SRNL-L6200-2009-00011

Date: March 18, 2009

To: Jeff Newman

From : Greg Flach

Subject: PORFLOW Sensitivity Cases for Saltstone PA

This memorandum documents the basis behind PORFLOW sensitivity cases related to uncertainty in the rate of vault degradation by sulfate attack. The nominal analysis (Flach et al. 2009) assumes that

1) Transport properties, with respect to predicting ettringite front position, are unchanged by passage of the front.

2) The presence of ettringite coincides with physical damage to concrete, for the purpose of estimating effective transport properties for Saltstone contaminant release.

To explore the sensitivity of PORFLOW simulations to these *Key Assumptions*, two alternatives are considered:

1) Diffusion coefficient, with respect to predicting ettringite front position, is assumed to locally increase after passage of the front.

2) Ettringite formation is assumed to not lead to damage.

Sensitivity Case 1 is contrary to Key Assumption 1, and produces faster vault degradation. Sensitivity Case 2 differs from Key Assumption 2, and implies no change to vault properties over time.

Accelerated degradation (Sensitivity Case 1): To assign an appropriate diffusion coefficient for Sensitivity Case 1, we consider the properties of cracked concrete, the presumed state of degraded concrete behind the advancing ettringite front. In a theoretical study of cracked cement-based materials, Gerard and Marchand (2000) conclude that "in most practical cases, the increase in diffusivity is limited to a factor of 10. In that respect, the influence of the crack network on the material diffusivity appears to be much less significant than its effect on the solid permeability". The latter statement is supported by a comparison of diffusion coefficient and hydraulic conductivity for materials in the Saltstone materials palette (Flach et al. 2009, Table 13). Figure 1 shows a cross plot of the two properties. An empirical curve fit indicates that diffusion coefficient varies as roughly the cube root of conductivity (power law exponent = 0.3187 ≈ 1/3):

$$\frac{D_e}{D_{ref}} \approx \left(\frac{K}{K_{ref}} \right)^{1/3} \quad (1)$$

A power law exponent of 1/3 means that a 1000x increase in conductivity corresponds to only a 10x increase in diffusion coefficient.

Equation (1) can be used to estimate changes in diffusion coefficient from conductivity variations. The conductivity of cracked concrete under unsaturated conditions can be estimated using the work of Or and Tuller (2000). Key specifications are the crack aperture and spacing. Wang et al. (1997) found that crack openings less than 50 μm had "little effect on concrete permeability", implying a similarly small effect on effective diffusion coefficient. In agreement with the latter, Ismail et al. (2004) found that apertures less than about 50 μm did not produce accelerated chloride penetration in cracked concrete. In another chloride propagation study, Sahmaran and Yaman (2008) report that "for crack widths less than about 135 μm, the effect of crack width on the effective diffusion coefficient . . . was found to be marginal when compared to virgin specimens". A hypothetical aperture of 127 μm (5 mil) is chosen for this sensitivity case. This crack opening is large enough to cause increased diffusion, but small enough to be consistent with microcracks presumed to occur with ettringite formation. Gerard and Marchand (2000) define a "mean crack spacing factor" as the ratio of crack spacing to aperture, and note that the parameter "rarely goes below 100, even for concrete samples severely degraded". For the assumed aperture of 127 μm, a mean crack spacing factor of 100 corresponds to a crack spacing of 1.27 cm. For this sensitivity study we assume a crack spacing of 1 cm, implying extensive damage from sulfate attack.

Using Vault 1/4 wall concrete as a basis, Figure 2 compares the unsaturated hydraulic conductivity of cracked and uncracked concrete for the chosen crack parameters. Soil suction levels under nominal Saltstone closure cap degradation conditions vary through space and time across a typical range of a few 10s to a few 100s of centimeters. In this suction range, the conductivity of cracked concrete ranges up to 3 orders of magnitude higher than K for uncracked concrete. Equation (1) suggests a corresponding increase in diffusion coefficient up to 10x, which is consistent with Gerard and Marchand (2000). Accordingly, a 10x higher diffusion coefficient is used to predict sulfate attack for Sensitivity Case 1.

The impact of a 10x increase in diffusion coefficient is summarized in Table 1. Figures 3 through 5 show the position of the ettringite front for this accelerated sulfate attack sensitivity case. Note that the time to complete failure is less than 10k years for Vault 2 components and the Vault 4 roof.

Table 1 - Vault component failure times for Case A Nominal and Case A Sensitivity Case 2.

