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CBP Toolbox Version 3.0 "Beta Testing" Performance Evaluation

F. G. Smith, III

July 2016

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REVIEWS AND APPROVALS

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EXECUTIVE SUMMARY

One function of the Cementitious Barriers Partnership (CBP) is to assess available models of cement degradation and to assemble suitable models into a "Toolbox" that would be made available to members of the partnership, as well as the DOE Complex. To this end, SRNL and Vanderbilt University collaborated to develop an interface using the GoldSim software to the STADIUM@ code developed by SIMCO Technologies, Inc. and LeachXS/ORCHESTRA developed by Energy research Centre of the Netherlands (ECN). Release of Version 3.0 of the CBP Toolbox is planned in the near future. As a part of this release, an increased level of quality assurance for the partner codes and the GoldSim interface has been developed.

This report documents results from evaluation testing of the ability of CBP Toolbox 3.0 to perform simulations of concrete degradation applicable to performance assessment of waste disposal facilities. Simulations of the behavior of Savannah River Saltstone Vault 2 and Vault 1/4 concrete subject to sulfate attack and carbonation over a 500- to 1000-year time period were run using a new and upgraded version of the STADIUM@ code and the version of LeachXS/ORCHESTRA released in Version 2.0 of the CBP Toolbox. Running both codes allowed comparison of results from two models which take very different approaches to simulating cement degradation. In addition, simulations of chloride attack on the two concretes were made using the STADIUM@ code. The evaluation sought to demonstrate that: 1) the codes are capable of running extended realistic simulations in a reasonable amount of time; 2) the codes produce "reasonable" results; the code developers have provided validation test results as part of their code QA documentation; and 3) the two codes produce results that are consistent with one another.

Results of the evaluation testing showed that the three criteria listed above were met by the CBP partner codes. Therefore, it is concluded that the codes can be used to support performance assessment. This conclusion takes into account the QA documentation produced for the partner codes and for the CBP Toolbox.

In particular, the author wishes to thank Brent Gutierrez of DOE Waste Disposal Engineering for his review of a draft of this report and the many helpful suggestions that significantly improved the quality of the final product.

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LIST OF ABBREVIATIONS

CBP	Cementitious Barriers Partnership
DOE	Department of Energy
ECN	Energy Corporation of the Netherlands
LXO	LeachXS/ORCHESTRA
NRG	Nuclear Research and consultancy Group (The Netherlands)
OPC	Ordinary Portland Cement
ORCHESTRA	Objects Representing CHEmical Speciation and TRAnsport models
SRNL	Savannah River National Laboratory
SRS	Savannah River Site

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1.0 Introduction

This report documents performance testing of the CBP Toolbox Version 3.0 (Brown, et al., 2015). Software QA for the CBP is controlled by two documents; 1) "CBP Software QA Work Plan" (CBP, 2015a) and 2) "Cementitious Barriers Partnership Software Quality Assurance Implementation Procedure" (CBP, 2015b). The QA Work Plan calls for verification testing. The "performance" testing, also called beta testing, described in this report is intended to provide verification of the performance of the integrated CBP Toolbox simulation package. As in previous versions of the CBP Toolbox (Brown, et al., 2013), the partner codes accessible through the toolbox are CBP STADIUM@ a product of SIMCO Technologies, Inc. (SIMCO) and LeachXS/ORCHESTRA (LXO) a product of the Energy Research Center of the Netherlands (ECN). The performance testing evaluates the suitability of using the latest available versions of CBP STADIUM@ and LXO for performance assessment applications. An updated version of LXO for use in the CBP Toolbox is under development but was not available when the evaluation testing was performed.

With previous versions of the CBP Toolbox, SIMCO has provided an executable version of STADIUM@ (stadium_win_v2016a.exe) that could be linked directly to the Toolbox and used to simulate concrete degradation. An interface to the code was developed using the GoldSim software (Version 11.1, GTG, 2014) that allow users to specify input for STADIUM@ and LXO simulations using preconfigured files, run simulations, and return results to GoldSim for plotting and further analysis (Brown et al., 2015). GoldSim also provided the capability of making multiple simulations drawing input from user specified parameter distributions for uncertainty analysis. It was intended to continue this approach in Version 3.0 of the Toolbox initially scheduled for release at the end of 2015. At the same time, a new approach to STADIUM@ simulations provided by SIMCO was also incorporated into Version 3.0 of the Toolbox (Brown, 2015). This approach allows the user to access a version of STADIUM@ on a SIMCO web server to perform simulations of concrete degradation. To access the web application at cbp.stadium-software.com the user must establish an account with SIMCO. The point of contact for opening a SIMCO account is Dr. Eric Sampson (esamson@simcotechnologies.com). Similarly, while LeachXS is available as stand-alone software, an interface to a version of LeachXS (ECN, 2012) coupled with ORCHESTRA (Meeussen and Brown, 2016) is provided through the CBP Toolbox.

