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date: January 24, 2013

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subject: Follow-up to questions concerning TAUFAIL flume testing raised during the November 14-15, 2012 technical exchange between the DOE and EPA

Sandia National Laboratories performed flume testing on samples made using three recipes of surrogate waste materials representing 50%, 75%, and 100% degradation of the iron and CPR in the waste after 10,000 years. The surrogate waste samples were subjected to two compaction pressures, 2.3 and 5.0 MPa. The samples were eroded in a vertical flume that simulates conditions occurring in a borehole where fluid flowing up the borehole applies a hydrodynamic shear stress on the material making up the wall. The results of these experiments were written up in Herrick et al. (2012) and presented to the EPA during a technical exchange videoconference between the DOE and EPA held on November 14-15, 2012. Several questions or uncertainties came up during that meeting to which the EPA needs responses to before CRA-2014 work can commence using a new value for the lower limit of TAUFAIL.

1 Compaction Pressure Origins and Recommendations

Two compaction pressures were used to make the samples for the flume tests, 5.0 and 2.3 MPa. It was recommended in Herrick et al. (2012) to use the results from the tests conducted using 5.0 MPa as the compaction pressure. One principle reason was that the 5.0 MPa compaction pressure was used to determine the experimental parameters for the Spallings model and by again using that pressure during the experimental evaluation of the waste shear strength consistency between models would be obtained. In addition, during the technical exchange meeting it was pointed out that it appeared that Hansen et al. (1997) had taken the CCA BRAGFLO porosity results and back-calculated the vertical stress necessary to produce the deformation of the drum stack. The BRAGFLO results are expected to be the best representation of possible repository conditions and should be used for predictive purposes.

The 2.3 MPa compaction pressure was obtained from structural calculations performed using the FEM code SANTOS to estimate compaction of the degraded waste with time (Herrick et al., 2007). The method used is identical to that used for the development of the porosity surface. The porosity surface is a compilation of time-dependent repository pressures and porosities under different gas generation rates. A scale factor (f) is used to multiply a base gas generation rate (f = 1) to produce the 3-D porosity surface representing changes in porosity as a function of pressure and time over the 10,000-year simulation period. The stress on the top of the waste stack for the possible values of f is shown in Figure 1. For the highest gas generation level (f = 1.2, Clayton 2007), the waste is compacted to 2.3 MPa.

