the underground structure becomes less important.

As an alternative to using a nonlinear elastic model, Callahan, 2004 suggested adopting a reduced deviatoric envelope in the crushable foam model used to describe the TRU waste (Callahan's Property Set 3). The reduced deviatoric envelope serves to reduce the out-of-plane tensile stresses producing more realistic stress results along the length of the disposal room. As another method to compare and verify SANTOS calculations, SANTOS was used to compute the no gas generation ($f = 0$) case with a reduced deviatoric envelope ($a_0 = 2.6$ MPa and $a_1 = 0.58$ instead of the original values $a_0 = 1.0$ MPa and $a_1 = 3.0$ included in Stone, 1997). This analysis was performed on the same finite element mesh as used by Callahan, 2004. The room porosity results obtained from SANTOS for this analysis are compared with those obtained by SPECTROM-32 in Figure 2. As shown in the Figure, the porosity results are very similar. The comparative trend of the two analyses is identical to the comparison seen in Figure 1 ($f = 0$) with the SPECTROM-32 porosity results being slightly higher than the SANTOS results earlier in time and slightly lower than the SANTOS results later in time. At 10,000 years, the SPECTROM-32 and SANTOS results differ by about 3.64% room porosity (i.e., 12.11% versus 15.75%). Figures 3 through 5 compare the horizontal, vertical, and out-of-plane stresses obtained from the SANTOS and SPECTROM-32 analyses, respectively. Note that tension is taken to be positive in these figures. The trends and magnitudes of the stresses are quite similar for the two calculations in all cases. The important item to notice is that the out-of-plane stresses are, for the most part, compressive as shown in Figure 5. The SPECTROM-32 out-of-plane compressive stresses are moderately smaller in magnitude than the SANTOS compressive stresses in the TRU waste.