1.1 Test Plan

The work described in this report involves performance testing of the CBP Toolbox Version 3.0 by exercising the partner codes to demonstrate that:

1. The codes are capable of running extended simulations required for PA applications in a reasonable amount of time.
2. The codes produce "physically reasonable" results. This is intended to simply be a subjective evaluation of the results that they fall within reasonable bounds and that the behavior over time is reasonably smooth.
3. STADIUM@ and LXO, which take different approaches to modeling concrete degradation, produce reasonably consistent results.

Code validation has been addressed by the developers in their respective QA documentation (SIMCO, 2015b and Meeussen and Brown, 2016). The validation must necessarily compare code performance to experimental results measuring concrete degradation over at most a few years. However, for performance assessment applications, concrete degradation over time periods on the order of 1000 years must be simulated. Thus, the testing described in this report was conducted to evaluate code performance for long term simulations. The testing was primarily conducted using concrete formulations for SRS Saltstone

Vault 1/4 and Vault 2 concrete (SIMCO, 2012) exposed to Saltstone waste material on one side and SRS backfill soil on the other.

The following CBP partner codes were tested:

1. STADIUM@ CBP accessed through the Toolbox as a web application.
2. An executable version of the STADIUM@ CBP code accessed directly through the Toolbox which was intended to give the same results as the web based application.
3. An executable version of the LeachXS/ORCHESTRA code (ORCHESTRA-LXS 2013 runtime system 26092013) accessed through the Toolbox. A revision of the LXO code is in progress and will be included in the next release of the CBP Toolbox (Version 3.1) at which time test results can be updated. Using LXO CBP Toolbox Version 2.0 provided code to code comparisons and including it in the testing provided a review of the CBP Toolbox 3.0 as it currently exists. However, because a new version of LXO is anticipated in the near future, the beta testing is primarily focused on STADIUM@.

The partner codes were evaluated for the three types of concrete degradation currently available using the CBP Toolbox:

1. Sulfate attack from exposure to pore solution leaching out of a representative SRS Saltstone waste material (SIMCO, 2010) having a high concentration of SO_4^{-2}.
2. Ingress of chloride into concrete from exposure to groundwater with high concentrations of Cl^- (simulation of chloride ingress is only available with STADIUM@ CBP).
3. Concrete carbonation:
    a. For STADIUM@, exposure to soil water having a high concentration of HCO_3^- under saturated conditions.
    b. For LXO, exposure to CO_2 in soil gas under unsaturated conditions.

LeachXS/ORCHESTRA also provides a model of fluid transport through porous concrete by percolation with radial diffusion (Sarkar, et al., 2013) that was not tested as part of this performance evaluation. SRNL has developed a CBP Toolbox module to calculate hydraulic properties of concrete. This module is described elsewhere (Smith and Flach, 2015) and was again not tested as part of this evaluation, which was focused on simulating concrete degradation mechanisms.

This report starts with a brief overview of the STADIUM@ CBP web application which is a new feature of the CBP Toolbox. This is followed by results obtained from testing the ability of the partner codes to simulate the three types of concrete degradation listed above. Model to model comparison of results obtained using the different codes to simulate the same concrete degradation process are provided. As noted above, the code developers have provided validation test results as part of QA documentation (SIMCO, 2015b and Meeussen and Brown, 2016). Input files for the executable version of STADIUM@ CBP are provided in a separate file that will be archived with this report and available on request. Identical inputs were entered to make the STADIUM@ CBP web application simulations. LXO input is contained in many separate files that could not be conveniently collected. Output from the simulations is provided as plots of mineral concentrations over the concrete depth at various times in the simulation. Copies of input and output files used in the testing will be archived an SRNL server where CBP storage space has been allocated but are not appended to this report to keep the size manageable.

2.0 STADIUM@ CBP Web Application

A full description of the STADIUM@ CBP application is given in the User Guide (SIMCO, 2015a). The STADIUM@ CBP web application provides the user with three types of simulations involving different material layers. The simulation types are: 1) Wasteform/Concrete/Soil, 2) Steel Liner/Concrete/Soil and 3) Wasteform Pore Solution/Concrete/Soil. The STADIUM@ CBP web application offers a limited number of materials for use in simulation of concrete degradation. Properties for two types of concrete are provided in the material selection menu that can be used to assess the behavior of Savannah River Site (SRS) Saltstone disposal Vaults 1/4 and 2. Properties are also provided for SRS compacted backfill soil and the Saltstone waste material (Samson, 2010). The soil composition in effect specifies the composition of water in contact with the concrete surface exposed to the environment. The user can change the water composition to simulate its effect on cement. In particular, this feature was used to model chloride attack and carbonation at the outer surface of the vault concrete. The user creates simulation input, runs the simulation and can plot results all within the web based interface. Plots and tabulated results can be downloaded.

Materials available in the STADIUM@ CBP web application are listed in Table 2-1. The material compositions were compared to those used to perform STADIUM@ simulations with the CBP Toolbox and the materials provided by the web application were found to be identical to the corresponding Toolbox materials. The correspondence between materials is shown in Table 2-1 and compositions of the materials are given in Table 2-2. Other than these materials, the STADIUM@ CBP Web application includes two additional concrete formulations (SIMCO Lab mix M1.1 0.35 water to cement Ordinary Portland Cement (OPC) and SIMCO Lab mix SUMMA2 0.45 water to cement OPC) which were not tested as part of this evaluation.

