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Verification of Sulfate Attack Penetration Rates for Saltstone Disposal Unit Modeling

G. P. Flach

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EXECUTIVE SUMMARY

Recent Special Analysis modeling of Saltstone Disposal Units consider sulfate attack on concrete and utilize degradation rates estimated from Cementitious Barriers Partnership software simulations. This study provides an independent verification of those simulation results using an alternative analysis method and an independent characterization data source. The sulfate penetration depths estimated herein are similar to the best-estimate values in SRNL-STI-2013-00118 Rev. 2 and well below the nominal values subsequently used to define Saltstone Special Analysis base cases.

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LIST OF ABBREVIATIONS

AFm	Monosulfoaluminate
BE	Best estimate
CE	Conservative estimate
C-S-H	Calcium-Silicate-Hydrate
LXO	LeachXS/Orchestra
NV	Nominal value
SDU	Saltstone Disposal Unit
SRNL	Savannah River National Laboratory
VCO	Vault Concrete One (SDU 1/4)
VCT	Vault Concrete Two (SDU 2/6)
VU	Vanderbilt University

1.0 Introduction

Recent Special Analysis modeling of Saltstone Disposal Units (SRR 2013, 2014) and supporting documents (Flach and Taylor 2014, SRR 2015) consider sulfate attack on SDU concrete and utilize degradation rates (Flach and Smith, 2013a, b, 2014) estimated from Cementitious Barriers Partnership (http://cementbarriers.org) software simulations. The purpose of this study is to provide an independent verification of the specific software results used for modeling following Procedure E7 2.31. Procedure E7 2.31 *Engineering Calculations*, Section 5.5 *Use of Engineering Calculation Software*, provides a means of assuring quality in software output without invoking Sections 5.5.2 *Software Management and Quality Assurance* and 5.5.3 *Functional Classification of Software*. Previous design checking of the Cementitious Barriers Partnership sulfate attack module use conducted under an E7 2.60 document review of SRNL-STI-2013-00118 Rev. 0 fulfills the E7 2.31 requirement that "the Verifier shall confirm that all formulae, inputs and outputs are correct". The present analysis fulfills the requirement that "the Verifier/Checker shall use a different method to validate the outputs are correct" such as "performing hand calculations to validate the outputs". The independent verification herein is based on an approximate analytic solution for a moving reaction front and reaction capacities based on initial mineral assemblage and stoichiometry.

2.0 General Moving Reaction Front

Figure 2-1 illustrates a reaction front that moves slowly through a porous medium compared to the time scale of diffusion for a dissolved reactant at exposure concentration c. Reaction with the solid phase is assumed to be instantaneous and complete, such that the reaction front is sharp and separates fully reacted and unreacted zones.

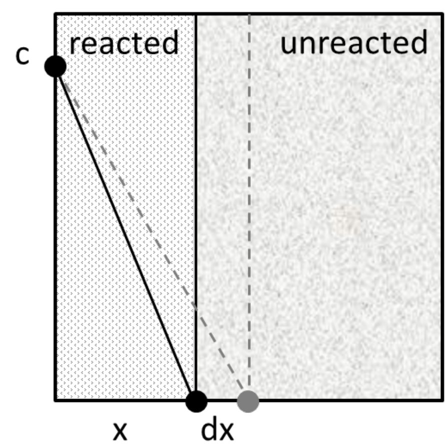

Figure 2-1. Generic slow-moving reaction front controlled by diffusion.

The differential molar balance for this generic moving front system is (Flach and Smith 2014)

$$Sn\tau D_m \frac{c}{x} dt = R(1-n)\rho_s dx \qquad (1)$$

where

S = saturation of fluid phase delivering reactant to moving front [cm^3 phase / cm^3 void]

n = porosity [cm^3 void / cm^3 total]

τ = tortuosity, defined here as the ratio of effective to molecular diffusion coefficient (< 1) [unitless]

D_m = molecular diffusion coefficient for fluid phase [cm^2/yr]

x = penetration depth [cm]

t = elapsed time [yr]

c = fixed concentration of fluid phase reactant at the exposure surface [mol / cm^3 phase]

R = reaction capacity of solid [mol / g solid], i.e., moles of fluid phase reactant consumed per mass of solid

ρ_s = solid / mineral density [g/cm^3 solid]

All material properties and the exposure concentration are assumed to have constant values. Integration of Equation (1) yields the following analytic expression for penetration depth as a function of exposure time

$$x = \left[\frac{2Sn\tau D_m ct}{(1-n)\rho_s R}\right]^{1/2} \tag{2}$$

The exposure and material property parameters can be lumped to form the rate constant

$$A \equiv \left[\frac{2Sn\tau D_m c}{(1-n)\rho_s R}\right]^{1/2} \tag{3}$$

and Equation (1) becomes

$$x = At^{1/2} \tag{4}$$

The reaction capacity R depends on the aqueous reactant at the exposure surface, mineral assemblage in the unreacted zone, and the stoichiometry of the reaction. Reaction capacities specific to sulfate attack on SDU concrete are estimated in the next section.

3.0 Reaction Capacities

Sodium sulfate attack involves ingress of sulfate ions through concrete pore water and reactions with calcium bearing minerals, including calcium hydroxide and C-S-H, that produce expansive products, principally ettringite and gypsum. Physical degradation occurs when sufficient ettringite and/or gypsum form to cause internal cracking. In the following sub-sections, sulfate reaction capacities are estimated for ettringite and gypsum formation based on material characterization by Simco Technologies and Vanderbilt University (VU).

3.1 Ettringite formation

The chemical formula for ettringite has been expressed in a number of equivalent forms including

$$Ca_6Al_2(SO_4)_3(OH)_{12} \cdot 26H_2O = 6CaO \cdot Al_2O_3 \cdot 3SO_3 \cdot 32H_2O = 3CaO \cdot Al_2O_3 \cdot 3CaSO_4 \cdot 32H_2O \quad (5)$$

and in the shorthand of cement chemist notation (http://en.wikipedia.org/wiki/Cement_chemist_notation)

$$C_6A\bar{S}_3H_{32} \quad (6)$$

Cement paste is calcium-rich compared to aluminum, so the latter is the limiting solid-phase reactant. The reaction capacity for ettringite formation based on aluminum availability can be estimated from laboratory characterization of Saltstone concrete.

Simco (2012) deduced mineral compositions for hydrated SDU concretes based on characterization of the dry mix components and thermodynamic considerations; these data summarized in Table 9 of Simco (2012) are reproduced in Table 3-1. The only aluminum-bearing phase is monosulfoaluminate (AFm). Equivalent chemical formulas for AFm in conventional and cement chemist notations include (Matschei et al. 2007)

$$Ca_4Al_2(SO_4)(OH)_{12} \cdot 6H_2O = 4CaO \cdot Al_2O_3 \cdot SO_3 \cdot 12H_2O \quad (7)$$

and

$$C_4A\bar{S}H_{12} \quad (8)$$

Table 3-2 presents a calculation of reaction capacity based on Table 3-1 and the stoichiometry indicated by Expressions (5) through (8). The availability of AFm for reaction is assumed to be 100% on the basis that formation of ettringite from AFm is thermodynamically favorable when additional sulfate enters the system (Matschei et al. 2007).

Ettringite reaction capacity can be similarly estimated from concrete characterization performed independently by Vanderbilt University on different concrete samples (Arnold et al. 2010), as summarized by input to the LeachXS/Orchestra sulfate attack module. These calculations are presented in Table 3-3. VU characterization is expressed on an elemental basis, thus the mass concentration of Al is directly specified.

The Al reaction capacities in Table 3-2 and Table 3-3 differ because different samples were tested, and more significantly, because of differing assumptions for the availability of aluminum for reaction.

Table 3-1. Simco (2012) characterization of SDU concretes.

Mineral phase	SDU 1/4 (g/kg)	SDU 2/6 (g/kg)
$C\text{-}S\text{-}H$	118.8	81.2
CH (Portlandite)	7.2	-
AFm	18.4	10.0
C_4FH_{13}	9.9	-

Table 3-2. Ettringite reaction capacity of AFm based on Simco (2012).

Parameter	SDU 1/4	SDU 2/6	Units	Comments
Mass concentration of AFm	18.4	10.0	g / kg solid	Simco (2012) Table 9
Molecular weight of AFm	622	622	g / mol	Approximate value calculated from chemical formula using round numbers for element molecular weights
Molar concentration of AFm	2.96e-2 2.96e-5	1.61e-2 1.61e-5	mol / kg solid mol / g solid	Calculated
Moles Al per mole AFm	2	2	mol Al / mol AFm	See Expression (7)
Molar concentration of Al	5.92e-5	3.22e-5	mol / g solid	Calculated
Moles SO_4 reacted per mol Al	1.5	1.5	mol SO_4 / mol Al	See Expression (5)
Reaction capacity, R	8.87e-5	4.82e-5	mol SO_4 / g solid	Calculated

Table 3-3. Ettringite reaction capacity based on VU characterization of total aluminum.

Parameter	SDU 1/4	SDU 2/6	Units	Comments
Mass concentration of Al	5373 5.373	6108 6.108	mg / kg solid g / kg solid	"Concrete_data.xls" input file
Molecular weight of Al	27	27	g / mol	
Molar concentration of Al	1.99e-1 1.99e-4	2.26e-1 2.26e-4	mol / kg solid mol / g solid	Calculated
Moles SO_4 reacted per mol Al	1.5	1.5	mol SO_4 / mol Al	See Expression (5)
Reaction capacity, R	2.99e-4	3.39e-4	mol SO_4 / g solid	Calculated

3.2 Gypsum formation

The chemical formula for gypsum can be expressed as

$$CaSO_4 \cdot 2H_2O = CaO \cdot SO_3 \cdot 2H_2O \tag{9}$$

or in cement chemist notation

$$C\bar{S}H_2 \tag{10}$$

Unlike ettringite, calcium availability defines the reaction capacity for gypsum formation. The availability of calcium for gypsum formation is assumed to be less than 100% and limited to that present as calcium hydroxide (Portlandite) following the sulfate attack model of Tixier and Mobasher (2003a, b).

Simco Technologies Inc. models $C\text{-}S\text{-}H$ gel as a mixture of calcium hydroxide and the calcium silicate hydrate mineral (true CSH)

$$C\text{-}S\text{-}H = 1.65CaO \cdot SiO_2 \cdot 1.65H_2O = 0.65Ca(OH)_2 + CaH_2SiO_4 \tag{11}$$

In cement chemist notation, Equation (11) becomes

$$C\text{-}S\text{-}H = 0.65CH + CSH \tag{12}$$

Table 3-4 presents a calculation of the reaction capacity for gypsum formation based on Ca available explicitly as $Ca(OH)_2 = CH$ and implicitly as the CH portion of $C\text{-}S\text{-}H$.