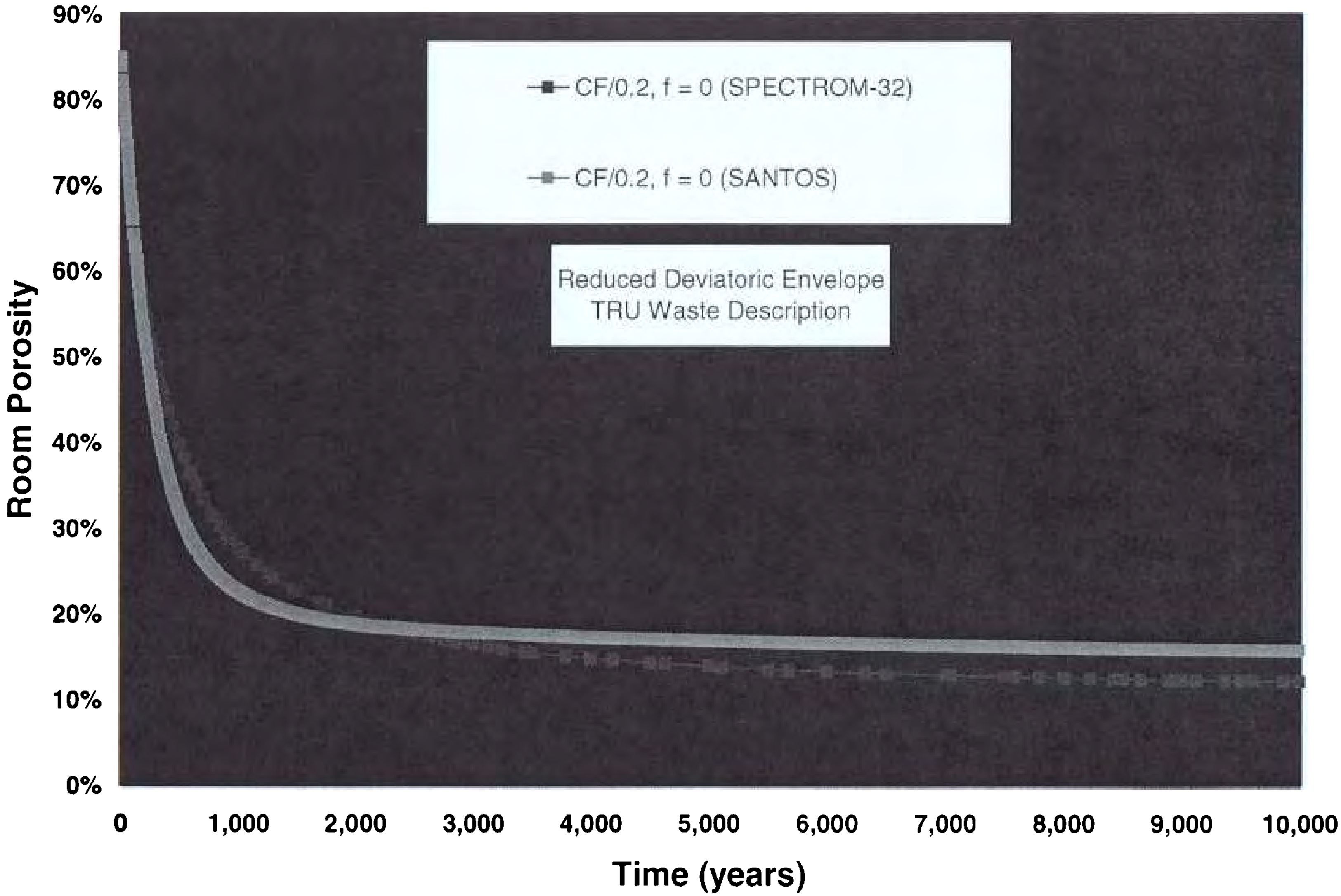

Figure 2. Comparison of SANTOS and SPECTROM-32 Room Porosity Results for a TRU Waste Reduced Deviatoric Envelope and No Gas Generation.