Time to complete failure	Nominal	10x higher De
Vault 1 wall	>100k	16000
Vault 1 floor	>100k	25000
Vault 1 roof	50000	12000
Vault 2 wall	18000	3000
Vault 2 floor	40000	5000
Vault 2 roof	40000	7000
Vault 4 wall	>100k	16000
Vault 4 floor	>100k	25000
Vault 4 roof	10000	3000

References

Flach, G. P., J. M. Jordan and T. Whiteside. 2009. Numerical Flow And Transport Simulations Supporting The Saltstone Disposal Facility Performance Assessment. SRNL-STI-2009-00115, Revision 0.

Gerard, B. and J. Marchand. 2000. Influence of cracking on the diffusion properties of cement-based materials; Part I: Influence of continuous cracks on the steady-state regime. Cement and Concrete Research. v30. 37-43.

Ismail, M., A. Toumi, R. Francois and R. Gagne. 2004. Effect of crack opening on the local diffusion coefficient of chloride in inert materials. Cement and Concrete Research. v34. 711-716.

Or, D. and M. Tuller, 2000, Flow in unsaturated fractured porous media: Hydraulic conductivity of rough surfaces, Water Resources Research, v. 36, n. 5, 1165-1177.

Sahmaran, M. and I. O. Yaman. 2008. Influence of transverse crack width on reinforcement corrosion initiation and propagation in mortar beams. Canadian Journal of Civil Engineering. v35. 236-245.

Wang, K., D. C. Jansen, S. P. Shah and A. F. Karr. 1997. Permeability study of cracked concrete. Cement and Concrete Research. v27. 381-393.

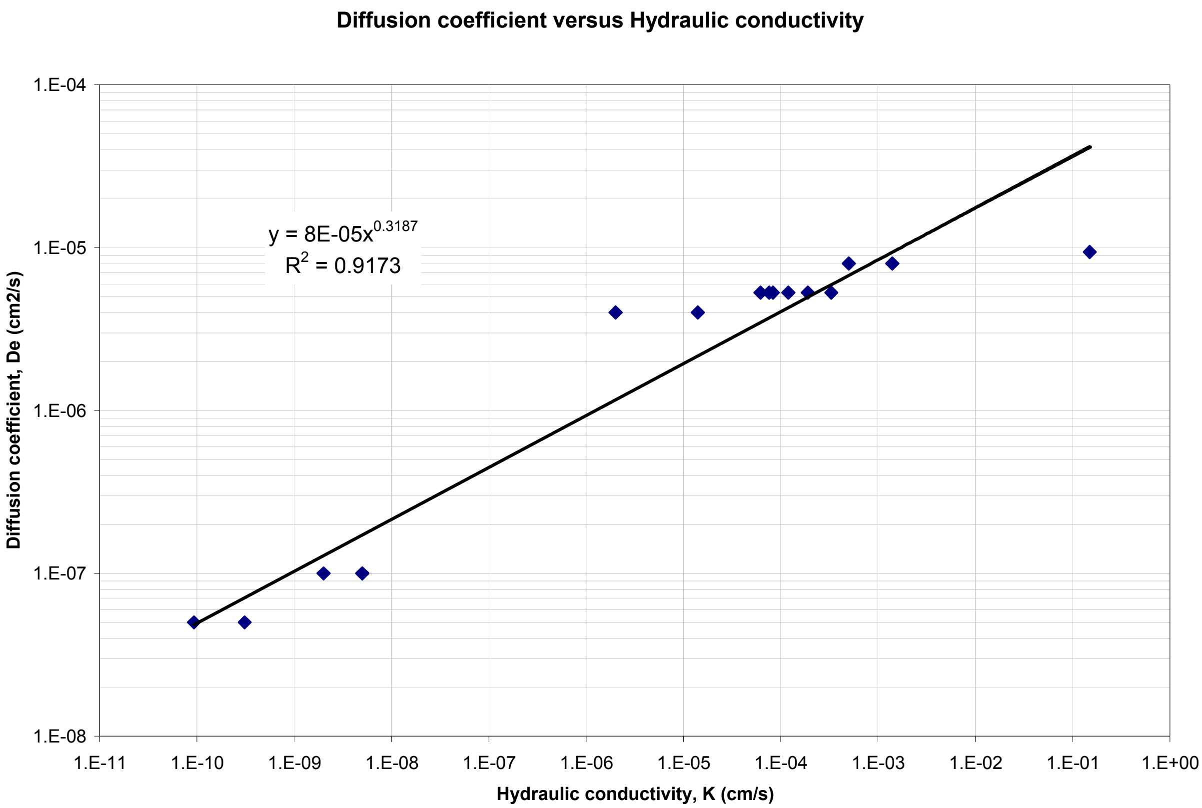

Figure 1 – Diffusion coefficient compared to hydraulic conductivity for Saltstone materials palette.