Table 2-1. STADIUM@ Material Comparison

STADIUM@ CBP Web Material	Corresponding Material in CBP Toolbox 3.0
SRS Saltstone Wasteform	Type 1 Saltwaste
CBP Vault1/4 Lab	Vault 1/4 Concrete
CBP Vault 2 Lab	Vault 2 Concrete
SRS CC Backfill	Type 1 Soil

While SIMCO plans to add the capability of performing uncertainty analysis to the web application this capability is not currently available. Therefore, it was decided that Version 3.0 of the CBP Toolbox would continue using an executable version of the STADIUM@ code so that the GoldSim software, which serves as a platform for the CBP Toolbox, could be used to perform uncertainty analysis. It was also desirable to continue with a Toolbox version of STADIUM@ for backward compatibility with existing CBP STADIUM@ simulations at least through Version 3.0 as the transition to a web based application is made.

Table 2-2. STADIUM Material Compositions

		Vault 1/4 Concrete	Vault 2 Concrete	Saltstone Type 1	SRS CC Backfill
Formulation (kg/m^3)	Type I/II Cement	255		135	
	Type V Cement		121		
	GGBFS (Blast Furnace Slag)	169	162	195	
	Class F Fly Ash		95	600	
	Force 1000 Silica Fume		27		
	Sand (Fine Aggregate)	691	548		
	Stone (Coarse Aggregate)	1096	1111		
	Water	161	154	553	
Hydration (%)	Cement	80	75	85	
	Slag	75	65	70	
	FlyAsh		35	50	
	Silica Fume		90		
Pore Fluid Species (mmol/L)	OH^-	244.4	113.9	484.6	0.50
	Na^+	73.9	26.5	4419.8	0.25
	K^+	140.7	35.8	119.3	0.25
	SO_4^{-2}	0.1	0.1	120.3	0
	Ca^{+2}	1.8	2.0	0.9	0
	AlO_4H_4	0.0	0.0	0.0	0
	Cl^-	4.8	4.2	8.9	0
	H_2SiO_4	0.0	0.0	0.0	0
	CO_3^{-2}	0.0	0.0	115.5	0
	NO_3^-	0.0	0.0	2000.0	0
	NO_2^-	0.0	0.0	1575.8	0
Initial Minerals (g/kg)	Portlandite	7.2	0.0	0.0	1.0E-10
	C-S-H	118.8	81.2	140.9	0
	Ettringite	0.0	0.0	0.0	0
	Monosulfate	18.4	10.0	39.0	0
	AFmOH	9.9	0.0	0.0	0
	Thaumasite	0.0	0.0	0.0	0
	Calcite	0.0	0.0	0.0	0
	Monocarboaluminate	0.0	0.0	0.0	0
	Gypsum	0.0	0.0	0.0	0
	Friedel_IX	0.0	0.0	0.0	0

3.0 Code Performance Modeling Sulfate Attack

3.1 STADIUM@ CBP Web Application

Three examples of sulfate attack were run using the STADIUM@ CBP Web application:

1. A 1000 yr simulation of 100 cm of Saltstone waste material in contact with 20 cm of Vault 2 concrete with 100 cm of soil against the outside surface.
2. A 250 yr simulation of 20 cm of Vault 2 concrete in contact with Saltstone pore solution.
3. A 1000 yr simulation of 100 cm of Saltstone waste material in contact with 45 cm of Vault 1/4 concrete with 100 cm of soil against the outside surface.

Properties of the Saltstone waste material and pore solution were obtained from SIMCO (2010) and properties of the concrete were obtained from SIMCO (2012). The pore solution represents the composition of pore fluids extracted from the waste form in SIMCO testing.

A nominal pore solution sulfate concentration of 123.6 mmol/L was used for these simulations. SIMCO (2010, Table 8) gives a value of 120.3 mmol/L for SO_4^{-2} in Saltstone pore solution. The slightly higher value has been used in previous simulations (Flach and Smith, 2014). Results of the modeling are shown in Figures 3-1 through 3-3. In these figures, the Vault 2 concrete material layer is between 1000 mm and 1200 mm and the Vault 4 concrete between 1000 mm and 1450 mm. The plots show concentrations of the sulfur containing minerals Al-AFt, AFm_SS and Friedel_SS throughout the concrete layer and in portions of the Saltstone waste and soil layers immediately adjacent to the concrete. The STADIUM@ damage factor is also plotted; for a description of the damage factor see Section 4.2.2 of the STADIUM@ QA Report (SIMCO 2015b). Table 3-1 shows the initial specification of the mineral species and the initial calculated equilibrium mineral compositions as determined by the STADIUM@ CBP web application.