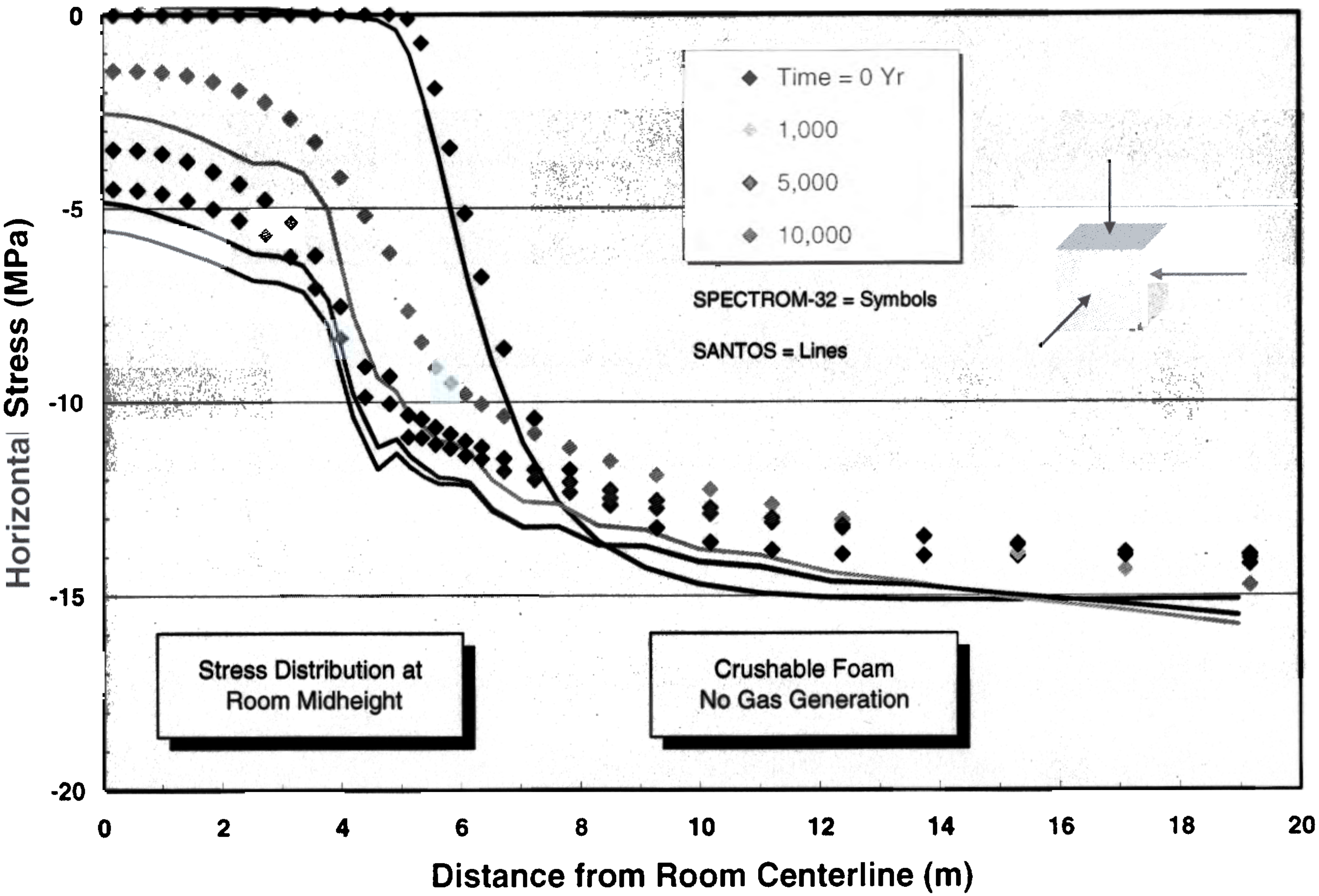

Figure 3. Comparison of SANTOS and SPECTROM-32 Horizontal Stress Results for a TRU Waste Reduced Deviatoric Envelope and No Gas Generation.