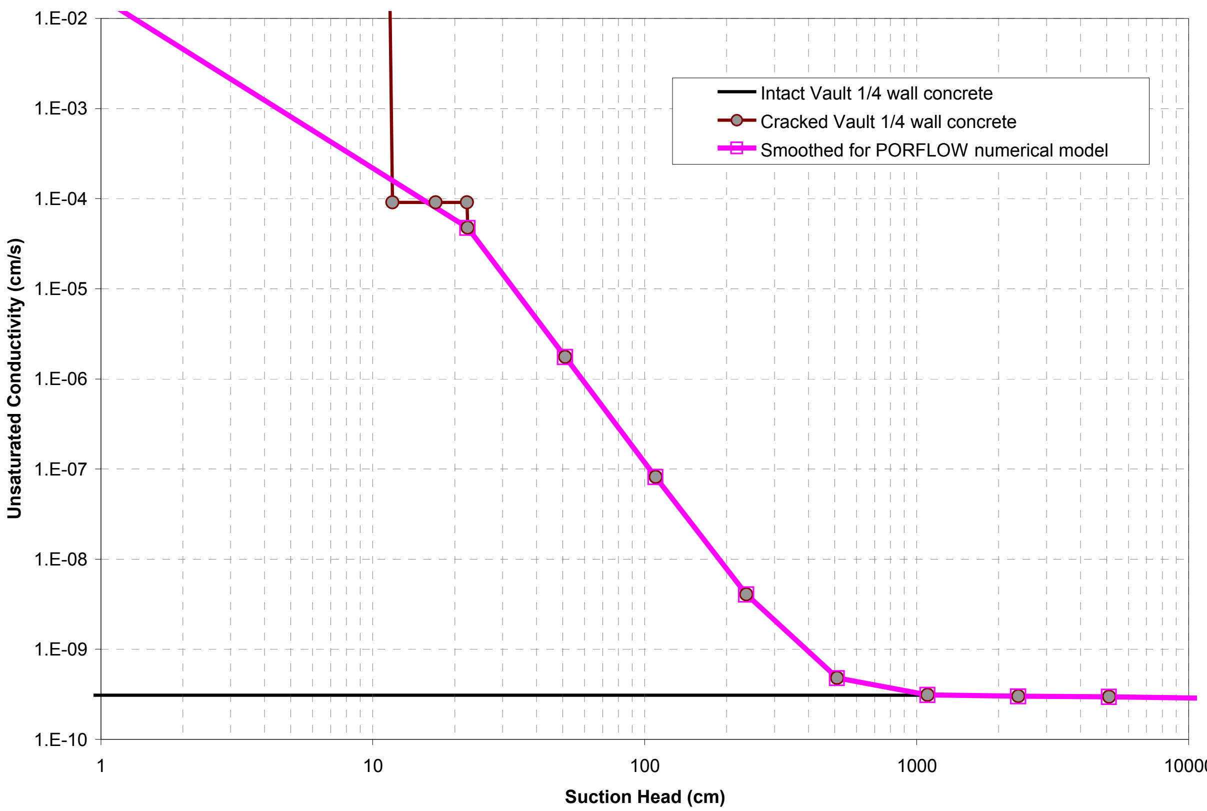

Figure 2 – Unsaturated hydraulic conductivity estimate for cracked and uncracked vault concrete (127 µm aperture, 1 cm crack spacing).