Table 3-1. Initial mineral composition (g/kg)

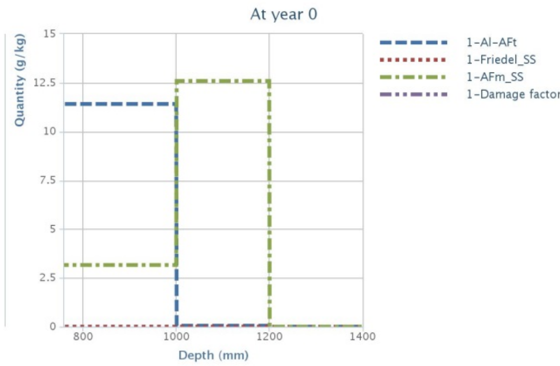
	Material	Al-AFt	Friedel_SS	AFm_SS
Initial Mineral Specification	Saltstone	0	0	11.82
	Vault 2 Concrete	0	0	12.63
	Vault 1 /4 Concrete	0	0	19.49
	Soil	0	0	0
Initial Equilibrium Mineral Composition	Saltstone	11.41	1.23e-4	3.16
	Vault 2 Concrete	4.97e-2	1.02e-3	12.59
	Vault 1/4 Concrete	2.72e-2	1.85e-3	19.48
	Soil	0	0	0

Sulfate attack starts at the Saltstone-concrete interface and progresses along a reaction front into the concrete. Previous results (Flach and Smith, 2013) obtained with CBP Toolbox Version 1.0 assumed that concrete degradation coincided with the formation of an Al-Ettringite mineral phase in the material. These results showed that at 1000 years the Al-Ettringite peak had progressed about 0.5 cm into Vault 2 concrete and 5.5 cm into Vault 1/4 concrete. These predictions of concrete damage were lower than those obtained using LeachXS/ORCHESTRA (ORCHESTRA-LXS 2008) and therefore, the LXO predictions were used in 2013 to provide conservative estimates of concrete life for the Saltstone Disposal Unit PA (SRR, 2009). The current version of STADIUM@ has increased the number of mineral phases available. Calcium-sulfoaluminate hydrates in the revised version of STADIUM@ are Al-AFt, which is the same mineral as Al-Ettringite with the same chemical properties, and AFm_SS. The assumption made for performance testing is that ingrowth of a sulfate containing mineral phase will be an indicator of sulfate attack on the concrete.

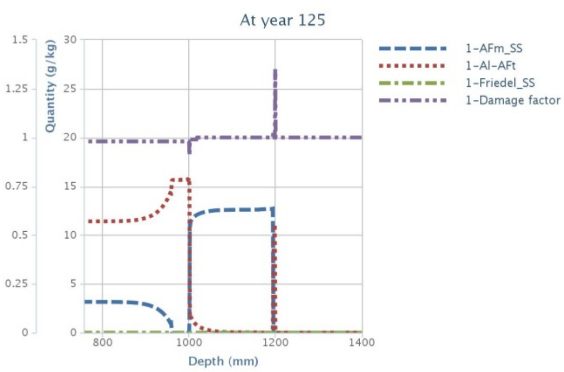
Results from the web based STADIUM@ application can be plotted online and the plots downloaded as jpeg files. Plots of results from the sulfate attack simulations are shown in Figures 3-1 through 3-3. Examining the results for Vault 2 concrete exposed to Saltstone waste material shown in Figure 3-1(b) through 3-1(e), Al-AFt steadily progresses into the concrete. At 1000 years Figure 3-1(e) shows that a significant Al-AFt concentration has penetrated about 17 cm (86% of the 20 cm thickness) into the concrete. Interpreting this result as concrete degradation would be in general agreement with the LXO results obtained previously (Flach and Smith, 2013 Table 2-2), which indicated full degradation of 20 cm of Vault 2 concrete at about 950 years. AFm_SS has been lost over the first 0.8 cm of the Vault 2 concrete which is in general agreement with the ingrowth of Al-Ettringite seen in the previous STADIUM@ CBP calculation. The damage factor peaks at the concrete-soil interface and does not appear to correlate with sulfate attack.

Figure 3-2, obtained from the simulation of sulfate attack on Vault 2 concrete exposed to Saltstone pore solution, provides similar results. At 125 years of exposure, Al-AFt has penetrated about 11 cm into the concrete (55% of the concrete depth) and the AFm_SS has been lost over a layer less than 1 cm in thickness near the Saltstone concrete interface. After 250 years of exposure, concentrations of Al-AFt > 0.1 g/kg occur up to 13.3 cm into the concrete while AFm_SS has now been lost over 2.4 cm. This result can be compared to Figure 3-1(c) which shows Al-AFt penetration to about 10 cm at 250 years. It was expected that simulating concrete in direct contact with the Saltstone pore solution would give a more aggressive sulfate attack response than that obtained by contact with the Saltstone waste material. While this was confirmed by the model simulations, the results were not extremely different. As noted in the Conclusions, the pore solution simulation ran considerably slower than the three layer simulation. Simulation of concrete in direct contact with pore solution would likely be used to model experimental results obtained over shorter exposure times than tested here while the three layer model would be used simulate actual waste disposal conditions.