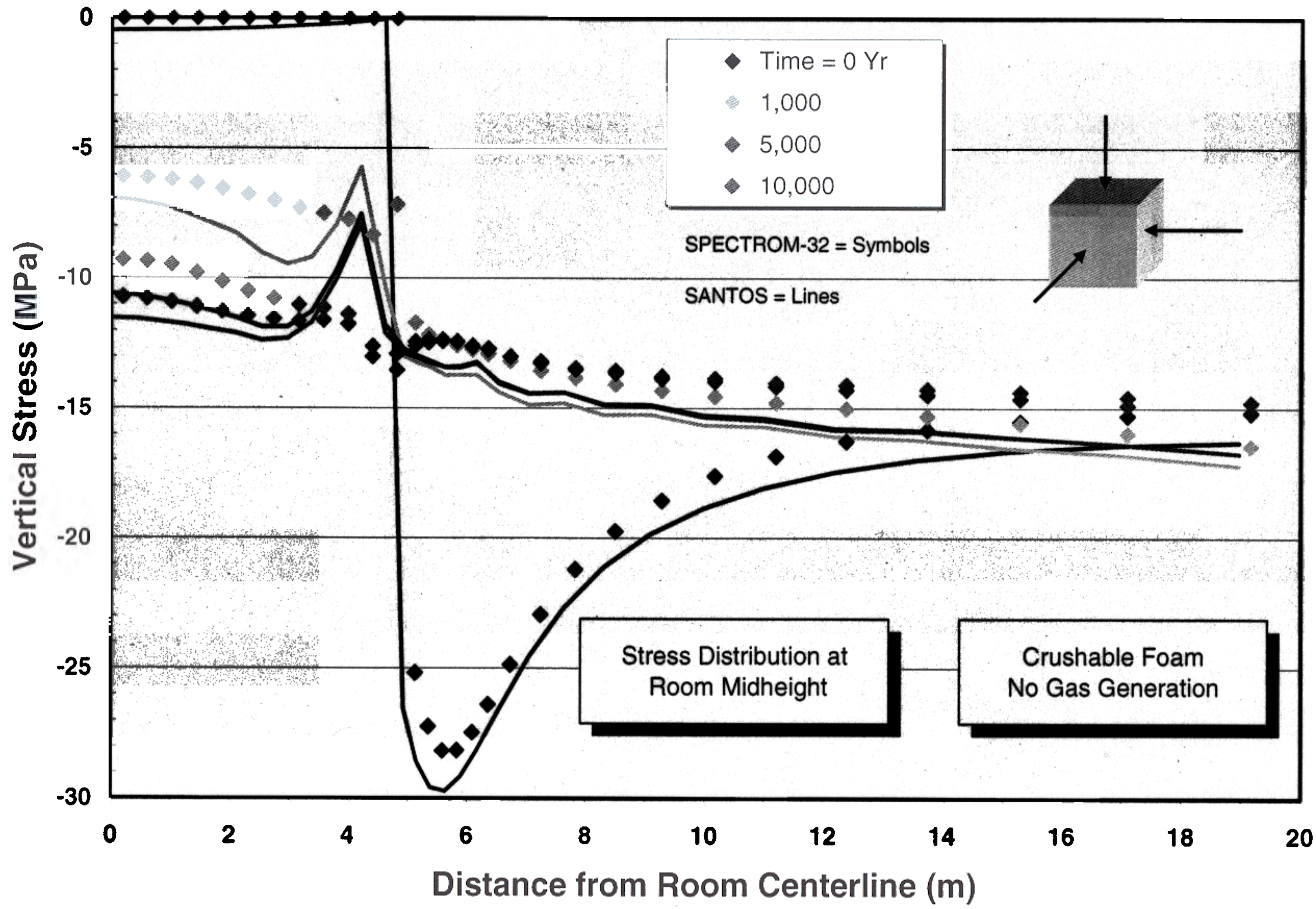

Figure 4. Comparison of SANTOS and SPECTROM-32 Vertical Stress Results for a TRU Waste Reduced Deviatoric Envelope and No Gas Generation.