A similar calculation can be performed based on VU characterization of VCO (SDU1/4) and VCT (SDU2/6) concretes (Arnold et al. 2010), and the resulting initial mineral assemblage in LeachXS/Orchestra sulfate attack module simulations. Inspection of LXO simulation output (Appendix) indicates that both Portlandite and siliceous hydrogarnet are consumed during sulfate ingress, so both minerals are assumed to contribute to gypsum reaction capacity. Chemical formulas for siliceous hydrogarnet include

$$C_3AS_{0.8}H_{4.4} = 3CaO \cdot Al_2O_3 \cdot 0.8SiO_2 \cdot 4.4H_2O \tag{13}$$

Table 3-5 presents a calculation of gypsum reaction capacity based on Ca being available in calcium hydroxide and siliceous hydrogarnet. As with Al reaction capacity, Ca reaction capacity differs between Table 3-4 and Table 3-5 due to differing assumptions for mineral availability. The LXO output file "output_profiles.dat" did not list the concentrations of $C\text{-}S\text{-}H$ components `C-S-H_tobermorite` and `C-S-H_jennite`. Presumably these minerals provided additional reaction capacity for gypsum formation. An upper bound on reaction capacity can be calculated by assuming all Ca present in the system is available for reaction. This calculation is presented in Table 3-6. The increases in reaction capacity are modest at +16% for SDU 1/4 concrete and +29% for SDU 2/6 concrete.

Table 3-4. Gypsum reaction capacity based on Simco (2012).

Parameter	SDU 1/4	SDU 2/6	Units	Comments
Mass concentration of CH	7.2	-	g / kg solid	Simco (2012) Table 9
Molecular weight of CH	74	74	g / mol	$Ca(OH)_2$
Molar concentration of CH	9.73e-2 9.73e-5	-	mol / kg solid mol / g solid	Calculated
Moles of Ca per mole of CH	1	1	mol Ca / mol CH	$CH = Ca(OH)_2$
Molar concentration of Ca as CH	9.73e-5	-	mol / g solid	Calculated
Mass conc. of Simco $C\text{-}S\text{-}H$	118.8	81.2	g / kg solid	Simco (2012) Table 9
Molecular weight of Simco $C\text{-}S\text{-}H$	182.1	182.1	g / mol	$1.65CaO \cdot SiO_2 \cdot 1.65H_2O$
Molar conc. of Simco $C\text{-}S\text{-}H$	6.52e-1 6.52e-4	4.46e-1 4.46e-4	mol / kg solid mol / g solid	Calculated
Moles of Ca as CH per mole of $C\text{-}S\text{-}H$	0.65	0.65	mol Ca / mol $C\text{-}S\text{-}H$	$0.65CH + CSH$
Molar conc. of Ca as $C\text{-}S\text{-}H$	4.24e-4	2.90e-4	mol / g solid	Calculated
Total molar concentration of Ca	5.21e-4	2.90e-4	mol / g solid	Calculated
Moles SO_4 reacted per mol Ca	1	1	mol SO_4 / mol Al	See Expression (9)
Reaction capacity, R	5.21e-4	2.90e-4	mol SO_4 / g solid	Calculated

Table 3-5. Gypsum reaction capacity based on VU characterization and LeachXS initialization.

Parameter	SDU 1/4	SDU 2/6	Units	Comments
Porosity	0.115	0.11	cm^3 void / cm^3 tot.	"Concrete_data.xls" input file
Saturation	1	1	cm^3 liq. / cm^3 void	Saturated exposure conditions
Solid density	2400	2310	kg / m^3 solid	"Concrete_data.xls" input file
Bulk density	2124 2.124	2056 2.056	kg / m^3 total g / cm^3 total	Calculated
Molar conc. of CH on a liquid basis	18.7	12.4	mol / L liquid	LeachXS initialization from "output_profiles.dat" (Appendix; unreacted concrete at depth)
Molar conc. of CH on a total volume basis	2.15 2.15e-3	1.36 1.36e-3	mol / L total mol / cm^3 total	Calculated
Molar conc. of CH on a solid basis	1.01e-3	6.63e-4	mol / g solid	Calculated
Moles of Ca per mole CH	1	1	mol Ca / mol CH	$CH = Ca(OH)_2$
Molar conc. of Ca in CH on a solid basis	1.01e-3	6.63e-4	mol / g solid	Calculated
Molar conc. of $C_3AS_{0.8}H_{4.4}$ on a liquid basis	1.15	1.09	mol / L liquid	LeachXS initialization from "output_profiles.dat" (Appendix; unreacted concrete at depth)
Molar conc. of $C_3AS_{0.8}H_{4.4}$ on a total volume basis	1.32e-1 1.32e-4	1.20e-1 1.20e-4	mol / L total mol / cm^3 total	Calculated
Molar conc. of $C_3AS_{0.8}H_{4.4}$ on a solid basis	6.23e-5	5.83e-5	mol / g solid	Calculated
Moles of Ca per mole $C_3AS_{0.8}H_{4.4}$	3	3	mol Ca / mol $C_3AS_{0.8}H_{4.4}$	$3CaO \cdot Al_2O_3 \cdot 0.8SiO_2 \cdot 4.4H_2O$
Molar conc. of Ca in $C_3AS_{0.8}H_{4.4}$ on a solid basis	1.87e-4	1.75e-4	mol / g solid	Calculated
Total molar conc. of Ca	1.20e-3	8.38e-4	mol / g solid	Calculated
Moles SO_4 reacted per mol Ca	1	1	mol SO_4 / mol Al	See Expression (9)
Reaction capacity, R	1.20e-3	8.38e-4	mol SO_4 / g solid	Calculated

Table 3-6. Gypsum reaction capacity based on VU characterization of total calcium.

Parameter	SDU 1/4	SDU 2/6	Units	Comments
Mass concentration of Ca	55579 55.579	43193 43.193	mg / kg solid g / kg solid	"Concrete_data.xls" input file
Molecular weight of Ca	40	40	g / mol	
Molar concentration of Ca	1.39 1.39e-3	1.08 1.08e-3	mol / kg solid mol / g solid	Calculated
Moles SO_4 reacted per mol Ca	1	1	mol SO_4 / mol Al	See Expression (9)
Reaction capacity, R	1.39e-3	1.08e-3	mol SO_4 / g solid	Calculated

3.3 Total reaction capacity

The total capacity of the solid to react with infiltrating sulfate is taken to be the sum of the capacities for reaction with AFm and any other aluminum phases (to form ettringite) and Portlandite (to form gypsum). Table 3-7 summarizes total reaction capacities based on independent material characterization performed by Simco Technologies and Vanderbilt University. The actual total reaction capacity based on VU characterization is expected to lie between the lower ("Portlandite calcium") and upper ("total calcium") estimates.

Table 3-7. Total reaction capacities.

Reaction capacity, *R* (mol SO_4 reacted / g solid)	**SDU 1/4**	**SDU 2/6**	**Comments**
Simco characterization			
Ettringite formation	8.87e-5	4.82e-5	Table 3-2
Gypsum formation	5.21e-4	2.90e-4	Table 3-4
Ettringite+gypsum formation	6.10e-4	3.38e-4	Total capacity
VU characterization			
Ettringite formation	2.99e-4	3.39e-4	Table 3-3
Gypsum formation, Portlandite calcium	1.20e-3	8.38e-4	Table 3-5
Gypsum formation, total calcium	1.39e-3	1.08e-3	Table 3-6
Ettringite+gypsum formation, Portlandite calcium	1.50e-3	1.18e-3	Lower estimate of total capacity
Ettringite+gypsum formation, total calcium	1.69e-3	1.42e-3	Upper estimate of total capacity

4.0 Penetration Depths

Table 4-1 summarizes the sulfate attack results from SRNL-STI-2013-00118 (Flach and Smith 2013a, b, 2014) that require verification per Procedure E7 2.31. The linear rate constants subsequently used to predict sulfate attack penetration depths for particular disposal unit components (floor, wall, roof) are computed as

$$A_\ell = \frac{x_0}{t_0} \tag{14}$$

Thus simulated penetration depth x_0 at the designated time t_0 defines the rate. For verification of SRNL-STI-2013-00118 A_ℓ results, x_0 values from Table 4-1 are compared to penetration depths computed from Equation (2) for the same exposure time t_0. Table 4-2 presents sulfate attack penetration depths for SDU 1/4 and 2/6 based on Simco (2012) characterization data, and Table 4-3 provides the analogous calculation for VU concrete characterization and LeachXS/Orchestra initialization. Table 4-4 compares these depths to those from SRNL-STI-2013-00118 (Flach and Smith 2013a, b, 2014).

Table 4-1. Summary of sulfate attack results from SRNL-STI-2013-00118 Rev. 2.

Parameter	SDU 2 CE[1]	SDU 2 NV[2]	SDU 2 BE[3]	SDU 1/4 CE[1]	SDU 1/4 NV[2]	SDU 1/4 BE[3]
Fractional porosity, b	0.3	0.45	0.6	0.3	0.45	0.6
Penetration depth, x_0 (cm)	9.4	7.4	3.8	23	18.5	7.7
Penetration time, t_0 (yr)	350	350	350	500	500	500
Linear rate constant, A_ℓ (cm/yr)	0.027	0.021	0.011	0.046	0.037	0.015

[1]CE – Conservative Estimate; [2]NV – Nominal Value; [3]BE – Best Estimate

Table 4-2. Penetration depth calculations based on Simco Technologies Inc. characterization.

Parameter	SDU 1/4	SDU 2/6	Units	Comments
Porosity, n	0.116	0.139	cm^3 void / cm^3 total	Simco (2012) Table 12 97 days
Bulk density, $\rho_b = (1-n)\rho_s$	2.330	2.309	g solid / cm^3 total	Simco (2012) Table 10
Saturation, S	1	1	cm^3 liquid / cm^3 void	Saturated exposure conditions
Effective diffusion coefficient, $D_e = \tau D_m$	2.6e-7 8.2	2.9e-8 0.91	cm^2/s cm^2/yr	Simco (2012) Table 13 97 day average
Exposure concentration, c	0.1 1.0e-4	0.1 1.0e-4	mol / L mol / cm^3	Concentration assumed in SRNL-STI-2013-00118
Reaction capacity, R	6.10e-4	3.38e-4	mol SO_4 reacted / g solid	Table 3-7
Rate coefficient, $A \equiv \left[\frac{2Sn\tau D_m c}{(1-n)\rho_s R}\right]^{1/2}$	0.37	0.18	cm/√yr	Calculated
Exposure time, t	500	350	yr	Table 4-1
Penetration depth, $x = At^{1/2}$	8.2	3.4	cm	Calculated

Table 4-3. Penetration depth calculations based on VU characterization.

Parameter	SDU 1/4	SDU 2/6	Units	Comments
Porosity, n	0.115	0.11	cm^3 void / cm^3 total	"Concrete_data.xls" input file
Solid density, ρ_s	2.40	2.31	g solid / cm^3 solid	"Concrete_data.xls" input file
Saturation, S	1	1	cm^3 liquid / cm^3 void	Saturated exposure conditions
Inverse of tortuosity, $1/\tau$	10	20.74	-	
Tortuosity, τ	0.1	0.0482	-	Calculated
Molecular diffusion coefficient, D_m	1.0e-9 1.0e-5 315	1.0e-9 1.0e-5 315	m^2/s cm^2/s cm^2/yr	Orchestra file "diffusion.inp"
Exposure concentration, c	0.1 1.0e-4	0.1 1.0e-4	mol / L mol / cm^3	Concentration assumed in SRNL-STI-2013-00118
Lower estimate reaction capacity, R	1.50e-3	1.18e-3	mol SO_4 / g solid	Table 3-7
Lower estimate reaction capacity, R	1.69e-3	1.42e-3	mol SO_4 / g solid	Table 3-7
Upper estimate rate coefficient, $A \equiv \left[\frac{2Sn\tau D_m c}{(1-n)\rho_s R}\right]^{1/2}$	0.48	0.37	cm/√yr	Calculated
Lower estimate rate coefficient, $A \equiv \left[\frac{2Sn\tau D_m c}{(1-n)\rho_s R}\right]^{1/2}$	0.45	0.34	cm/√yr	Calculated
Exposure time, t	500	350	yr	Table 4-1
Upper estimate penetration depth, $x = At^{1/2}$	10.7	7.0	cm	Calculated
Lower estimate penetration depth, $x = At^{1/2}$	10.1	6.3	cm	Calculated

Table 4-4. Penetration depth comparisons.