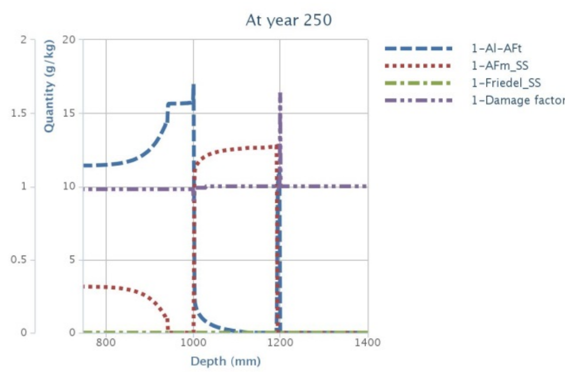
The results obtained for sulfate attack on Vault 1/4 concrete exposed to Saltstone waste material shown in Figure 3-3(b) through 3-3(e) are somewhat puzzling. At 1000 years Al-Aft appears to have barely penetrated into the concrete. This result is in contrast to the results obtained with the previous version of STADIUM@ CBP which indicated about 12% of the concrete had degraded after 1000 year of exposure to Saltstone. Examining the numerical results, there is in fact a very low concentration of Al-AFt 27 cm into the concrete while AFm_SS has been lost over the first 0.6 cm. This Al-AFt result would again be in general agreement with the LXO results obtained previously (Flach and Smith, 2013 Table 2-4) which predicted full degradation of 45 cm of Vault 1/4 concrete at about 1200 years. However, the Al-Ettringite peak previously used as a marker of sulfate attack was easily observable on a linear plot of the results and it is difficult to associate the low concentration of Al-AFt obtained in the current simulation with any significant concrete degradation. Comparing Figure 3-3 with Figure 3-1, the two concretes show significantly different behavior at both the Saltstone and soil interfaces. This difference was not observed in the 2013 simulations. Figure 3-3 also shows some growth of Al-AFt into the soil layer which is not apparent in Figure 3-1.



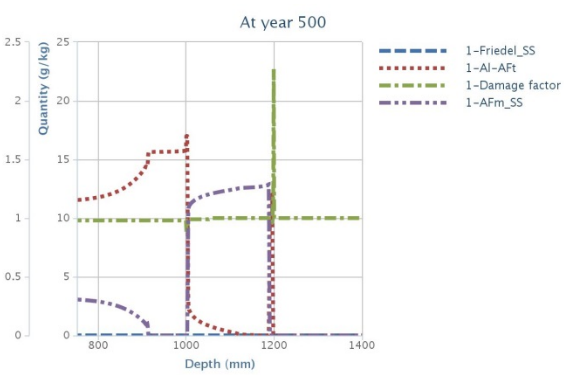
(a)



(b)



(c)



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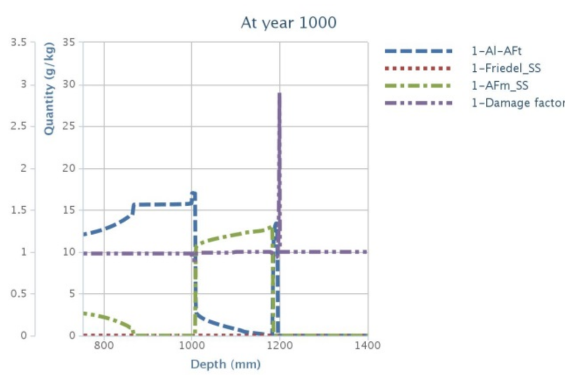


(e)

Figure 3-1. Progression of sulfate attack on 20 cm of Vault 2 concrete over 1000 years predicted by STADIUM[@] CBP Web application.