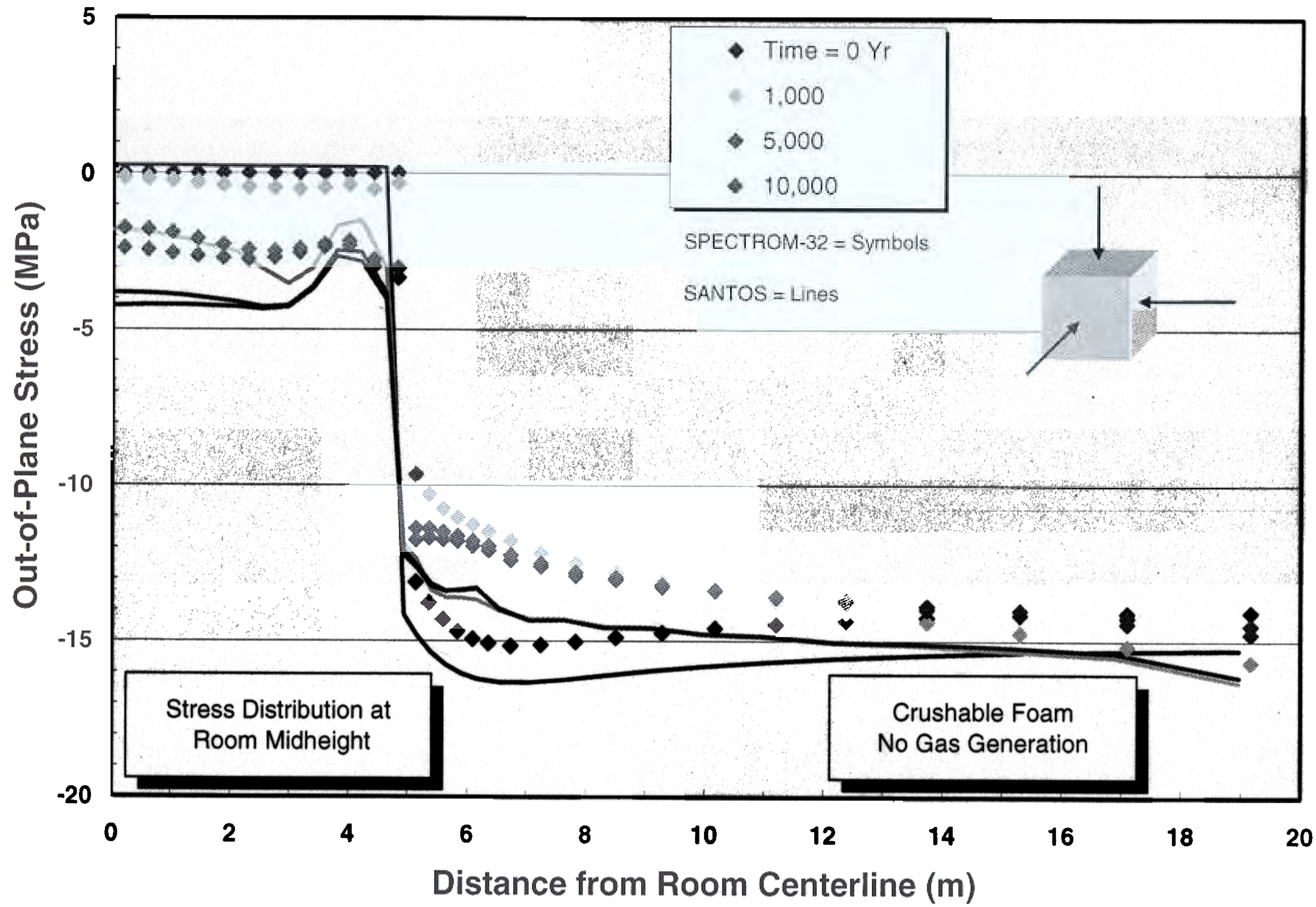

Figure 5. Comparison of SANTOS and SPECTROM-32 Out-of-Plane Stress Results for a TRU Waste Reduced Deviatoric Envelope and No Gas Generation.

REFERENCES

Butcher, B. M. and F. T. Mendenhall, 1993. *A Summary of the Models Used for the Mechanical Response of Disposal Rooms in the Waste Isolation Pilot Plant with Regard to Compliance with 40 CFR 191, Subpart B,* SAND92-0427, Sandia National Laboratories, Albuquerque, NM.

Callahan, G. D., 2004. *Disposal Room Calculations with Alternative Waste Models,* RSI-1783, prepared by RE/SPEC Inc., Rapid City, SD for Sandia National Laboratories, Albuquerque, NM. ERMS#536804

Stone, C. M., 1997. *Final Disposal Room Structural Response Calculations,* SAND97-0795, Sandia National Laboratories, Albuquerque, NM, August.

EPA Comment
G-8-2

The initial stress on the waste is assumed in DRSPALL to be the lithostatic stress of 15 MPa. However, SANTOS calculations now appear to predict an average stress on standard waste that is less than 5 MPa, even after 10,000 years. If, after reviewing and confirming the SANTOS results, the actual stress on the waste is found to be less than 15 MPa for most of the regulatory time frame, the sensitivity of DRSPALL results to lower initial stresses should be studied. The need for and details of this second sensitivity study will be determined following completion of DOE's SANTOS model evaluation. DOE needs to verify SANTOS' predicted stress of 5 MPa and run DRSPALL sensitivity test at 5 MPa to verify the performance of this model.