Parameter	SDU 1/4	SDU 2/6	Units	Comments
Penetration time	500	350	yr	Table 4-1
Conservative Estimate (CE) penetration depth	23	9.4	cm	Table 4-1
Nominal Value (NV) penetration depth	18.5	7.4	cm	Table 4-1
Best Estimate (BE) penetration depth	7.7	3.8	cm	Table 4-1
Penetration depth based on Simco characterization	8.2	3.4	cm	Table 4-2
Penetration depth based on VU characterization, upper estimate	10.7	7.0	cm	Table 4-3
Penetration depth based on VU characterization, lower estimate	10.1	6.3	cm	Table 4-3

5.0 Discussion of Results

Sulfate attack simulations were originally performed using a two-layer (saltstone / concrete) STADIUM model and a single-layer (concrete) LeachXS/Orchestra (LXO) model (Flach and Smith 2013a, b, 2014). STADIUM simulations produced slower degradation rates in part because depletion of sulfate in saltstone over time lowered the exposure concentration for concrete at their interface. LXO simulations assumed a non-depleting sulfate concentration at the concrete exposure surface. The simulations also incorporated a damage mechanics model that increased tortuosity behind the reaction front. For conservatism, LXO predictions were used to define degradation rates for SDU components in SRNL-STI-2013-00118. Among the LXO penetration depths presented in Table 4-4, the most important are the nominal values (NV) because Special Analysis evaluation cases are based on the NV values whereas the conservative- and best-estimate values are used for sensitivity/alternative cases (SRR 2013, 2014). With this consideration, primary emphasis will be placed on verification of the NV values.

The LXO simulations underlying the penetration depths presented in Table 4-4 involve equilibrium chemistry calculations, diffusive transport of multiple species, and evolving porosity and tortuosity. The analytic solution given by Equation (2) and supporting calculations for reaction capacity are based on a number of simplifying assumptions, including:

- The chemical system is reduced to sulfate ions reacting completely and instantaneously with AFm (or total Al) and Ca as Portlandite
- Diffusion of ions other than sulfate are ignored, most importantly Ca^{2+} diffusion
- All material properties including the effective diffusion coefficient are constant

Because of model differences, exact agreement between LXO results and those using Equation (2) is not to be expected. It should also be noted that events and processes in the distant future are inherently uncertain, and precise predictions are not possible. Accordingly, Performance Assessments include an explicit assessment of uncertainties in the overall chain of dose calculation.

The penetration depths estimated from Simco Technologies Inc. characterization data are independent of LXO predictions, in both input data source and calculation method. Thus comparison to Simco estimates affords the opportunity for full verification of the LXO results. The Simco-based penetration depths in Table 4-4 are observed to lie near the BE values and well below the NV values for both disposal unit concrete types. The similarity with BE values is consistent with the LXO BE simulations using a large fractional porosity which minimizes modification of transport properties in response to damage. The close agreement between Equation (2) and the BE values validates the latter. Furthermore, the NV values are verified as being modestly more conservative than the best-estimate scenario.

The penetration depths estimated from Vanderbilt University characterization data share the same data source as the LXO simulations (the former being taken directly from LXO input files) while an independent calculation method was used. Comparisons to the VU based penetration data thus represent a verification of the numerical algorithms embodied in LXO but not inputs. The VU-based penetration depths lie between the BE and NV values (Table 4-4). A likely explanation is that the LXO simulations allow significant migration of Ca^{2+} ions from unreacted concrete, where the concentration is high, to the reaction front, where aqueous calcium is being depleted. This phenomenon effectively represents a migration of reaction capacity from the unreacted zone to the reaction front, which is not considered in Equation (2). Diffusion of dissolved calcium to the reaction front would slow advance of the latter and produce lower BE values. In any case, VU-based penetration depths are less than, and validate, the NV values.

The VU characterization data indicate effective diffusion coefficients (τD_m) of 1.0e-6 and 4.8e-7 cm^2/s for SDU 1/4 and SDU 2/6 concrete, respectively. These values are much higher than those from Simco characterization (Table 4-2), and concrete values recommended by Phifer et al. (2006, Table 6-47) and used in the 2009 Performance Assessment and subsequent Special Analyses. The Phifer et al. (2006) values for concrete range from 5.0e-8 to 1.0e-7 cm^2/s. The comparatively high diffusion coefficients are largely responsible for greater predicted penetration depths in Table 4-3 versus Table 4-2, and may represent a conservatism embedded in the LXO simulations of sulfate attack.

6.0 Conclusions

Sulfate penetration depths estimated herein, using an independent analysis method and characterization data source, are similar to the best-estimate (BE) values in SRNL-STI-2013-00118 and well below the nominal values (NV) subsequently used to define Saltstone Special Analysis base cases. The independent results validate the sulfate attack degradation inputs to recent Saltstone Special Analyses and, together with prior design checking of LXO simulations, satisfy the requirements of Procedure E7 2.31 *Engineering Calculations* for software use outside of E7 Section 5.5 *Use of Engineering Calculation Software*.

7.0 References

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Appendix

This appendix contains input data to the verification calculation extracted from the following electronic files archived on a project CD created 4/27/2015 from original files stored by Frank Smith on a personal hard-drive.

Concrete_Data.xls	7/29/2013	1:39PM	198KB
VCO_SO4_45cm_500yr.xlsx	1/18/2013	10:51AM	388KB
VCT_SO4_20cm_500yr.xlsx	1/22/2013	6:52AM	383KB

VCO simulation input (Concrete_Data.xls, "VCO")

Chemicals (mmol/L)	**Concrete**
OH	0.00
Na	0.00
K	0.00
SO4	0.00
Ca	0.00
AlO4H4	0.00
Cl	0.00
H2SiO4	0.00
CO3	0.00
NO3	0.00
NO2	0.00
Minerals (g/kg)	**Concrete**
Portlandite	0.00
CaH2SiO4	0.00
Ettringite	0.00
Monosulfate	0.00
AFmOH	0.00
Thaumasite	0.00
Calcite	0.00
Monocarboaluminate	0.00
Gypsum	0.00
Friedel_IX	0.00
Properties	**Concrete**
Temperature, C	23
Water/Binder Ratio	0.38
Binder, kg/m3	424
Aggregates, kg/m3	1787
Binder Density, kg/m3	2885
Porosity	0.115
Permeability, m2	1.80E-21
OH Diffusion Coefficient, m2/s	1.40E-11
Isotherm Parameter b	-25.928
Isotherm Parameter d	0.4285
Relative Permeability	18
Initial Hydration, days	28
Reference Time, days	28
Hydration Parameter a	0.8
Hydration Parameter a, 1/s	0.015
Thermal Conductivity, W/m/C	2
Specific Heat, J/kg/C	1000

Tortuosity	10.00
LeachXS/ORCHESTRA Parameters	
pH	11.5
pe	3.5
Density (kg/dm3)	2.40
	mg/kg
Al+3	5.37E+03
Ca+2	5.56E+04
H2CO3	1.52E+02
Fe+3	1.75E+03
Mg+2	4.40E+03
Na+	1.99E+02
H4SiO4	1.26E+04
SO4-2	2.32E+03
OH-	1.00E-12
K+	1.19E+03
Cl-	2.97E+00
NO3-	1.84E+01
NO2-	1.00E-12
H+	1.00E-12
Ag+	1.00E-12
H3AsO4	1.40E+00
H3BO3	7.31E+00
Ba+2	2.69E+01
Br-	1.00E-12
Cd+2	6.23E-02
CrO4-2	1.64E+01
Cu+2	7.19E+00
F-	3.12E+02
Hg+2	1.00E-12
I-	1.00E-12
Li+	2.05E+01
Mn+2	1.62E+02
MoO4-2	2.64E-01
NH4+	1.00E-12
Ni+2	2.86E+00
PO4-3	1.66E+02
Pb+2	1.25E+00
Sb[OH]6-	1.94E-01
SeO4-2	1.87E-01
Sr+2	8.32E+01
Th+4	1.00E-12
UO2+	1.61E+00
VO2+	6.53E+00
Zn+2	2.03E+01
Polynomial coefficients	
c0	-5.181E+00
c1	-2.902E-02
c2	-1.388E-02
c3	4.303E-03
c4	-4.352E-04
c5	1.513E-05
Other parameters	

L/S	10
Clay (kg/kg)	1.00E-03
HFO (kg/kg)	1.00E-03
SHA (kg/kg)	3.00E-04
DHA (kg/L)	0
Paste Volume	**Quantity**
Cement	255
Slag	169
Fly ash	0
Silica Fume	0
Water	161
Fine Aggregates	691
Coarse Aggregates	1096
Paste Volume	0.31
	2372

VCO simulation output – selected fields at 500 years – fractional porosity = 0.3

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
5.00E+02	0	1	1	0	0
5.00E+02	4.50E-03	15.482108	8.36E-02	0	0
5.00E+02	9.00E-03	21.8207307	5.90E-02	0	0
5.00E+02	1.35E-02	20.6640215	6.29E-02	0	0
5.00E+02	1.80E-02	20.4413412	6.37E-02	0	0
5.00E+02	2.25E-02	20.3101473	6.42E-02	0	0
5.00E+02	2.70E-02	20.2344419	6.44E-02	0	0
5.00E+02	3.15E-02	20.1964899	6.46E-02	0	0
5.00E+02	3.60E-02	20.1716339	6.47E-02	0	0
5.00E+02	4.05E-02	20.9558023	6.19E-02	0	0
5.00E+02	4.50E-02	42.3303941	1.15E-02	0	0
5.00E+02	4.95E-02	42.3303941	1.15E-02	0	0
5.00E+02	5.40E-02	41.2635315	1.33E-02	0	0
5.00E+02	5.85E-02	39.3441224	1.67E-02	8.85860055	0
5.00E+02	6.30E-02	40.0995217	1.54E-02	13.532704	0
5.00E+02	6.75E-02	39.5971141	1.63E-02	13.2953247	0
5.00E+02	7.20E-02	39.0623942	1.73E-02	13.0391573	0
5.00E+02	7.65E-02	38.5869385	1.81E-02	12.8084341	0
5.00E+02	8.10E-02	38.1681336	1.89E-02	12.6028128	0
5.00E+02	8.55E-02	37.7982698	1.96E-02	12.4193952	0
5.00E+02	9.00E-02	37.4733397	2.02E-02	12.2568388	0
5.00E+02	9.45E-02	37.1880663	2.08E-02	12.1129679	0
5.00E+02	9.90E-02	36.9313126	2.13E-02	11.9825992	0
5.00E+02	1.04E-01	36.7022307	2.17E-02	11.865471	0
5.00E+02	1.08E-01	36.4982269	2.21E-02	11.7607373	0
5.00E+02	1.13E-01	36.3097022	2.25E-02	11.6632414	0
5.00E+02	1.17E-01	36.1383215	2.28E-02	11.5743608	0
5.00E+02	1.22E-01	35.985721	2.31E-02	11.494837	0
5.00E+02	1.26E-01	35.851069	2.34E-02	11.4245478	0