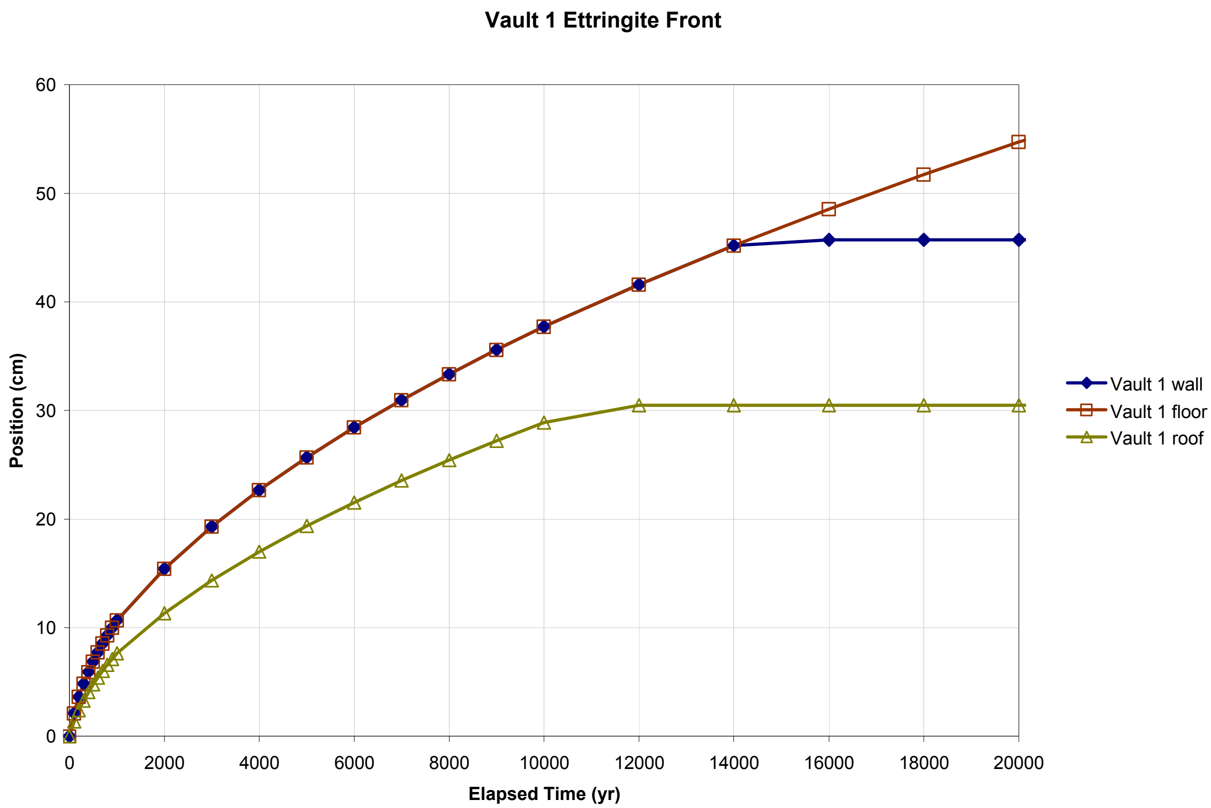

Figure 3 – Ettringite front position for accelerated sulfate attack in Vault 1.