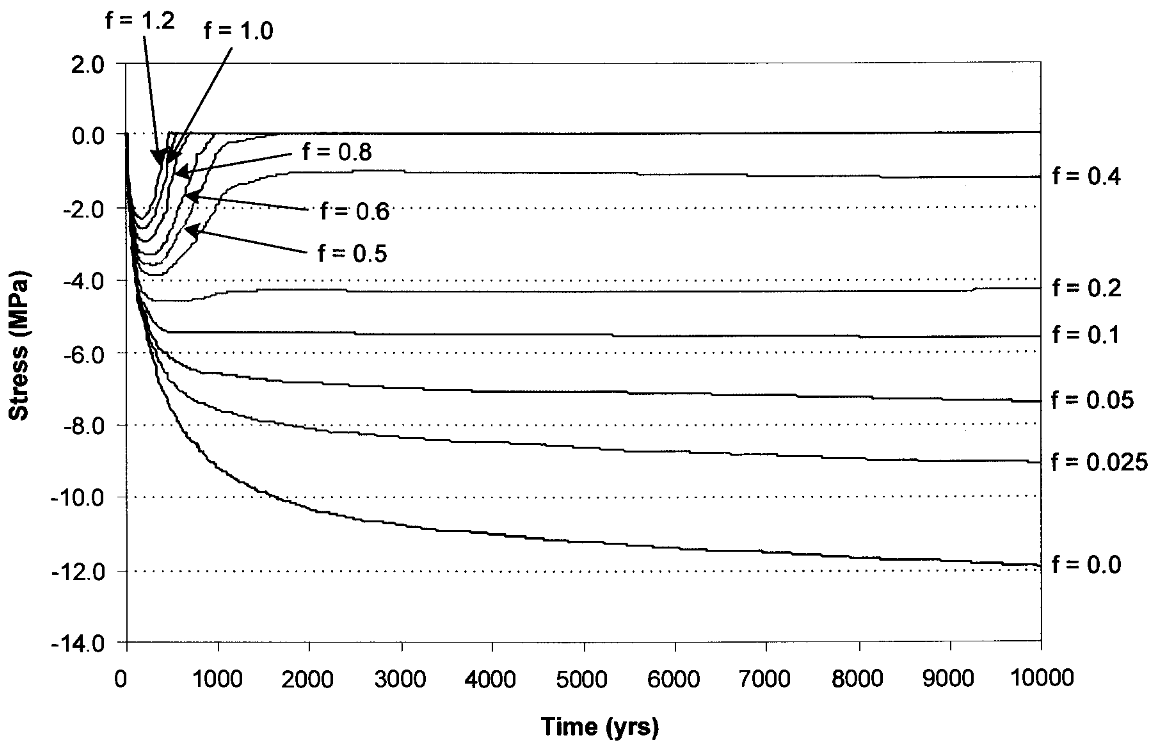

Figure 1. Stresses applied to the waste by salt creep for various gas generation factors from SANTOS structural calculations by Herrick et al. (2007). Negative stress values indicate a compressive stress.

It was presented during the technical exchange that the BRAGFLO results represent possible repository conditions better than the structural code calculations because the chemical and environmental processes that lead to gas generation are accounted for in BRAGFLO rather than assuming a fixed gas generation rate as is done in the porosity surface calculations. A slower gas generation rate would allow for more salt creep in early times, which would lead to more compaction and higher stresses in the waste. As will be shown next, the 2.3 MPa compaction pressure is a conservative underestimate since the actual gas generation rates predicted from BRAGFLO are not as fast as those modeled in the structural calculations.

It appears that Hansen et al. (1997) estimated the vertical stress needed represent the waste compaction using BRAGFLO porosity results from the CCA. Room closure and compaction are discussed in Appendix D of Hansen et al. (1997). In Appendix D, Larson used the end state BRAGFLO waste disposal area porosities for the undisturbed (Scenario S1) and an E1 intrusion at 1000 years (Scenario S3) for Replicate R1 to estimate the room closure. He obtained calculated room heights ranging from 0.9 to 1.5 m.

To obtain the best estimate of the least amount of room closure the minimum largest BRAGFLO porosity should be used. These values correspond to the smallest pressures acting on the waste stack before gas pressure pushes back against the creeping salt. For the CCA results, the selection of these points is shown in Figure 2 and Figure 3. Notice in Figure 2 that the largest BRAGFLO porosity increases with time indicating that the generated gas pressures are able to overcome the lithostatic stress leading to salt creep and reopen the room up by a small amount. Therefore, the stress on the waste drum stack estimated using the end state conditions, the time Larson used, would be less than the stress at 1,400 years.