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
5.00E+02	1.31E-01	35.7258853	2.37E-02	11.3587397	0
5.00E+02	1.35E-01	35.6095091	2.39E-02	1.13E+01	0
5.00E+02	1.40E-01	35.5077433	2.41E-02	11.2439299	0
5.00E+02	1.44E-01	35.4147038	2.43E-02	11.1947719	0
5.00E+02	1.49E-01	35.3268948	2.45E-02	11.1482287	0
5.00E+02	1.53E-01	35.2481195	2.46E-02	11.1064383	0
5.00E+02	1.58E-01	35.1771778	2.48E-02	11.0688578	0
5.00E+02	1.62E-01	35.1096015	2.49E-02	11.0328371	0
5.00E+02	1.67E-01	35.0477581	2.50E-02	10.999938	0
5.00E+02	1.71E-01	34.9928944	2.52E-02	10.9708395	0
5.00E+02	1.76E-01	34.9401138	2.53E-02	10.9426433	0
5.00E+02	1.80E-01	34.8917884	2.54E-02	10.9169306	0
5.00E+02	1.85E-01	34.8483652	2.55E-02	10.8939414	0
5.00E+02	1.89E-01	34.8059134	2.55E-02	10.8713152	0
5.00E+02	1.94E-01	34.7673218	2.56E-02	10.8508681	0
5.00E+02	1.98E-01	34.7324884	2.57E-02	10.8325582	0
5.00E+02	2.03E-01	34.6978026	2.58E-02	10.8142414	0
5.00E+02	2.07E-01	34.6665284	2.58E-02	10.7979353	0
5.00E+02	2.12E-01	34.6380271	2.59E-02	10.7832806	0
5.00E+02	2.16E-01	34.6087149	2.59E-02	10.7682685	0
5.00E+02	2.21E-01	34.5789716	2.60E-02	10.7529264	0
5.00E+02	2.25E-01	27.7158801	4.19E-02	12.7395438	0
5.00E+02	2.30E-01	12.7464765	9.76E-02	17.4171333	8.34E-01
5.00E+02	2.34E-01	10.0036206	1.15E-01	18.7286415	1.14476545
5.00E+02	2.39E-01	10.0018799	1.15E-01	18.7296703	1.14499241
5.00E+02	2.43E-01	10.0017988	1.15E-01	18.7297029	1.14500218
5.00E+02	2.48E-01	10.0017205	1.15E-01	18.7297341	1.14501159
5.00E+02	2.52E-01	10.0016442	1.15E-01	18.7297643	1.14502075
5.00E+02	2.57E-01	10.0015698	1.15E-01	18.7297936	1.14502967
5.00E+02	2.61E-01	10.0014974	1.15E-01	18.7298221	1.14503836
5.00E+02	2.66E-01	10.0014268	1.15E-01	18.7298497	1.14504681
5.00E+02	2.70E-01	10.001358	1.15E-01	18.7298764	1.14505504
5.00E+02	2.75E-01	10.0012911	1.15E-01	18.7299023	1.14506304
5.00E+02	2.79E-01	10.001226	1.15E-01	18.7299273	1.14507082
5.00E+02	2.84E-01	10.0011627	1.15E-01	18.7299516	1.14507838
5.00E+02	2.88E-01	10.0011011	1.15E-01	18.7299751	1.15E+00
5.00E+02	2.93E-01	10.0010413	1.15E-01	18.7299978	1.14509285
5.00E+02	2.97E-01	10.0009833	1.15E-01	18.7300197	1.14509977
5.00E+02	3.02E-01	10.0009269	1.15E-01	18.7300409	1.14510647
5.00E+02	3.06E-01	10.0008723	1.15E-01	18.7300613	1.14511297
5.00E+02	3.11E-01	10.0008194	1.15E-01	18.7300811	1.14511926
5.00E+02	3.15E-01	10.0007681	1.15E-01	18.7301	1.14512534
5.00E+02	3.20E-01	10.0007186	1.15E-01	18.7301183	1.14513122
5.00E+02	3.24E-01	10.0006707	1.15E-01	18.7301359	1.1451369
5.00E+02	3.29E-01	10.0006245	1.15E-01	18.7301528	1.14514237
5.00E+02	3.33E-01	10.00058	1.15E-01	18.7301691	1.14514764

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
5.00E+02	3.38E-01	10.0005371	1.15E-01	18.7301846	1.14515272
5.00E+02	3.42E-01	10.0004959	1.15E-01	18.7301995	1.14515759
5.00E+02	3.47E-01	10.0004563	1.15E-01	18.7302137	1.14516226
5.00E+02	3.51E-01	10.0004184	1.15E-01	18.7302273	1.14516674
5.00E+02	3.56E-01	10.0003821	1.15E-01	18.7302403	1.14517102
5.00E+02	3.60E-01	10.0003475	1.15E-01	18.7302526	1.14517511
5.00E+02	3.65E-01	10.0003145	1.15E-01	18.7302643	1.14517899
5.00E+02	3.69E-01	10.0002832	1.15E-01	18.7302753	1.14518268
5.00E+02	3.74E-01	10.0002535	1.15E-01	18.7302858	1.14518618
5.00E+02	3.78E-01	10.0002255	1.15E-01	18.7302956	1.14518948
5.00E+02	3.83E-01	10.0001991	1.15E-01	18.7303049	1.14519258
5.00E+02	3.87E-01	10.0001743	1.15E-01	18.7303135	1.14519549
5.00E+02	3.92E-01	10.0001512	1.15E-01	18.7303215	1.14519821
5.00E+02	3.96E-01	10.0001298	1.15E-01	18.730329	1.14520073
5.00E+02	4.01E-01	10.0001099	1.15E-01	18.7303358	1.14520306
5.00E+02	4.05E-01	10.0000918	1.15E-01	18.7303421	1.14520519
5.00E+02	4.10E-01	10.0000753	1.15E-01	18.7303478	1.14520713
5.00E+02	4.14E-01	10.0000604	1.15E-01	18.7303529	1.14520887
5.00E+02	4.19E-01	10.0000472	1.15E-01	18.7303575	1.14521042
5.00E+02	4.23E-01	10.0000356	1.15E-01	18.7303614	1.14521178
5.00E+02	4.28E-01	10.0000257	1.15E-01	18.7303648	1.14521294
5.00E+02	4.32E-01	10.0000174	1.15E-01	18.7303677	1.14521391
5.00E+02	4.37E-01	10.0000108	1.15E-01	18.7303699	1.14521469
5.00E+02	4.41E-01	10.0000059	1.15E-01	18.7303716	1.14521527
5.00E+02	4.46E-01	10.0000025	1.15E-01	18.7303727	1.14521566
5.00E+02	4.50E-01	10.0000009	1.15E-01	18.7303733	1.14521585

VCO simulation output – selected fields at 500 years – fractional porosity = 0.45

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
5.00E+02	0	1	1	0.00E+00	0
5.00E+02	4.50E-03	1.51E+01	8.54E-02	0.00E+00	0
5.00E+02	9.00E-03	2.18E+01	5.91E-02	0	0
5.00E+02	1.35E-02	2.07E+01	6.28E-02	0.00E+00	0
5.00E+02	1.80E-02	2.05E+01	6.34E-02	0.00E+00	0
5.00E+02	2.25E-02	2.04E+01	6.39E-02	0	0
5.00E+02	2.70E-02	2.03E+01	6.42E-02	0	0
5.00E+02	3.15E-02	2.03E+01	6.44E-02	0	0
5.00E+02	3.60E-02	2.02E+01	6.46E-02	0	0
5.00E+02	4.05E-02	4.16E+01	1.27E-02	0	0
5.00E+02	4.50E-02	4.23E+01	1.15E-02	0	0
5.00E+02	4.95E-02	4.23E+01	1.15E-02	0	0
5.00E+02	5.40E-02	3.94E+01	1.66E-02	0	0
5.00E+02	5.85E-02	3.85E+01	1.83E-02	7.83E-01	0
5.00E+02	6.30E-02	3.91E+01	1.72E-02	13.0568122	0

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
5.00E+02	6.75E-02	3.91E+01	1.71E-02	13.0764472	0
5.00E+02	7.20E-02	3.87E+01	1.80E-02	12.8502533	0
5.00E+02	7.65E-02	3.82E+01	1.88E-02	12.6415911	0
5.00E+02	8.10E-02	3.79E+01	1.95E-02	12.4559736	0
5.00E+02	8.55E-02	3.75E+01	2.01E-02	12.2934327	0
5.00E+02	9.00E-02	3.72E+01	2.07E-02	12.1450709	0
5.00E+02	9.45E-02	3.70E+01	2.12E-02	12.0137106	0
5.00E+02	9.90E-02	3.68E+01	2.16E-02	11.8967953	0
5.00E+02	1.04E-01	3.66E+01	2.20E-02	11.7893489	0
5.00E+02	1.08E-01	3.64E+01	2.24E-02	11.6961345	0
5.00E+02	1.13E-01	3.62E+01	2.27E-02	11.6086066	0
5.00E+02	1.17E-01	3.60E+01	2.30E-02	11.5279954	0
5.00E+02	1.22E-01	3.59E+01	2.33E-02	11.458701	0
5.00E+02	1.26E-01	3.58E+01	2.35E-02	11.3925728	0
5.00E+02	1.31E-01	3.57E+01	2.38E-02	11.3334146	0
5.00E+02	1.35E-01	3.56E+01	2.40E-02	11.2794903	0
5.00E+02	1.40E-01	3.55E+01	2.42E-02	11.2274535	0
5.00E+02	1.44E-01	3.54E+01	2.43E-02	11.183032	0
5.00E+02	1.49E-01	3.53E+01	2.45E-02	11.1404668	0
5.00E+02	1.53E-01	3.52E+01	2.47E-02	11.0990927	0
5.00E+02	1.58E-01	3.52E+01	2.48E-02	11.0649954	0
5.00E+02	1.62E-01	3.51E+01	2.49E-02	1.10E+01	0
5.00E+02	1.67E-01	3.50E+01	2.51E-02	1.10E+01	0
5.00E+02	1.71E-01	3.50E+01	2.52E-02	1.10E+01	0
5.00E+02	1.76E-01	3.49E+01	2.53E-02	1.09E+01	0
5.00E+02	1.80E-01	3.47E+01	2.59E-02	1.08E+01	0
5.00E+02	1.85E-01	1.53E+01	8.45E-02	1.64E+01	6.01E-01
5.00E+02	1.89E-01	1.00E+01	1.15E-01	1.87E+01	1.14451061
5.00E+02	1.94E-01	1.00E+01	1.15E-01	1.87E+01	1.14492652
5.00E+02	1.98E-01	1.00E+01	1.15E-01	1.87E+01	1.14493755
5.00E+02	2.03E-01	1.00E+01	1.15E-01	1.87E+01	1.14494804
5.00E+02	2.07E-01	1.00E+01	1.15E-01	1.87E+01	1.14495827
5.00E+02	2.12E-01	1.00E+01	1.15E-01	1.87E+01	1.14496824
5.00E+02	2.16E-01	1.00E+01	1.15E-01	1.87E+01	1.14497795
5.00E+02	2.21E-01	1.00E+01	1.15E-01	1.87E+01	1.14498742
5.00E+02	2.25E-01	1.00E+01	1.15E-01	1.87E+01	1.14499665
5.00E+02	2.30E-01	1.00E+01	1.15E-01	1.87E+01	1.14500565
5.00E+02	2.34E-01	1.00E+01	1.15E-01	1.87E+01	1.14501442
5.00E+02	2.39E-01	1.00E+01	1.15E-01	1.87E+01	1.14502297
5.00E+02	2.43E-01	1.00E+01	1.15E-01	1.87E+01	1.14503131
5.00E+02	2.48E-01	1.00E+01	1.15E-01	1.87E+01	1.14503943
5.00E+02	2.52E-01	1.00E+01	1.15E-01	1.87E+01	1.14504734
5.00E+02	2.57E-01	1.00E+01	1.15E-01	1.87E+01	1.14505504
5.00E+02	2.61E-01	1.00E+01	1.15E-01	1.87E+01	1.14506254
5.00E+02	2.66E-01	1.00E+01	1.15E-01	1.87E+01	1.14506985
5.00E+02	2.70E-01	1.00E+01	1.15E-01	1.87E+01	1.14507695