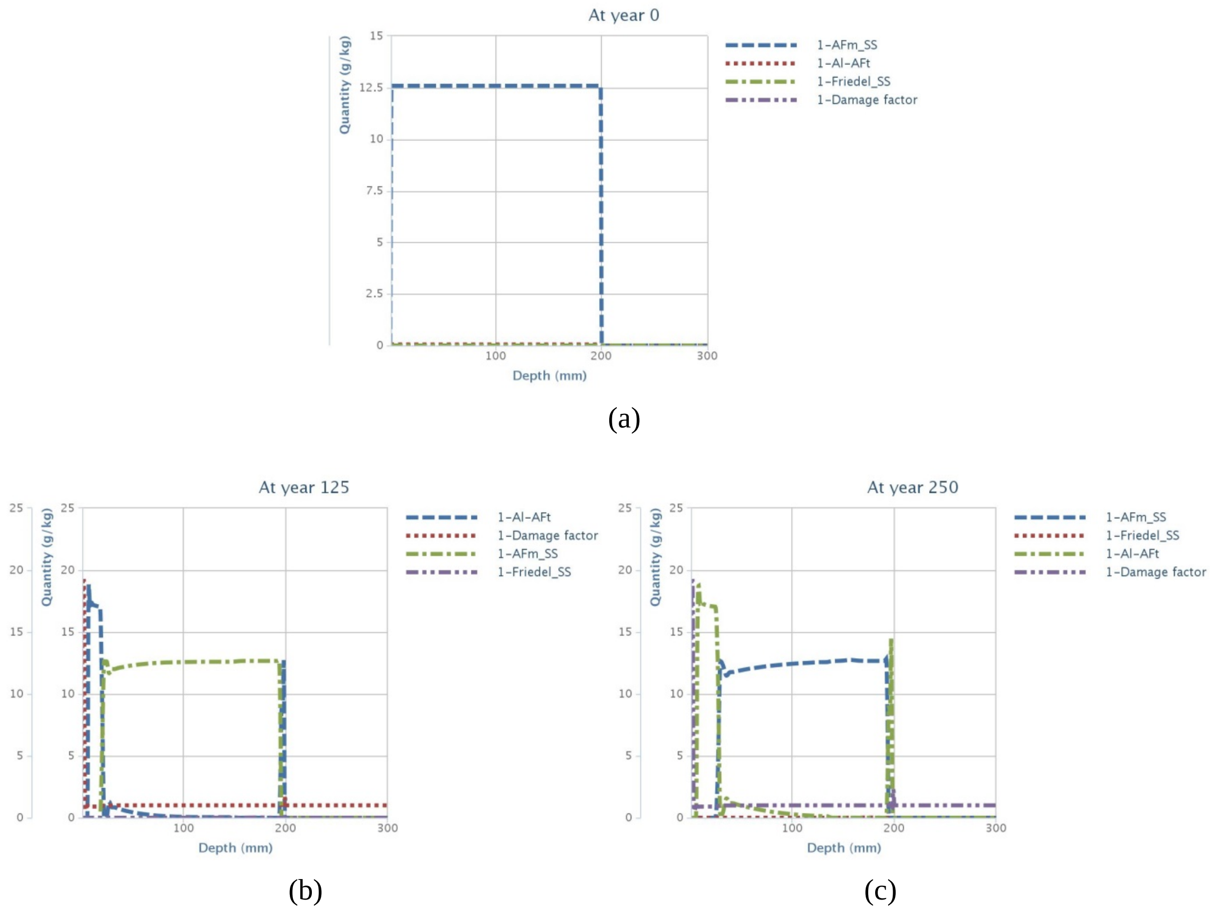


Figure 3-2. Progression of sulfate attack on 20 cm of Vault 2 concrete in contact with Saltstone pore solution over 250 years predicted by STADIUM@ CBP Web application.