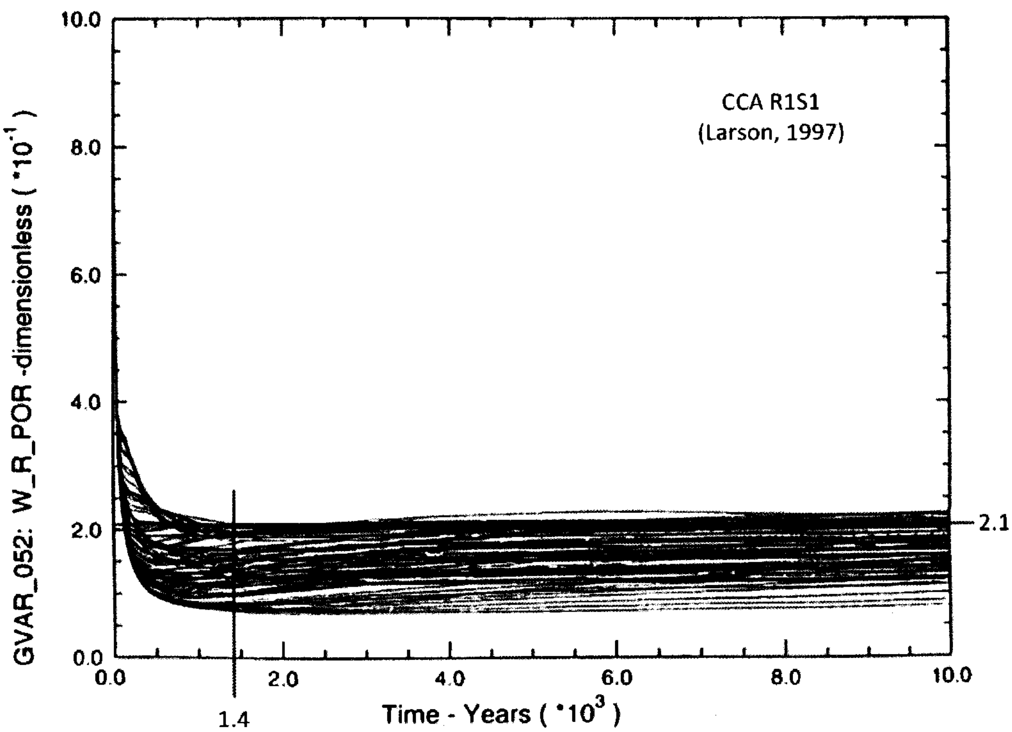

Figure 2. The minimum largest BRAGFLO porosity value (0.21) for the undisturbed case from the CCA Replicate R1 (Larson 1997, Appendix D in Hanson et al. 1997)