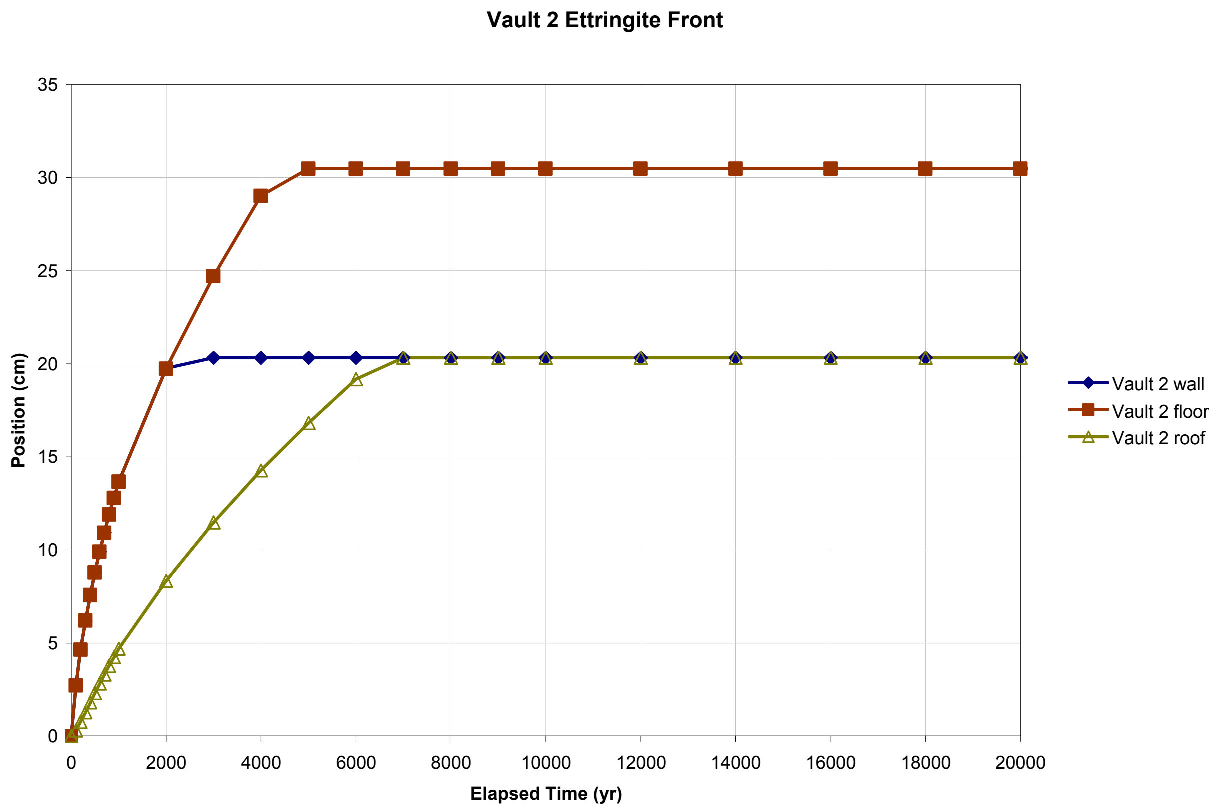

Figure 4 – Ettringite front position for accelerated sulfate attack in Vault 2.

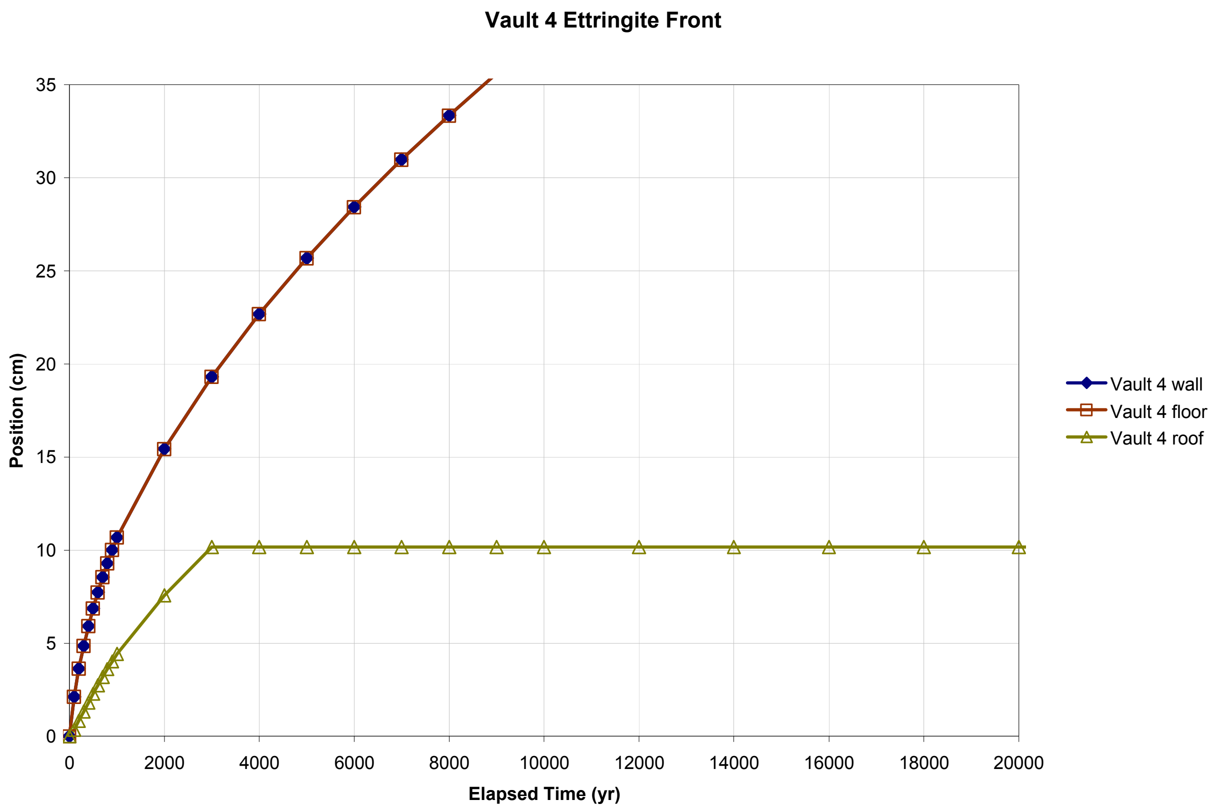

Figure 5 – Ettringite front position for accelerated sulfate attack in Vault 4.