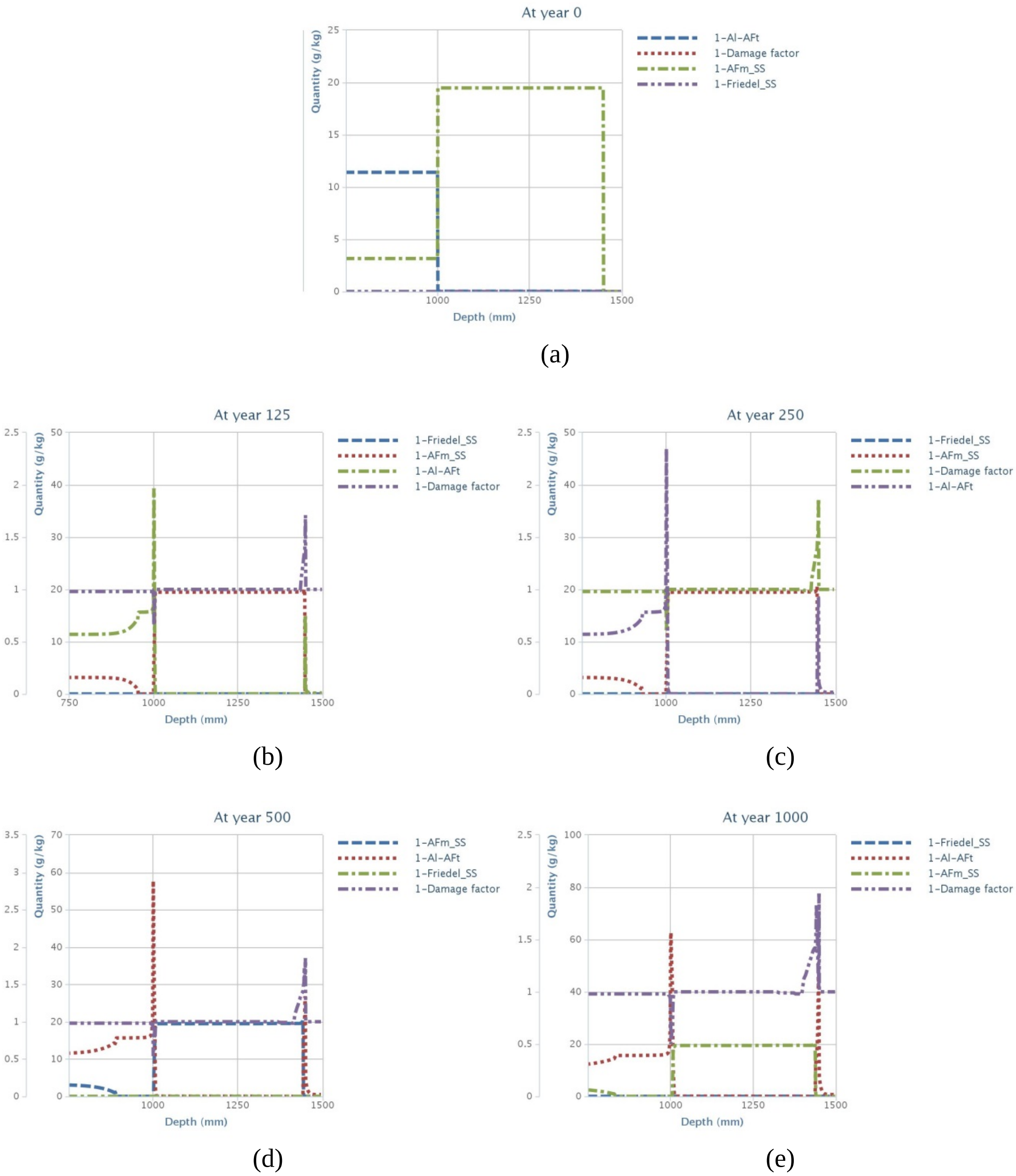


Figure 3-3. Progression of sulfate attack on 45 cm of Vault 1/4 concrete over 1000 years predicted by STADIUM@ CBP Web application.

3.2 STADIUM@ CBP Toolbox Executable

The Toolbox version of STADIUM@ CBP provides three types of simulations: 1) A one-layer model of concrete with liquid ponding on one side, 2) A two-layer Wasteform/Concrete model, and 3) A three-layer Wasteform/Concrete/Soil model. To obtain shorter run times, previous modeling of Saltstone vault concrete by SRNL used the two-layer model which does not directly translate into an equivalent web version. Previous modeling (Flach and Smith, 2013) used 120 cm of Saltstone contacting 20 cm of Vault 2 concrete and 270 cm of Saltstone contacting 45 cm of Vault 1/4 concrete. Model results showed that the relatively large extent of the Saltstone layer in the models was not necessary and effects from reactions at the Saltstone boundary did not propagate beyond 50 cm into the Saltstone over 1000 years.

Two examples of sulfate attack were run using the STADIUM@ CBP Toolbox executable:

1. A 1000 yr simulation of 100 cm of Saltstone waste material in contact with 20 cm of Vault 2 concrete with 100 cm of soil against the outside surface.
2. A 1000 yr simulation of 100 cm of Saltstone waste material in contact with 45 cm of Vault 1/4 concrete with 100 cm of soil against the outside surface.

Saltstone waste material with a nominal sulfate concentration of 123.6 mmol/L was used for these simulations. These tests duplicate two of the web based runs described in Section 3.1 and used identical computational meshes. Results of the modeling are shown in Figures 3-4 and 3-5. Input files used to make the simulations are provided in a separate file that will be archived with this report and available on request. In Figure 3-4, the Vault 2 concrete material layer is between 100 cm and 120 cm and in Figure 3-5, the Vault 1/4 concrete is between 100 cm and 145 cm. The plots show concentrations of the minerals Al-AFt, AFm_SS and Friedel_SS in the concrete layer and in portions of the Saltstone waste and soil layers immediately adjacent to the concrete. The damage factor was not included as one of the Toolbox plotting options although it will be added as a plotting option in future releases.

Table 3-2 shows the initial specification of the mineral species and the model calculated initial equilibrium mineral compositions as determined by the STADIUM@ CBP Toolbox executable. The STADIUM@ CBP web based application and Toolbox executable should behave the same, the different equilibrium Saltstone mineralization results in Tables 3-1 and 3-2 indicate that there are some differences in the input to the two models. Concrete mineralization is almost identical in both versions but the Saltstone is evidently different.

Table 3-2. Initial mineral composition (g/kg)

	Material	**Al-AFt**	**Friedel_SS**	**AFm_SS**
Initial Mineral Specification	Saltstone	0	0	11.82
	Vault 2 Concrete	0	0	12.63
	Vault 1 /4 Concrete	0	0	19.49
	Soil	0	0	0
Initial Equilibrium Mineral Speciation	Saltstone	6.28	4.10e-4	6.94
	Vault 2 Concrete	5.23e-2	9.07e-4	12.58
	Vault 1/4 Concrete	2.67e-2	1.85e-3	19.48
	Soil	0	0	0

Comparing the Vault 2 concrete simulations shown in Figure 3-1 with Figure 3-4 shows the results appear to be very similar if not identical. A quantitative comparison of the position of the Al-AFt front in Vault 2 concrete obtained with the two versions of the STADIUM@ model is provided in Table 3-3. These results would suggest slight differences in the performance of the two versions of the STADIUM@ code. However; the differences are small and are probably within the predictive capability of the models although the uncertainty in model results has not been quantified.