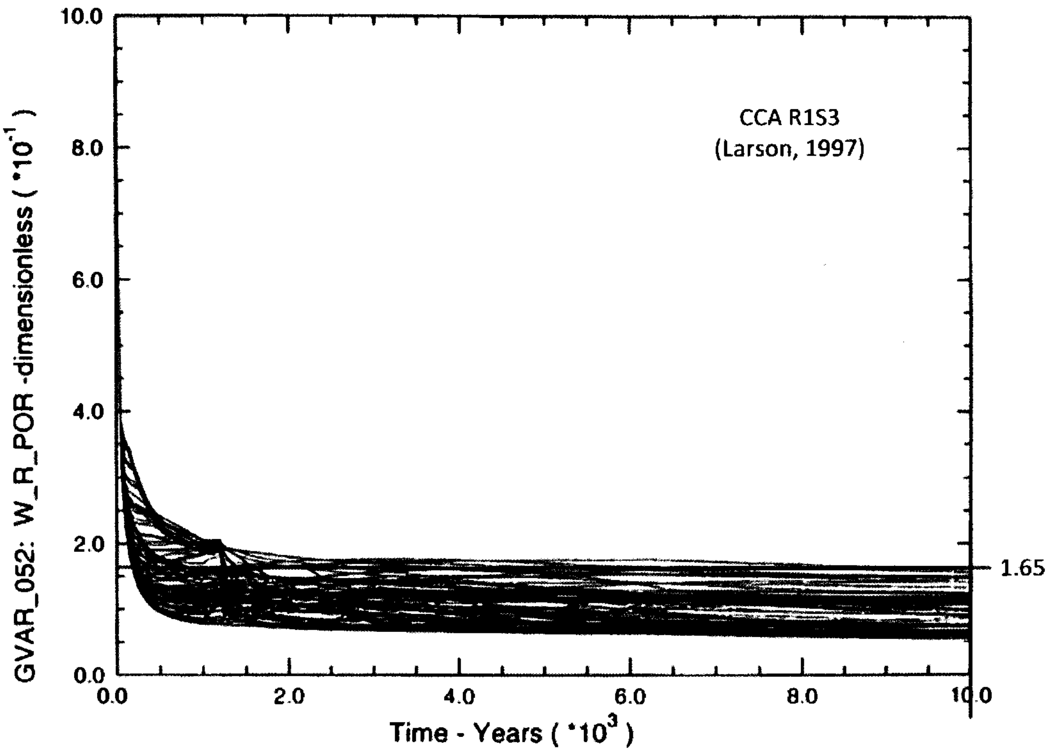

Figure 3. The minimum largest BRAGFLO porosity value (0.165) for Scenario S3 from the CCA Replicate R1 (Larson 1997, Appendix D in Hanson et al. 1997)

The porosity calculated by a structural code (ϕ) is the intrinsic, or true, porosity, which is defined as the ratio of the void volume to the current volume of an element of waste. In contrast, porosity in BRAGFLO (ϕ_B) is defined as the ratio of void volume to the original volume of an element of waste. The BRAGFLO porosities are related to the porosities calculated by a structural code by correcting for deformation of the waste during repository closure. The relationship between ϕ_B and ϕ is given by (CRA-2009 Appendix PORSURF):

$$\phi = \frac{\phi_B}{\phi_B + (1 - \phi_0)}$$

where ϕ_0 is initial waste porosity (0.848).

Once the intrinsic porosity is determined, the definition of porosity is used to determine the amount of room closure and waste compaction. For simplification, the solid component is considered incompressible compared to the void volume. The maximum room heights due to salt creep and waste compaction for CCA Scenarios S1 and S3 are given in Table 1. The same calculations were performed for the CRA-2009 PABC Replicate R1 results (Nemer 2010), Scenarios S1, S2, and S3. The results are also given in Table 1.

Table 1. Calculated maximum room heights based on BRAGFLO porosities

Case	BRAGFLO Porosity	Intrinsic Porosity	Room Height (m)	Source
1	0.21	0.58	1.43	Larson (1997): R1 S1 at ≈ 1400 years
2	0.165	0.52	1.26	Larson (1997): R1 S3 at 10,000 years
3	0.20	0.57	1.39	Nemer (2010): R1 S1 at ≈ 600 years
4	0.195	0.56	1.37	Nemer (2010): R1 S2 at ≈ 1100 years
5	0.195	0.56	1.37	Nemer (2010): R1 S4 at ≈ 600 years

Once the maximum room heights are determined, the degree to which the waste stack is crushed can be determined. This is estimated in Table 2 as volumetric strain ($\Delta V/V$). The pressure to cause a certain volumetric strain is determined by interpolation of the original experimental results performed to develop the constitutive model for the waste as reported in Stone (1997). Finally, the equivalent vertical stress is backed out from the pressure. The estimated minimum vertical stresses for the CCA and CRA-2009 PABC results are given in Table 2.

The compaction pressure used for the experiments performed to develop the Spallings model parameters was rounded from Larson's (1997) estimate of 4.8 MPa to 5.0 MPa (Table 2). Many of those experiments were tensile in nature, and thus the results were not affected by the compaction pressure used to make the samples. The estimated vertical stresses estimated from back-calculation using BRAGFLO porosities from the CRA-2009 are fairly consistent at 4.3 – 4.4 MPa regardless of the scenario, but are somewhat lower than the upper compaction pressure used in the experiments. These pressures are considered more credible than the FEM code estimates of 2.3 MPa because of the more realistic assumptions about gas generation employed in BRAGFLO. However, because the flume experiment results are strongly dependent on the compaction pressure, in contrast to the experiments designed to measure tensile strength, data from the 5.0 MPa samples are likely to bias the estimated value for the lower limit of TAUFAIL somewhat high for the current BRAGFLO estimates of compaction pressure. The shape of the shear strength versus compaction pressure curve can't be estimated using only two compaction pressures, but is more likely to be concave than linear or convex. Therefore, to be conservative, Sandia National Laboratories recommends using the experimental results from the 50% degraded surrogate waste samples fabricated using the considerably lower compaction pressure of 2.3 MPa rather than interpolating from the data to a 4.3 MPa compaction pressure. We believe that the average shear stress value from the experimental samples compacted at 2.3 MPa (2.22 Pa) represents a conservative, but defendable estimate of the lower bound on the range representing uncertainty in TAUFAIL.