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
5.00E+02	2.75E-01	1.00E+01	1.15E-01	1.87E+01	1.14508387
5.00E+02	2.79E-01	1.00E+01	1.15E-01	1.87E+01	1.14509059
5.00E+02	2.84E-01	1.00E+01	1.15E-01	1.87E+01	1.14509712
5.00E+02	2.88E-01	1.00E+01	1.15E-01	1.87E+01	1.14510346
5.00E+02	2.93E-01	1.00E+01	1.15E-01	1.87E+01	1.14510962
5.00E+02	2.97E-01	1.00E+01	1.15E-01	1.87E+01	1.1451156
5.00E+02	3.02E-01	1.00E+01	1.15E-01	1.87E+01	1.14512139
5.00E+02	3.06E-01	1.00E+01	1.15E-01	1.87E+01	1.14512701
5.00E+02	3.11E-01	1.00E+01	1.15E-01	1.87E+01	1.14513244
5.00E+02	3.15E-01	1.00E+01	1.15E-01	1.87E+01	1.1451377
5.00E+02	3.20E-01	1.00E+01	1.15E-01	1.87E+01	1.14514278
5.00E+02	3.24E-01	1.00E+01	1.15E-01	1.87E+01	1.14514768
5.00E+02	3.29E-01	1.00E+01	1.15E-01	1.87E+01	1.14515241
5.00E+02	3.33E-01	1.00E+01	1.15E-01	1.87E+01	1.14515697
5.00E+02	3.38E-01	1.00E+01	1.15E-01	1.87E+01	1.14516135
5.00E+02	3.42E-01	1.00E+01	1.15E-01	1.87E+01	1.14516556
5.00E+02	3.47E-01	1.00E+01	1.15E-01	1.87E+01	1.1451696
5.00E+02	3.51E-01	1.00E+01	1.15E-01	1.87E+01	1.14517346
5.00E+02	3.56E-01	1.00E+01	1.15E-01	1.87E+01	1.14517716
5.00E+02	3.60E-01	1.00E+01	1.15E-01	1.87E+01	1.14518069
5.00E+02	3.65E-01	1.00E+01	1.15E-01	1.87E+01	1.14518404
5.00E+02	3.69E-01	1.00E+01	1.15E-01	1.87E+01	1.14518723
5.00E+02	3.74E-01	1.00E+01	1.15E-01	1.87E+01	1.14519025
5.00E+02	3.78E-01	1.00E+01	1.15E-01	1.87E+01	1.1451931
5.00E+02	3.83E-01	1.00E+01	1.15E-01	1.87E+01	1.14519578
5.00E+02	3.87E-01	1.00E+01	1.15E-01	1.87E+01	1.14519829
5.00E+02	3.92E-01	1.00E+01	1.15E-01	1.87E+01	1.14520063
5.00E+02	3.96E-01	1.00E+01	1.15E-01	1.87E+01	1.14520281
5.00E+02	4.01E-01	1.00E+01	1.15E-01	1.87E+01	1.14520482
5.00E+02	4.05E-01	1.00E+01	1.15E-01	1.87E+01	1.14520666
5.00E+02	4.10E-01	1.00E+01	1.15E-01	1.87E+01	1.14520833
5.00E+02	4.14E-01	1.00E+01	1.15E-01	1.87E+01	1.14520984
5.00E+02	4.19E-01	1.00E+01	1.15E-01	1.87E+01	1.14521118
5.00E+02	4.23E-01	1.00E+01	1.15E-01	1.87E+01	1.14521235
5.00E+02	4.28E-01	1.00E+01	1.15E-01	1.87E+01	1.14521335
5.00E+02	4.32E-01	1.00E+01	1.15E-01	1.87E+01	1.14521419
5.00E+02	4.37E-01	1.00E+01	1.15E-01	1.87E+01	1.14521485
5.00E+02	4.41E-01	1.00E+01	1.15E-01	1.87E+01	1.14521536
5.00E+02	4.46E-01	1.00E+01	1.15E-01	1.87E+01	1.14521569
5.00E+02	4.50E-01	1.00E+01	1.15E-01	1.87E+01	1.14521586

VCO simulation output – selected fields at 500 years – fractional porosity = 0.6

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
5.00E+02	0	1	1	0.00E+00	0
5.00E+02	4.50E-03	1.42E+01	8.99E-02	0.00E+00	0
5.00E+02	9.00E-03	2.14E+01	6.05E-02	0	0
5.00E+02	1.35E-02	2.12E+01	6.10E-02	0.00E+00	0
5.00E+02	1.80E-02	2.09E+01	6.22E-02	0.00E+00	0
5.00E+02	2.25E-02	2.18E+01	5.92E-02	0	0
5.00E+02	2.70E-02	4.23E+01	1.15E-02	0	0
5.00E+02	3.15E-02	4.23E+01	1.15E-02	0	0
5.00E+02	3.60E-02	4.23E+01	1.15E-02	0	0
5.00E+02	4.05E-02	4.23E+01	1.15E-02	0	0
5.00E+02	4.50E-02	4.23E+01	1.15E-02	0	0
5.00E+02	4.95E-02	4.23E+01	1.15E-02	0	0
5.00E+02	5.40E-02	4.23E+01	1.15E-02	0	0
5.00E+02	5.85E-02	4.23E+01	1.15E-02	0.00E+00	0
5.00E+02	6.30E-02	3.89E+01	1.75E-02	8.77759029	0
5.00E+02	6.75E-02	2.46E+01	5.04E-02	14.0273079	0
5.00E+02	7.20E-02	1.04E+01	1.12E-01	18.4968879	1.0901004
5.00E+02	7.65E-02	1.00E+01	1.15E-01	18.7286523	1.1446967
5.00E+02	8.10E-02	1.00E+01	1.15E-01	18.7288312	1.14474017
5.00E+02	8.55E-02	1.00E+01	1.15E-01	18.7288919	1.14475773
5.00E+02	9.00E-02	1.00E+01	1.15E-01	18.7289489	1.14477431
5.00E+02	9.45E-02	1.00E+01	1.15E-01	18.729003	1.14479005
5.00E+02	9.90E-02	1.00E+01	1.15E-01	18.7290544	1.14480503
5.00E+02	1.04E-01	1.00E+01	1.15E-01	18.7291034	1.14481935
5.00E+02	1.08E-01	1.00E+01	1.15E-01	18.7291502	1.14483305
5.00E+02	1.13E-01	1.00E+01	1.15E-01	18.7291949	1.14484619
5.00E+02	1.17E-01	1.00E+01	1.15E-01	18.7292379	1.14485881
5.00E+02	1.22E-01	1.00E+01	1.15E-01	18.7292791	1.14487096
5.00E+02	1.26E-01	1.00E+01	1.15E-01	18.7293188	1.14488268
5.00E+02	1.31E-01	1.00E+01	1.15E-01	18.729357	1.14489398
5.00E+02	1.35E-01	1.00E+01	1.15E-01	18.7293938	1.14490491
5.00E+02	1.40E-01	1.00E+01	1.15E-01	18.7294294	1.14491548
5.00E+02	1.44E-01	1.00E+01	1.15E-01	18.7294637	1.14492571
5.00E+02	1.49E-01	1.00E+01	1.15E-01	18.7294969	1.14493563
5.00E+02	1.53E-01	1.00E+01	1.15E-01	18.729529	1.14494526
5.00E+02	1.58E-01	1.00E+01	1.15E-01	18.7295601	1.1449546
5.00E+02	1.62E-01	1.00E+01	1.15E-01	1.87E+01	1.14496367
5.00E+02	1.67E-01	1.00E+01	1.15E-01	1.87E+01	1.14497248
5.00E+02	1.71E-01	1.00E+01	1.15E-01	1.87E+01	1.14498106
5.00E+02	1.76E-01	1.00E+01	1.15E-01	1.87E+01	1.1449894
5.00E+02	1.80E-01	1.00E+01	1.15E-01	1.87E+01	1.14499751
5.00E+02	1.85E-01	1.00E+01	1.15E-01	1.87E+01	1.15E+00
5.00E+02	1.89E-01	1.00E+01	1.15E-01	1.87E+01	1.1450131

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
5.00E+02	1.94E-01	1.00E+01	1.15E-01	1.87E+01	1.1450206
5.00E+02	1.98E-01	1.00E+01	1.15E-01	1.87E+01	1.1450279
5.00E+02	2.03E-01	1.00E+01	1.15E-01	1.87E+01	1.14503501
5.00E+02	2.07E-01	1.00E+01	1.15E-01	1.87E+01	1.14504194
5.00E+02	2.12E-01	1.00E+01	1.15E-01	1.87E+01	1.1450487
5.00E+02	2.16E-01	1.00E+01	1.15E-01	1.87E+01	1.14505528
5.00E+02	2.21E-01	1.00E+01	1.15E-01	1.87E+01	1.1450617
5.00E+02	2.25E-01	1.00E+01	1.15E-01	1.87E+01	1.14506796
5.00E+02	2.30E-01	1.00E+01	1.15E-01	1.87E+01	1.14507405
5.00E+02	2.34E-01	1.00E+01	1.15E-01	1.87E+01	1.14508
5.00E+02	2.39E-01	1.00E+01	1.15E-01	1.87E+01	1.14508579
5.00E+02	2.43E-01	1.00E+01	1.15E-01	1.87E+01	1.14509143
5.00E+02	2.48E-01	1.00E+01	1.15E-01	1.87E+01	1.14509693
5.00E+02	2.52E-01	1.00E+01	1.15E-01	1.87E+01	1.14510228
5.00E+02	2.57E-01	1.00E+01	1.15E-01	1.87E+01	1.14510749
5.00E+02	2.61E-01	1.00E+01	1.15E-01	1.87E+01	1.14511257
5.00E+02	2.66E-01	1.00E+01	1.15E-01	1.87E+01	1.14511751
5.00E+02	2.70E-01	1.00E+01	1.15E-01	1.87E+01	1.14512231
5.00E+02	2.75E-01	1.00E+01	1.15E-01	1.87E+01	1.14512698
5.00E+02	2.79E-01	1.00E+01	1.15E-01	1.87E+01	1.14513153
5.00E+02	2.84E-01	1.00E+01	1.15E-01	1.87E+01	1.14513594
5.00E+02	2.88E-01	1.00E+01	1.15E-01	1.87E+01	1.14514022
5.00E+02	2.93E-01	1.00E+01	1.15E-01	1.87E+01	1.14514438
5.00E+02	2.97E-01	1.00E+01	1.15E-01	1.87E+01	1.14514841
5.00E+02	3.02E-01	1.00E+01	1.15E-01	1.87E+01	1.14515232
5.00E+02	3.06E-01	1.00E+01	1.15E-01	1.87E+01	1.14515611
5.00E+02	3.11E-01	1.00E+01	1.15E-01	1.87E+01	1.14515977
5.00E+02	3.15E-01	1.00E+01	1.15E-01	1.87E+01	1.14516332
5.00E+02	3.20E-01	1.00E+01	1.15E-01	1.87E+01	1.14516674
5.00E+02	3.24E-01	1.00E+01	1.15E-01	1.87E+01	1.14517005
5.00E+02	3.29E-01	1.00E+01	1.15E-01	1.87E+01	1.14517323
5.00E+02	3.33E-01	1.00E+01	1.15E-01	1.87E+01	1.1451763
5.00E+02	3.38E-01	1.00E+01	1.15E-01	1.87E+01	1.14517925
5.00E+02	3.42E-01	1.00E+01	1.15E-01	1.87E+01	1.14518208
5.00E+02	3.47E-01	1.00E+01	1.15E-01	1.87E+01	1.1451848
5.00E+02	3.51E-01	1.00E+01	1.15E-01	1.87E+01	1.1451874
5.00E+02	3.56E-01	1.00E+01	1.15E-01	1.87E+01	1.14518989
5.00E+02	3.60E-01	1.00E+01	1.15E-01	1.87E+01	1.14519226
5.00E+02	3.65E-01	1.00E+01	1.15E-01	1.87E+01	1.14519452
5.00E+02	3.69E-01	1.00E+01	1.15E-01	1.87E+01	1.14519666
5.00E+02	3.74E-01	1.00E+01	1.15E-01	1.87E+01	1.14519868
5.00E+02	3.78E-01	1.00E+01	1.15E-01	1.87E+01	1.1452006
5.00E+02	3.83E-01	1.00E+01	1.15E-01	1.87E+01	1.1452024
5.00E+02	3.87E-01	1.00E+01	1.15E-01	1.87E+01	1.14520409
5.00E+02	3.92E-01	1.00E+01	1.15E-01	1.87E+01	1.14520566
5.00E+02	3.96E-01	1.00E+01	1.15E-01	1.87E+01	1.14520712