DOE Response

Recent calculations (Callahan, 2004 and summarized by Hansen 2004) corroborate the stress results from the SANTOS calculations. By significant re-examination of the constitutive model for the waste, the stresses can be modeled perhaps slightly better than previously calculated by SANTOS, but the trends and magnitudes yielded by SANTOS are correct. Thus, independent calculations have confirmed SANTOS results and stress in the waste is less than lithostatic, even after 10,000 years. The second half of comment G-8-2 cannot be executed exactly as described because gas pore pressure must exceed the 8 MPa pressure in the wellbore before spall can occur. At the same time the pore pressure cannot exceed the minimum principal stress. Thus, the spall event could not occur when stress in the waste is 5 MPa. However, an additional calculation in which the initial pore pressure and the far field stress are set equivalent at 10 MPa was run. Spall releases were less than the most extreme cases already run for the re-certification, which sets the pore pressure and the far field stress near hydrostatic levels.

References

Callahan, G. D., 2004. *Disposal Room Calculations With Alternative TRU Waste Models*, RSI-1783, prepared by RESPEC, Rapid City, SD, for Sandia National Laboratories, Albuquerque, NM: ERMS#536804

Hansen, F.D., Lord, D.L., Callahan G.D., Rudeen, D. 2004. *Spall Sensitivity to Initial Stress EPA Question G-8-2*, ERMS#536308, Carlsbad, NM: Sandia National Laboratories.

EPA Comment

C-23-5 Ch 6, pg 6-91, lines 1 to 6

As a result of approved changes to the MgO placement scheme (i.e., elimination of mini-sacks), the safety factor of 2.45 is not valid and needs to be recomputed. The actual MgO safety factor is well below the assumed value of 2.45.

In fact, as described in our approval for MgO changes, and in our recent approval of compressed waste from the Advanced Mixed Waste Treatment Facility, DOE must assure that a safety factor of 1.67 be maintained, and modify the text of the CRA documentation accordingly.

DOE Response

DOE will take necessary measures to ensure, per 40 CFR 191.14 and EPA's certification of WIPP, that sufficient amounts of magnesium oxide (MgO), an engineered barrier, are emplaced within the repository.

Specific DOE methodologies for calculating an MgO safety factor, the technical justification for the methodology used to calculate a safety factor and a regulatory discussion regarding the engineered barrier are being developed by the Carlsbad Field Office (CBFO) and will be provided to EPA via separate cover letter. Shortly after EPA receives these documents DOE proposes EPA and DOE have a technical exchange regarding these issues, and make the final determination on CRA text changes, if any, that may be warranted.

EPA Comment
C-23-10 Ch 6, pg 6-166, lines 23 to 24

The CRA states that "spallings are assumed to be derived from a sufficiently large volume of waste that container-scale variability can be neglected." While we accepted this assumption in the original certification decision, since then DOE has used a number of different container configurations-such as ten drum overpacks and supercompacted waste-with greater frequency than estimated earlier. In addition, the new DRSPALL code generally predicts much lower release volumes. For these reasons, neglecting container-scale variability may not be a valid assumption.

DOE must fully justify the existing waste spall model given the changes in waste container since the CCA and the new spallings model results or must rerun the CRA PA with assumptions that better reflect the container variation.

DOE Response

The following is from Dunagan and Vugrin (2004).

In response to EPA's request in a letter dated May 20, 2004 (C-23-10, EPA 2004), a study was conducted to analyze the impact of container-scale variability on the current spallings model. In the CRA, spallings releases were calculated using the average radioactivity in all CH-TRU waste streams. The spallings model uses the repository-average radioactivity because the impact of container-scale variability on mean releases was considered negligible. The current spallings model predicts lower release volumes than the spallings model for the CCA. To evaluate the impact of heterogeneity in the waste on the spallings model, three waste streams were randomly sampled for each spallings event, and the release was calculated using the average of these three waste streams. Three waste streams were chosen to be sampled because waste containers are typically stacked three high in the repository.