Table 2. Estimated minimum vertical stress required to bring about waste stack deformation

Case	Source	$\frac{\Delta V}{V}$	Pressure (MPa)	Vertical Stress (MPa)
1	Larson (1997): R1 S1 at ≈ 1400 years	0.46	1.4	4.2
2	Larson (1997): R1 S3 at 10,000 years	0.53	1.6	4.8
3	Nemer (2010): R1 S1 at ≈ 600 years	0.48	1.4	4.3
4	Nemer (2010): R1 S2 at ≈ 1100 years	0.49	1.5	4.4
5	Nemer (2010): R1 S4 at ≈ 600 years	0.49	1.5	4.4

2 Variabilities in Results of the Flume Experiments

The EPA asked the DOE to consider uncertainties in the experimental data when defining the minimum value for TAUFAIL. For the following discussion, only the results from 50% degraded surrogate waste material samples are considered. Five replicates at each compaction pressure (2.3 and 5.0 MPa) were used.

TAUFAIL is modeled as a constant representing the average shear strength of repository waste. However, because there is variability in the waste and the waste form is expected to change, particularly in cases where the repository is inundated, uncertainty exists about the value used to represent the waste shear strength. The upper bound on probable values of TAUFAIL is 77 Pa, based on the assumption that the degradation of the waste is limited. The lower bound is assumed to be associated with waste that has become massively degraded physically over time. Having waste degrade by at most 50% seems reasonable based on results for iron corrosion and CPR degradation in BRAGFLO.

The average values of the experimental shear strengths were given in Herrick et al. (2012), Table 14, p. 79 for three methods of data analysis. Based on how well the experimental data fit the analysis method, the University of Florida (UF) method was recommended because it consistently fit the data well with almost no exceptions and only those results are considered. Variability in the experimental values arises from random error in the measurements and variability in the composition and construction of the samples. The measured mean shear strength across the five samples compacted at 2.3 MPa was 2.22 Pa with a standard error ($\sigma_{\bar{X}}$) of 0.269. In contrast, the measured mean shear strength across the five samples compacted at 5.0 MPa was 5.05 Pa with $\sigma_{\bar{X}} = 0.347$. The mean of the 2.3 MPa samples (2.22 Pa) is significantly different from the mean of the 5.0 MPa samples (5.05 Pa) at 95% confidence. Linear interpolation across the means to estimate a shear strength at 4.3 MPa compression (4.32 Pa) may produce a somewhat biased estimate of that shear strength, but nevertheless that value would also be well above the 95% confidence interval on the mean of 2.22 Pa ([1.47, 2.97]). Thus, 2.22 Pa represents a conservative lower bound for TAUFAIL at the expected compression pressure.

3 Why Water Was Used as the Eroding Fluid

Water was used as the eroding fluid for all the flume experiments. There are several reasons for this choice.

The shear strength of a material is assumed to be a property of the material. Another term for it, and perhaps a better description, is critical shear stress for the initiation of erosion of a material subjected to a hydrodynamic shear stress. It is modeled as a constant, and experimental evidence has always supported this idea. It is, therefore, independent of the eroding fluid used to measure it.