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
5.00E+02	4.01E-01	1.00E+01	1.15E-01	1.87E+01	1.14520847
5.00E+02	4.05E-01	1.00E+01	1.15E-01	1.87E+01	1.1452097
5.00E+02	4.10E-01	1.00E+01	1.15E-01	1.87E+01	1.14521083
5.00E+02	4.14E-01	1.00E+01	1.15E-01	1.87E+01	1.14521184
5.00E+02	4.19E-01	1.00E+01	1.15E-01	1.87E+01	1.14521273
5.00E+02	4.23E-01	1.00E+01	1.15E-01	1.87E+01	1.14521352
5.00E+02	4.28E-01	1.00E+01	1.15E-01	1.87E+01	1.14521419
5.00E+02	4.32E-01	1.00E+01	1.15E-01	1.87E+01	1.14521475
5.00E+02	4.37E-01	1.00E+01	1.15E-01	1.87E+01	1.1452152
5.00E+02	4.41E-01	1.00E+01	1.15E-01	1.87E+01	1.14521554
5.00E+02	4.46E-01	1.00E+01	1.15E-01	1.87E+01	1.14521576
5.00E+02	4.50E-01	1.00E+01	1.15E-01	1.87E+01	1.14521587

VCO simulation input (Concrete_Data.xls, "VCO")

Chemicals (mmol/L)	**Concrete**
OH	0.00
Na	0.00
K	0.00
SO4	0.00
Ca	0.00
AlO4H4	0.00
Cl	0.00
H2SiO4	0.00
CO3	0.00
NO3	0.00
NO2	0.00
Minerals (g/kg)	**Concrete**
Portlandite	0.00
CaH2SiO4	0.00
Ettringite	0.00
Monosulfate	0.00
AFmOH	0.00
Thaumasite	0.00
Calcite	0.00
Monocarboaluminate	0.00
Gypsum	0.00
Friedel_IX	0.00
Properties	**Concrete**
Temperature, C	23
Water/Binder Ratio	0.38
Binder, kg/m3	405
Aggregates, kg/m3	1659
Binder Density, kg/m3	2885
Porosity	0.11
Permeability, m2	1.80E-21
OH Diffusion Coefficient, m2/s	1.40E-11
Isotherm Parameter b	-25.928
Isotherm Parameter d	0.4285
Relative Permeability	18
Initial Hydration, days	28
Reference Time, days	28
Hydration Parameter a	0.8
Hydration Parameter a, 1/s	0.015
Thermal Conductivity, W/m/C	2
Specific Heat, J/kg/C	1000
Tortuosity	20.74
LeachXS/ORCHESTRA Parameters	
pH	13.0
pe	7.0
Density (kg/dm3)	2.31
	mg/kg
Al+3	6.11E+03
Ca+2	4.32E+04
H2CO3	2.34E+02

Fe+3	1.84E+03
Mg+2	6.36E+03
Na+	1.45E+02
H4SiO4	1.60E+04
SO4-2	1.76E+03
OH-	1.00E-12
K+	1.14E+03
Cl-	2.31E+00
NO3-	1.66E+01
NO2-	1.00E-12
H+	1.00E-12
Ag+	1.00E-12
H3AsO4	4.40E+00
H3BO3	1.15E+01
Ba+2	3.64E+01
Br-	1.00E-12
Cd+2	4.80E-02
CrO4-2	8.03E+00
Cu+2	6.28E+00
F-	2.39E+02
Hg+2	1.00E-12
I-	1.00E-12
Li+	8.89E+00
Mn+2	2.26E+02
MoO4-2	5.51E-01
NH4+	1.00E-12
Ni+2	1.79E+00
PO4-3	1.06E+02
Pb+2	1.64E+00
SbOH6+	1.44E-01
SeO4-2	8.50E-02
Sr+2	7.54E+01
Th+4	1.00E+00
UO2+	1.36E+00
VO2+	9.67E+00
Zn+2	1.89E+01
Polynomial coefficients	
c0	-5.296E+00
c1	-7.837E-01
c2	3.169E-01
c3	-5.518E-02
c4	4.195E-03
c5	-1.124E-04
Other parameters	
L/S	10.0000
Clay (kg/kg)	1.000E-03
HFO (kg/kg)	1.000E-03
SHA (kg/kg)	3.000E-04
DHA (kg/L)	0.000E+00
Paste Volume	**Quantity**
Cement	121
Slag	162
Fly ash	95

Silica Fume	27
Water	154
Fine Aggregates	548
Coarse Aggregates	1111
Paste Volume	0.32
	2218

VCT simulation output – selected fields at 350 years – fractional porosity = 0.3

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
3.50E+02	2.00E-03	20.9593926	1.09E-01	0	0
3.50E+02	4.00E-03	25.6854023	9.39E-02	0	0
3.50E+02	6.00E-03	36.5172338	6.74E-02	0	0
3.50E+02	8.00E-03	39.6425934	6.12E-02	0	0
3.50E+02	1.00E-02	71.5019064	1.68E-02	0	0
3.50E+02	1.20E-02	70.7531489	1.76E-02	0	0
3.50E+02	1.40E-02	70.3498364	1.80E-02	0	0
3.50E+02	1.60E-02	69.9957761	1.84E-02	0	0
3.50E+02	1.80E-02	69.7682565	1.86E-02	0	0
3.50E+02	2.00E-02	69.6117658	1.88E-02	0	0
3.50E+02	2.20E-02	69.5001256	1.89E-02	0	0
3.50E+02	2.40E-02	69.4278972	1.90E-02	0	0
3.50E+02	2.60E-02	69.3649079	1.91E-02	0	0
3.50E+02	2.80E-02	69.3130925	1.91E-02	0	0
3.50E+02	3.00E-02	69.2683821	1.92E-02	0	0
3.50E+02	3.20E-02	69.2398778	1.92E-02	0	0
3.50E+02	3.40E-02	69.2443331	1.92E-02	0	0
3.50E+02	3.60E-02	68.9789697	1.95E-02	0	0
3.50E+02	3.80E-02	67.686452	2.09E-02	0	0
3.50E+02	4.00E-02	67.6779908	2.09E-02	0	0
3.50E+02	4.20E-02	67.6757538	2.09E-02	0	0
3.50E+02	4.40E-02	67.6713034	2.09E-02	0	0
3.50E+02	4.60E-02	67.6625987	2.09E-02	0	0
3.50E+02	4.80E-02	76.6465462	1.15E-02	2.6082238	0
3.50E+02	5.00E-02	77.2041344	1.10E-02	4.22885491	0
3.50E+02	5.20E-02	77.2041344	1.10E-02	4.04746837	0
3.50E+02	5.40E-02	77.2041344	1.10E-02	3.87300006	0
3.50E+02	5.60E-02	77.2041344	1.10E-02	3.71577821	0
3.50E+02	5.80E-02	77.2041344	1.10E-02	3.57498973	0
3.50E+02	6.00E-02	77.2041344	1.10E-02	3.44982799	0
3.50E+02	6.20E-02	77.2041344	1.10E-02	3.3349823	0
3.50E+02	6.40E-02	77.2041344	1.10E-02	3.23206963	0
3.50E+02	6.60E-02	77.2041344	1.10E-02	3.14135109	0
3.50E+02	6.80E-02	77.2041344	1.10E-02	3.05928518	0
3.50E+02	7.00E-02	77.2041344	1.10E-02	2.98562502	0
3.50E+02	7.20E-02	77.2041344	1.10E-02	2.91939345	0
3.50E+02	7.40E-02	77.2041344	1.10E-02	2.85936117	0