Figure 1 shows the 100 complementary cumulative distribution functions (CCDFs) for CRA Replicate 1 spallings releases that were computed using the average radioactivity across all CH waste streams. Fifty-eight of the 100 vectors fall off-scale with values too low to plot. Figure 2 shows the 100 CCDFs for CRA Replicate 1 spallings releases that were computed using the randomly sampled waste streams. Fifty-seven of the 100 vectors fall off-scale.

Figure 3 shows the mean and 90th percentile curves for both the spallings releases calculated using the average radioactivity of all the waste streams and the spallings releases calculated using the radioactivity of the randomly selected waste streams. The two mean CCDFs are nearly identical everywhere except at very low probabilities. The 90th percentile curve calculated using the randomly selected waste streams shows higher releases than the 90th percentile curve calculated using the total average radioactivity, but the largest deviations occur at low probabilities. It is not surprising that the 90th percentile curves differ somewhat because the second method of computing spallings releases introduces greater variability. Thus, we expect the 90th percentile curve for the random sampling method to show higher releases than the 90th percentile curve for the average radioactivity method shows.

Therefore, this analysis concludes that calculation of spallings releases is not significantly affected by waste-scale variability.

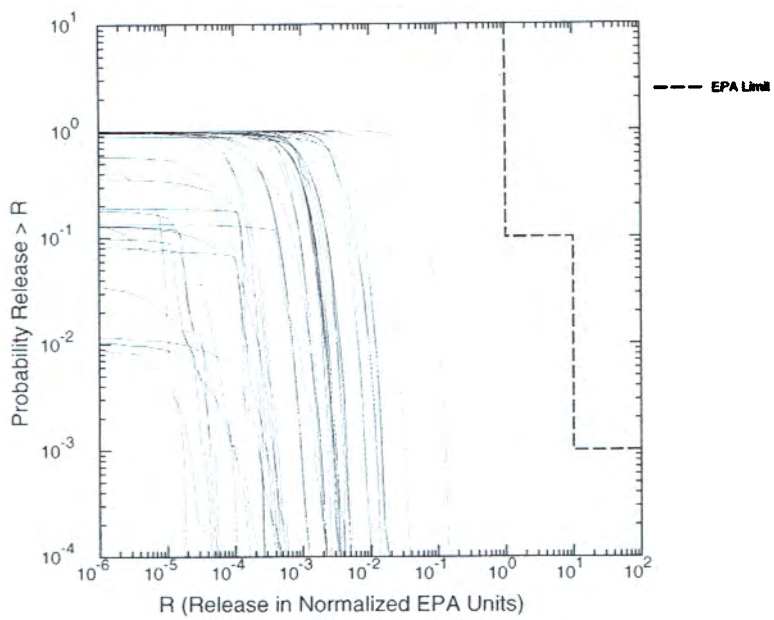

Figure 1. Spallings Releases Calculated Using the Average Radioactivity Over All CH-TRU Waste Streams