Flow of fluids through pipes has been studied extensively with theories and laws have been developed which relate the mean flow rate to the wall shear stress. The equations governing the design of the vertical flume are discussed in Section 2.3 of Test Plan 09-01 (Roberts and Herrick 2009), among many other places. Of importance is that the fluid properties, such as density and viscosity, can be accurately determined so that the flow can be sufficiently regulated to subject the samples to a known hydrodynamic shear stress. The properties of water are well known having been extensively studied, as are the effects of water quality measurements such as temperature and conductivity. Over the course of an experiment, the temperature of the fluid may rise a couple degrees. At the beginning of erosion, the change in conductivity of the water is attributable to the change in temperature, not to material being carried along in the current. Therefore, the hydrodynamic shear stress using water can be determined accurately. Special testing would be required to characterize the properties of any other eroding fluid, requiring methods and procedures to be developed and extra time spent to conduct these fluid characterization tests.

In experimental laboratories of Sandia National Laboratories Defense Waste Management Programs, brine is typically considered a hazardous waste. The two supply tanks for the vertical flume are 300 gallons (1135 L) each. The tanks are cleaned after each sample is eroded. The volume of potentially hazardous waste to dispose of was considered cost prohibitive if an alternative could be found. Plain water was the obvious choice.

There is a small amount of salt in each specimen. Water is expected to at least partially dissolve the salt. The dissolution of salt from the experimental samples would only make erosion easier. Therefore, the use of water makes the experimental TAUFAIL results conservative.

The laboratory equipment is well suited for use with water. It was not known what effect brine would have on the equipment since it can deteriorate stainless steel and salt and other minerals may precipitate out and cake on the channels and measuring equipment, interfering with their operation.

4 Comparison of Surrogate Waste Material Recipe with the PAIR

The experimental samples were made using weight fractions of the various constituents. Starting with Butcher et al. (1991), the waste inventory has been divided into major five categories for purposes of surrogate material development. The EPA asked for a comparison between the original surrogate waste material development inventory and the present inventory. This is given in Table 3 below, along with the inventory used for the last CRA. Based on the fluctuation that occurs whenever the inventory is compiled, the slight difference between the present inventory and the inventory used by Hansen et al. (1997) to develop the surrogate waste recipes is not sufficient grounds to justify a change.

Table 3. Inventories by weight fraction of the major waste components as compared to the surrogate waste material recipes developed by Hansen et al. (1997).

Waste Composition	CCA Hansen et al. (1997)	CRA-2009 PABC Crawford et al. (2009)	CRA-2014 Van Soest (2012)
Metals	52	47	49
Cellulosics	7	8	5
Rubbers and Plastics	9	10	10
Sorbents	4	6	7
Sludges	28	29	28

5 Recommendations

Based on back calculation of the most recent PA baseline, CRA-2009 PABC, the compaction pressure applied to the waste is at a consistent minimum 4.3 – 4.4 MPa. This number is slightly less than the 5.0 MPa used to make the samples recommended in Herrick et al. (2012) to establish the lower limit of TAUFAIL. On the other hand, the 4.3 – 4.4 MPa range is considerably higher than 2.3 MPa, the compaction pressure obtained based on FEM analyses.

The shear strength of the surrogate waste material is dependent on the compaction pressure. To be conservative, Sandia National Laboratories recommends using the experimental results from the 50% degraded surrogate waste samples fabricated using the considerably lower compaction pressure of 2.3 MPa rather than the 5.0 MPa compaction pressure results or by interpolating from the data to a 4.3 MPa compaction pressure. We believe that the average shear stress value from the experimental results of samples compacted at 2.3 MPa (2.22 Pa) represents a conservative, but defendable estimate of the lower bound on the range representing uncertainty in TAUFAIL. Table 4 contains updated information related to this distribution that will be input into the parameter database.

Table 4. Statistics for BOREHOLE : TAUFAIL to be entered into the parameter database.

Minimum	2.22 Pa
Maximum	77.00 Pa
Distribution	Uniform
Mean	39.61 Pa
Median	39.61 Pa
Standard Deviation	21.59 Pa

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Acknowledgments

Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security Administration. This research is funded by WIPP programs administered by the Office of Environmental Management (EM) of the U.S Department of Energy.