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
3.50E+02	7.60E-02	77.2041344	1.10E-02	2.80479498	0
3.50E+02	7.80E-02	77.1020318	1.11E-02	2.75684395	0
3.50E+02	8.00E-02	76.9373372	1.13E-02	2.71322061	0
3.50E+02	8.20E-02	76.7912098	1.14E-02	2.67460756	0
3.50E+02	8.40E-02	76.6579553	1.15E-02	2.63948265	0
3.50E+02	8.60E-02	76.5322444	1.17E-02	2.60651361	0
3.50E+02	8.80E-02	76.4175271	1.18E-02	2.57671597	0
3.50E+02	9.00E-02	76.3154137	1.19E-02	2.55077247	0
3.50E+02	9.20E-02	75.9929987	1.22E-02	2.46666786	0
3.50E+02	9.40E-02	29.9852639	8.22E-02	10.2122601	5.69E-01
3.50E+02	9.60E-02	20.7556672	1.10E-01	12.3911852	1.08651378
3.50E+02	9.80E-02	20.7467836	1.10E-01	12.3939586	1.08712637
3.50E+02	1.00E-01	20.7463653	1.10E-01	12.3940427	1.08715276
3.50E+02	1.02E-01	20.7459646	1.10E-01	12.3941215	1.08717795
3.50E+02	1.04E-01	20.7455737	1.10E-01	12.3941976	1.08720248
3.50E+02	1.06E-01	20.7451923	1.10E-01	12.394271	1.08722636
3.50E+02	1.08E-01	20.7448202	1.10E-01	12.3943418	1.08724963
3.50E+02	1.10E-01	20.7444572	1.10E-01	12.39441	1.08727227
3.50E+02	1.12E-01	20.7441032	1.10E-01	12.3944758	1.08729432
3.50E+02	1.14E-01	20.743758	1.10E-01	12.3945391	1.08731578
3.50E+02	1.16E-01	20.7434214	1.10E-01	12.3946001	1.08733666
3.50E+02	1.18E-01	20.7430933	1.10E-01	12.3946587	1.08735698
3.50E+02	1.20E-01	20.7427737	1.10E-01	12.3947151	1.08737673
3.50E+02	1.22E-01	20.7424623	1.10E-01	12.3947694	1.08739593
3.50E+02	1.24E-01	20.7421592	1.10E-01	12.3948214	1.08741459
3.50E+02	1.26E-01	20.7418642	1.10E-01	12.3948714	1.08743271
3.50E+02	1.28E-01	20.7415772	1.10E-01	12.3949193	1.0874503
3.50E+02	1.30E-01	20.7412982	1.10E-01	12.3949652	1.08746737
3.50E+02	1.32E-01	20.7410271	1.10E-01	12.3950092	1.08748392
3.50E+02	1.34E-01	20.7407639	1.10E-01	12.3950513	1.08749995
3.50E+02	1.36E-01	20.7405085	1.10E-01	12.3950915	1.08751548
3.50E+02	1.38E-01	20.7402609	1.10E-01	12.39513	1.0875305
3.50E+02	1.40E-01	20.7400211	1.10E-01	12.3951666	1.08754503
3.50E+02	1.42E-01	20.7397889	1.10E-01	12.3952016	1.08755906
3.50E+02	1.44E-01	20.7395645	1.10E-01	12.3952349	1.0875726
3.50E+02	1.46E-01	20.7393477	1.10E-01	12.3952665	1.08758565
3.50E+02	1.48E-01	20.7391386	1.10E-01	12.3952966	1.08759821
3.50E+02	1.50E-01	20.7389372	1.10E-01	12.3953251	1.08761029
3.50E+02	1.52E-01	20.7387434	1.10E-01	12.3953522	1.08762189
3.50E+02	1.54E-01	20.7385572	1.10E-01	12.3953778	1.08763301
3.50E+02	1.56E-01	20.7383787	1.10E-01	12.3954019	1.08764366
3.50E+02	1.58E-01	20.7382078	1.10E-01	12.3954247	1.08765384
3.50E+02	1.60E-01	20.7380446	1.10E-01	12.3954462	1.08766354
3.50E+02	1.62E-01	20.7378891	1.10E-01	12.3954664	1.08767277
3.50E+02	1.64E-01	20.7377412	1.10E-01	12.3954853	1.08768153
3.50E+02	1.66E-01	20.737601	1.10E-01	12.395503	1.08768983

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
3.50E+02	1.68E-01	20.7374684	1.10E-01	12.3955195	1.08769765
3.50E+02	1.70E-01	20.7373436	1.10E-01	12.3955348	1.08770502
3.50E+02	1.72E-01	20.7372265	1.10E-01	12.395549	1.08771192
3.50E+02	1.74E-01	20.7371171	1.10E-01	12.3955622	1.08771835
3.50E+02	1.76E-01	20.7370155	1.10E-01	12.3955742	1.08772432
3.50E+02	1.78E-01	20.7369216	1.10E-01	12.3955852	1.08772984
3.50E+02	1.80E-01	20.7368355	1.10E-01	12.3955953	1.08773488
3.50E+02	1.82E-01	20.7367571	1.10E-01	12.3956043	1.08773947
3.50E+02	1.84E-01	20.7366866	1.10E-01	12.3956123	1.0877436
3.50E+02	1.86E-01	20.7366239	1.10E-01	12.3956195	1.08774727
3.50E+02	1.88E-01	20.7365689	1.10E-01	12.3956256	1.08775048
3.50E+02	1.90E-01	20.7365219	1.10E-01	12.3956309	1.08775323
3.50E+02	1.92E-01	20.7364826	1.10E-01	12.3956353	1.08775552
3.50E+02	1.94E-01	20.7364512	1.10E-01	12.3956388	1.08775736
3.50E+02	1.96E-01	20.7364276	1.10E-01	12.3956414	1.08775873
3.50E+02	1.98E-01	20.7364119	1.10E-01	12.3956431	1.08775965
3.50E+02	2.00E-01	20.736404	1.10E-01	12.395644	1.08776011

VCT simulation output – selected fields at 350 years – fractional porosity = 0.45

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
3.50E+02	0	1	1	0	0
3.50E+02	2.00E-03	20.8665726	1.10E-01	0	0
3.50E+02	4.00E-03	26.4238748	9.17E-02	0	0
3.50E+02	6.00E-03	36.2770007	6.79E-02	0	0
3.50E+02	8.00E-03	44.4176716	5.26E-02	0	0
3.50E+02	1.00E-02	71.3771394	1.69E-02	0	0
3.50E+02	1.20E-02	70.6552923	1.77E-02	0	0
3.50E+02	1.40E-02	70.2003449	1.82E-02	0	0
3.50E+02	1.60E-02	69.896391	1.85E-02	0	0
3.50E+02	1.80E-02	69.6739052	1.87E-02	0	0
3.50E+02	2.00E-02	69.5259229	1.89E-02	0	0
3.50E+02	2.20E-02	69.4309052	1.90E-02	0	0
3.50E+02	2.40E-02	69.3582292	1.91E-02	0	0
3.50E+02	2.60E-02	69.3064758	1.91E-02	0	0
3.50E+02	2.80E-02	69.2622456	1.92E-02	0	0
3.50E+02	3.00E-02	69.2276228	1.92E-02	0	0
3.50E+02	3.20E-02	69.2057537	1.92E-02	0	0
3.50E+02	3.40E-02	69.1891273	1.93E-02	0	0
3.50E+02	3.60E-02	69.1833826	1.93E-02	0	0
3.50E+02	3.80E-02	69.1749471	1.93E-02	0	0
3.50E+02	4.00E-02	67.6919259	2.09E-02	0	0
3.50E+02	4.20E-02	67.6387386	2.10E-02	0	0
3.50E+02	4.40E-02	67.6339793	2.10E-02	0	0
3.50E+02	4.60E-02	67.6284119	2.10E-02	0	0

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
3.50E+02	4.80E-02	67.6232318	2.10E-02	0	0
3.50E+02	5.00E-02	76.0635248	1.21E-02	2.45484696	0
3.50E+02	5.20E-02	77.2041344	1.10E-02	4.10511368	0
3.50E+02	5.40E-02	77.2041344	1.10E-02	3.88516397	0
3.50E+02	5.60E-02	77.2041344	1.10E-02	3.68736271	0
3.50E+02	5.80E-02	77.2041344	1.10E-02	3.52786718	0
3.50E+02	6.00E-02	77.2041344	1.10E-02	3.39460907	0
3.50E+02	6.20E-02	77.2041344	1.10E-02	3.28679746	0
3.50E+02	6.40E-02	77.2041344	1.10E-02	3.19389846	0
3.50E+02	6.60E-02	77.2041344	1.10E-02	3.11202694	0
3.50E+02	6.80E-02	77.2041344	1.10E-02	3.04455836	0
3.50E+02	7.00E-02	76.7825629	1.14E-02	2.67579343	0
3.50E+02	7.20E-02	32.3307193	7.66E-02	9.79177496	4.64E-01
3.50E+02	7.40E-02	20.7579851	1.10E-01	12.3907831	1.09E+00
3.50E+02	7.60E-02	20.7494376	1.10E-01	12.3934506	1.09E+00
3.50E+02	7.80E-02	20.7489777	1.10E-01	12.3935471	1.09E+00
3.50E+02	8.00E-02	20.7485364	1.10E-01	12.3936384	1.09E+00
3.50E+02	8.20E-02	20.7481066	1.10E-01	12.3937264	1.09E+00
3.50E+02	8.40E-02	20.7476879	1.10E-01	12.3938115	1.09E+00
3.50E+02	8.60E-02	20.7472798	1.10E-01	12.3938936	1.09E+00
3.50E+02	8.80E-02	20.7468819	1.10E-01	12.393973	1.09E+00
3.50E+02	9.00E-02	20.7464939	1.10E-01	12.3940496	1.09E+00
3.50E+02	9.20E-02	20.7461154	1.10E-01	12.3941237	1.09E+00
3.50E+02	9.40E-02	20.7457463	1.10E-01	12.3941952	1.09E+00
3.50E+02	9.60E-02	20.7453861	1.10E-01	12.3942642	1.09E+00
3.50E+02	9.80E-02	20.7450347	1.10E-01	12.3943308	1.09E+00
3.50E+02	1.00E-01	20.7446918	1.10E-01	12.3943951	1.09E+00
3.50E+02	1.02E-01	20.7443573	1.10E-01	12.3944572	1.09E+00
3.50E+02	1.04E-01	20.7440309	1.10E-01	12.394517	1.09E+00
3.50E+02	1.06E-01	20.7437124	1.10E-01	12.3945747	1.09E+00
3.50E+02	1.08E-01	20.7434018	1.10E-01	12.3946303	1.09E+00
3.50E+02	1.10E-01	20.7430988	1.10E-01	12.3946838	1.09E+00
3.50E+02	1.12E-01	20.7428033	1.10E-01	12.3947354	1.09E+00
3.50E+02	1.14E-01	20.7425153	1.10E-01	12.394785	1.09E+00
3.50E+02	1.16E-01	20.7422345	1.10E-01	12.3948328	1.09E+00
3.50E+02	1.18E-01	20.7419608	1.10E-01	12.3948787	1.09E+00
3.50E+02	1.20E-01	20.7416943	1.10E-01	12.3949228	1.09E+00
3.50E+02	1.22E-01	20.7414347	1.10E-01	12.3949652	1.09E+00
3.50E+02	1.24E-01	20.7411821	1.10E-01	12.3950058	1.09E+00
3.50E+02	1.26E-01	20.7409362	1.10E-01	12.3950448	1.09E+00
3.50E+02	1.28E-01	20.7406972	1.10E-01	12.3950822	1.09E+00
3.50E+02	1.30E-01	20.7404649	1.10E-01	12.395118	1.09E+00
3.50E+02	1.32E-01	20.7402392	1.10E-01	12.3951522	1.09E+00
3.50E+02	1.34E-01	20.7400201	1.10E-01	12.395185	1.09E+00
3.50E+02	1.36E-01	20.7398076	1.10E-01	12.3952163	1.09E+00
3.50E+02	1.38E-01	20.7396017	1.10E-01	12.3952461	1.09E+00