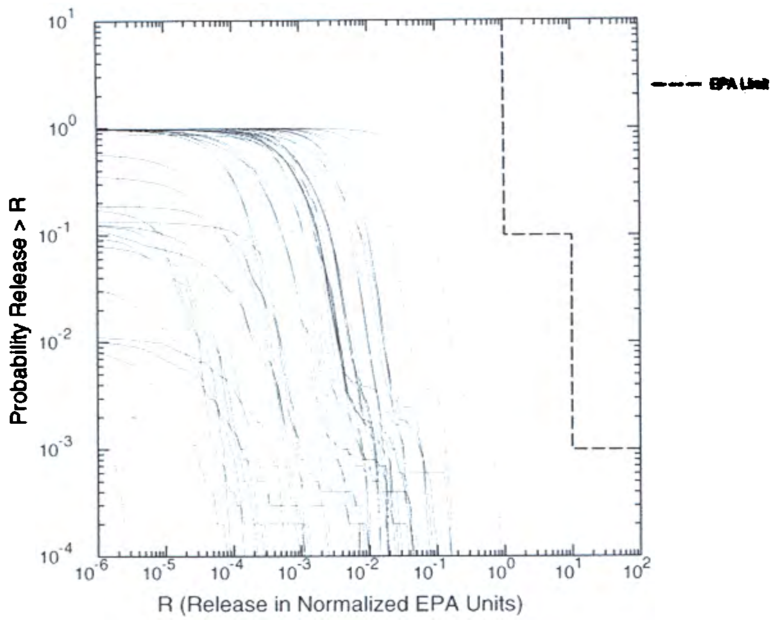

Figure 2. **Spallings Releases Calculated Using the Average Radioactivity of 3 Randomly Sampled CH-TRU Waste Streams**

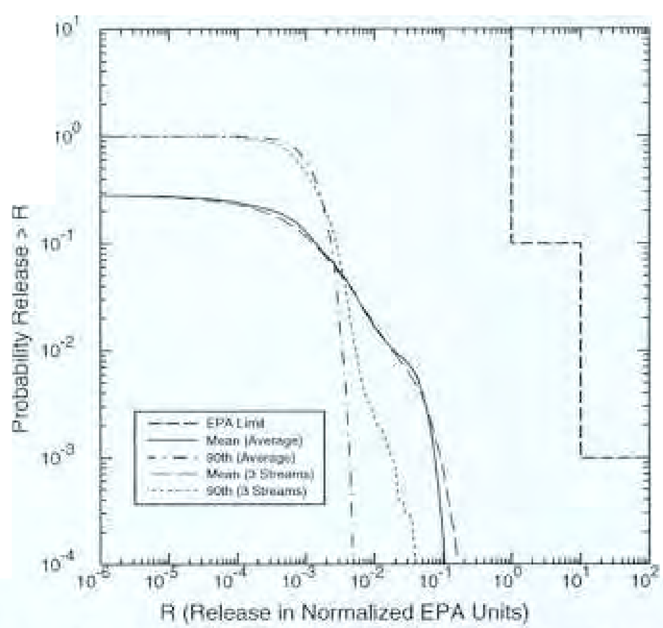

Figure 3. Sensitivity of Spallings Releases to Assumptions About Container-Scale Variability

References

Dunagan, S. D. and E. D. Vugrin. 2004. "Waste container-scale variability and DRSPALL in response to C-23-10." Memorandum to David Kessel. August 4, 2004. Sandia National Laboratories. Carlsbad, NM. ERMS# 536314.

U. S. Environmental Protection Agency (EPA). Letter from Elizabeth Cotsworth to Dr. R. Paul Detwiler. May 20, 2004. ERMS# 535554.

EPA Comment (Received during EPA Run Control Inspection for the Week of August 9, 2004)
Investigate how CCDFGF and SUMMARIZE are checked/verified/tested for capturing the correct code CDB data streams.

DOE Response

Dunagan (2004) describes the procedure used to verify that SUMMARIZE and CCDFGF have captured the correct code Computational Database (CDB) data streams. The actual processing of CDB data streams is verified in advance because the codes which manipulate CDB data streams have been validated and verified for this purpose in accordance with Sandia National Laboratories (SNL) software quality assurance procedure NP 19-1. The selection of CDB data streams to process is controlled by scripts that are part of the Performance Assessment Run Control System (PA RCS). Verifying that these scripts choose the appropriate data streams is accomplished by comparing the script input files with PA RCS log files.

References

Dunagan, S. 2004. "Explanation of how SUMMARIZE and CCDFGF are checked/verified/tested for capturing the correct CDB data streams in the WIPP CRA-2004 Performance Assessment." Memorandum to David Kessel dated September 16, 2004. Sandia National Laboratories. Carlsbad, NM. ERMS # 536767.