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
3.50E+02	1.40E-01	20.7394022	1.10E-01	12.3952746	1.09E+00
3.50E+02	1.42E-01	20.7392092	1.10E-01	12.3953017	1.09E+00
3.50E+02	1.44E-01	20.7390227	1.10E-01	12.3953276	1.09E+00
3.50E+02	1.46E-01	20.7388426	1.10E-01	12.3953521	1.09E+00
3.50E+02	1.48E-01	20.7386689	1.10E-01	12.3953754	1.09E+00
3.50E+02	1.50E-01	20.7385017	1.10E-01	12.3953975	1.09E+00
3.50E+02	1.52E-01	20.7383408	1.10E-01	12.3954184	1.09E+00
3.50E+02	1.54E-01	20.7381864	1.10E-01	12.3954382	1.09E+00
3.50E+02	1.56E-01	20.7380383	1.10E-01	12.3954569	1.09E+00
3.50E+02	1.58E-01	20.7378966	1.10E-01	12.3954746	1.09E+00
3.50E+02	1.60E-01	20.7377613	1.10E-01	12.3954912	1.09E+00
3.50E+02	1.62E-01	20.7376323	1.10E-01	12.3955067	1.09E+00
3.50E+02	1.64E-01	20.7375098	1.10E-01	12.3955213	1.09E+00
3.50E+02	1.66E-01	20.7373937	1.10E-01	12.395535	1.09E+00
3.50E+02	1.68E-01	20.7372839	1.10E-01	12.3955477	1.09E+00
3.50E+02	1.70E-01	20.7371806	1.10E-01	12.3955596	1.09E+00
3.50E+02	1.72E-01	20.7370836	1.10E-01	12.3955705	1.09E+00
3.50E+02	1.74E-01	20.7369931	1.10E-01	12.3955806	1.09E+00
3.50E+02	1.76E-01	20.736909	1.10E-01	12.3955899	1.09E+00
3.50E+02	1.78E-01	20.7368314	1.10E-01	12.3955984	1.09E+00
3.50E+02	1.80E-01	20.7367602	1.10E-01	12.3956062	1.09E+00
3.50E+02	1.82E-01	20.7366954	1.10E-01	12.3956131	1.09E+00
3.50E+02	1.84E-01	20.7366371	1.10E-01	12.3956193	1.09E+00
3.50E+02	1.86E-01	20.7365852	1.10E-01	12.3956248	1.09E+00
3.50E+02	1.88E-01	20.7365398	1.10E-01	12.3956296	1.09E+00
3.50E+02	1.90E-01	20.7365009	1.10E-01	12.3956336	1.09E+00
3.50E+02	1.92E-01	20.7364685	1.10E-01	12.395637	1.09E+00
3.50E+02	1.94E-01	20.7364425	1.10E-01	12.3956397	1.09E+00
3.50E+02	1.96E-01	20.736423	1.10E-01	12.3956417	1.09E+00
3.50E+02	1.98E-01	20.73641	1.10E-01	12.395643	1.09E+00
3.50E+02	2.00E-01	20.7364035	1.10E-01	12.3956437	1.09E+00

VCT simulation output – selected fields at 350 years – fractional porosity = 0.6

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
3.50E+02	0	1	1	0	0
3.50E+02	2.00E-03	19.5741955	1.14E-01	0	0
3.50E+02	4.00E-03	24.7501406	9.67E-02	0	0
3.50E+02	6.00E-03	30.2795547	8.15E-02	0	0
3.50E+02	8.00E-03	35.2037006	7.01E-02	0	0
3.50E+02	1.00E-02	34.1741671	7.24E-02	0	0
3.50E+02	1.20E-02	33.802297	7.32E-02	0	0
3.50E+02	1.40E-02	33.6318907	7.36E-02	0	0
3.50E+02	1.60E-02	33.3675718	7.42E-02	0	0
3.50E+02	1.80E-02	64.1317713	2.50E-02	0	0

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
3.50E+02	2.00E-02	70.2104861	1.82E-02	0	0
3.50E+02	2.20E-02	69.8448202	1.85E-02	0	0
3.50E+02	2.40E-02	69.6519064	1.88E-02	0	0
3.50E+02	2.60E-02	69.4980612	1.89E-02	0	0
3.50E+02	2.80E-02	77.2041344	1.10E-02	0	0
3.50E+02	3.00E-02	77.2041344	1.10E-02	0	0
3.50E+02	3.20E-02	77.2041344	1.10E-02	0	0
3.50E+02	3.40E-02	77.2041344	1.10E-02	0	0
3.50E+02	3.60E-02	43.0457371	5.50E-02	8.20963457	6.79E-02
3.50E+02	3.80E-02	20.7862196	1.10E-01	12.3824387	1.08445044
3.50E+02	4.00E-02	20.7546455	1.10E-01	12.392433	1.08663344
3.50E+02	4.20E-02	20.7539329	1.10E-01	12.3925923	1.08667922
3.50E+02	4.40E-02	20.753319	1.10E-01	12.3927228	1.08671831
3.50E+02	4.60E-02	20.7527334	1.10E-01	12.3928467	1.08675556
3.50E+02	4.80E-02	20.7521733	1.10E-01	12.3929645	1.08679117
3.50E+02	5.00E-02	20.7516363	1.10E-01	12.393077	1.08682527
3.50E+02	5.20E-02	20.7511205	1.10E-01	12.3931844	1.086858
3.50E+02	5.40E-02	20.7506241	1.10E-01	12.3932872	1.08688947
3.50E+02	5.60E-02	20.7501457	1.10E-01	12.3933857	1.08691977
3.50E+02	5.80E-02	20.749684	1.10E-01	12.3934802	1.08694898
3.50E+02	6.00E-02	20.7492378	1.10E-01	12.393571	1.08697717
3.50E+02	6.20E-02	20.7488062	1.10E-01	12.3936582	1.08700442
3.50E+02	6.40E-02	20.7483882	1.10E-01	12.393742	1.08703078
3.50E+02	6.60E-02	20.7479831	1.10E-01	12.3938227	1.08705629
3.50E+02	6.80E-02	20.7475901	1.10E-01	12.3939004	1.08708101
3.50E+02	7.00E-02	20.7472086	1.10E-01	12.3939753	1.08710498
3.50E+02	7.20E-02	20.7468381	1.10E-01	12.3940474	1.09E+00
3.50E+02	7.40E-02	20.7464779	1.10E-01	12.3941169	1.09E+00
3.50E+02	7.60E-02	20.7461276	1.10E-01	12.3941839	1.09E+00
3.50E+02	7.80E-02	20.7457868	1.10E-01	12.3942486	1.09E+00
3.50E+02	8.00E-02	20.745455	1.10E-01	12.3943109	1.09E+00
3.50E+02	8.20E-02	20.745132	1.10E-01	12.394371	1.09E+00
3.50E+02	8.40E-02	20.7448173	1.10E-01	12.394429	1.09E+00
3.50E+02	8.60E-02	20.7445107	1.10E-01	12.394485	1.09E+00
3.50E+02	8.80E-02	20.7442119	1.10E-01	12.394539	1.09E+00
3.50E+02	9.00E-02	20.7439206	1.10E-01	12.394591	1.09E+00
3.50E+02	9.20E-02	20.7436366	1.10E-01	12.3946412	1.09E+00
3.50E+02	9.40E-02	20.7433597	1.10E-01	12.3946896	1.09E+00
3.50E+02	9.60E-02	20.7430896	1.10E-01	12.3947362	1.09E+00
3.50E+02	9.80E-02	20.7428262	1.10E-01	12.3947812	1.09E+00
3.50E+02	1.00E-01	20.7425693	1.10E-01	12.3948245	1.09E+00
3.50E+02	1.02E-01	20.7423188	1.10E-01	12.3948662	1.09E+00
3.50E+02	1.04E-01	20.7420744	1.10E-01	12.3949063	1.09E+00
3.50E+02	1.06E-01	20.7418361	1.10E-01	12.394945	1.09E+00
3.50E+02	1.08E-01	20.7416038	1.10E-01	12.3949822	1.09E+00
3.50E+02	1.10E-01	20.7413773	1.10E-01	12.395018	1.09E+00

time_years	depth	tortuosity	porosity	AA_Portlandite.min	Cem07_C3AS0.8H4.4.min
3.50E+02	1.12E-01	20.7411565	1.10E-01	12.3950523	1.09E+00
3.50E+02	1.14E-01	20.7409413	1.10E-01	12.3950854	1.09E+00
3.50E+02	1.16E-01	20.7407316	1.10E-01	12.3951171	1.09E+00
3.50E+02	1.18E-01	20.7405274	1.10E-01	12.3951475	1.09E+00
3.50E+02	1.20E-01	20.7403285	1.10E-01	12.3951767	1.09E+00
3.50E+02	1.22E-01	20.740135	1.10E-01	12.3952047	1.09E+00
3.50E+02	1.24E-01	20.7399467	1.10E-01	12.3952315	1.09E+00
3.50E+02	1.26E-01	20.7397635	1.10E-01	12.3952571	1.09E+00
3.50E+02	1.28E-01	20.7395855	1.10E-01	12.3952817	1.09E+00
3.50E+02	1.30E-01	20.7394125	1.10E-01	12.3953052	1.09E+00
3.50E+02	1.32E-01	20.7392446	1.10E-01	12.3953276	1.09E+00
3.50E+02	1.34E-01	20.7390817	1.10E-01	12.395349	1.09E+00
3.50E+02	1.36E-01	20.7389237	1.10E-01	12.3953694	1.09E+00
3.50E+02	1.38E-01	20.7387707	1.10E-01	12.3953888	1.09E+00
3.50E+02	1.40E-01	20.7386225	1.10E-01	12.3954073	1.09E+00
3.50E+02	1.42E-01	20.7384792	1.10E-01	12.3954249	1.09E+00
3.50E+02	1.44E-01	20.7383408	1.10E-01	12.3954416	1.09E+00
3.50E+02	1.46E-01	20.7382071	1.10E-01	12.3954574	1.09E+00
3.50E+02	1.48E-01	20.7380783	1.10E-01	12.3954725	1.09E+00
3.50E+02	1.50E-01	20.7379543	1.10E-01	12.3954867	1.09E+00
3.50E+02	1.52E-01	20.7378351	1.10E-01	12.3955002	1.09E+00
3.50E+02	1.54E-01	20.7377207	1.10E-01	12.3955129	1.09E+00
3.50E+02	1.56E-01	20.737611	1.10E-01	12.3955248	1.09E+00
3.50E+02	1.58E-01	20.7375061	1.10E-01	12.3955361	1.09E+00
3.50E+02	1.60E-01	20.737406	1.10E-01	12.3955467	1.09E+00
3.50E+02	1.62E-01	20.7373106	1.10E-01	12.3955566	1.09E+00
3.50E+02	1.64E-01	20.7372199	1.10E-01	12.3955659	1.09E+00
3.50E+02	1.66E-01	20.7371341	1.10E-01	12.3955746	1.09E+00
3.50E+02	1.68E-01	20.7370529	1.10E-01	12.3955827	1.09E+00
3.50E+02	1.70E-01	20.7369765	1.10E-01	12.3955902	1.09E+00
3.50E+02	1.72E-01	20.7369049	1.10E-01	12.3955971	1.09E+00
3.50E+02	1.74E-01	20.7368381	1.10E-01	12.3956035	1.09E+00
3.50E+02	1.76E-01	20.7367759	1.10E-01	12.3956094	1.09E+00
3.50E+02	1.78E-01	20.7367186	1.10E-01	12.3956147	1.09E+00
3.50E+02	1.80E-01	20.736666	1.10E-01	12.3956196	1.09E+00
3.50E+02	1.82E-01	20.7366182	1.10E-01	12.3956239	1.09E+00
3.50E+02	1.84E-01	20.7365752	1.10E-01	12.3956278	1.09E+00
3.50E+02	1.86E-01	20.7365369	1.10E-01	12.3956313	1.09E+00
3.50E+02	1.88E-01	20.7365034	1.10E-01	12.3956343	1.09E+00
3.50E+02	1.90E-01	20.7364747	1.10E-01	12.3956368	1.09E+00
3.50E+02	1.92E-01	20.7364508	1.10E-01	12.3956389	1.09E+00
3.50E+02	1.94E-01	20.7364316	1.10E-01	12.3956406	1.09E+00
3.50E+02	1.96E-01	20.7364173	1.10E-01	12.3956419	1.09E+00
3.50E+02	1.98E-01	20.7364077	1.10E-01	12.3956427	1.09E+00
3.50E+02	2.00E-01	20.7364029	1.10E-01	12.3956431	1.09E+00

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