Table 3-3. Comparison of Al_AFt front position calculated by STADIUM@ web application and Toolbox executable for Vault 2 concrete.

SDU Concrete	STADIUM@ Code	Simulation Time (Years)	Al-AFt > 0.06 (cm)
Vault 2	Web Application	100	8.1
		300	11.0
		500	13.3
		1000	16.8
	Toolbox Executable	100	7.3
		300	10.0
		500	12.6
		1000	16.8

Comparing the Vault 1/4 concrete simulations shown in Figure 3-3 with Figure 3-5 shows the results again appear to be very similar. The damage factor in Figure 3-3 may indicate decalcification occurring at the soil boundary. This penetrates into the Vault 1/4 concrete but is localized at the surface of the Vault 2 concrete as shown in Figure 3-1(c). The STADIUM@ damage factor is indicative of the formation of microcracks in the concrete (SIMCO, 2015a).

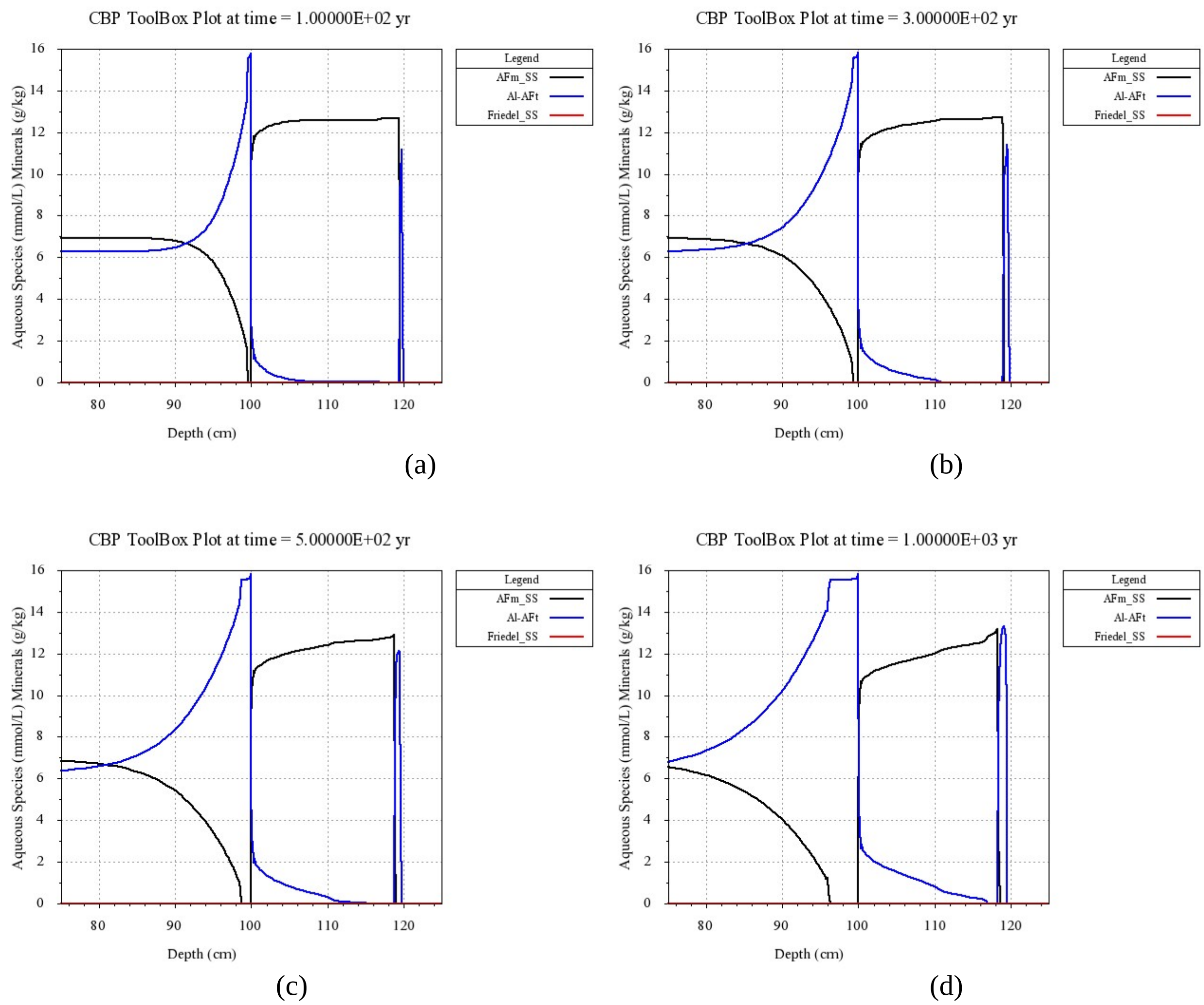


Figure 3-4. Progression of sulfate attack on 20 cm of Vault 2 concrete over 1000 years predicted by STADIUM@ CBP Toolbox executable.

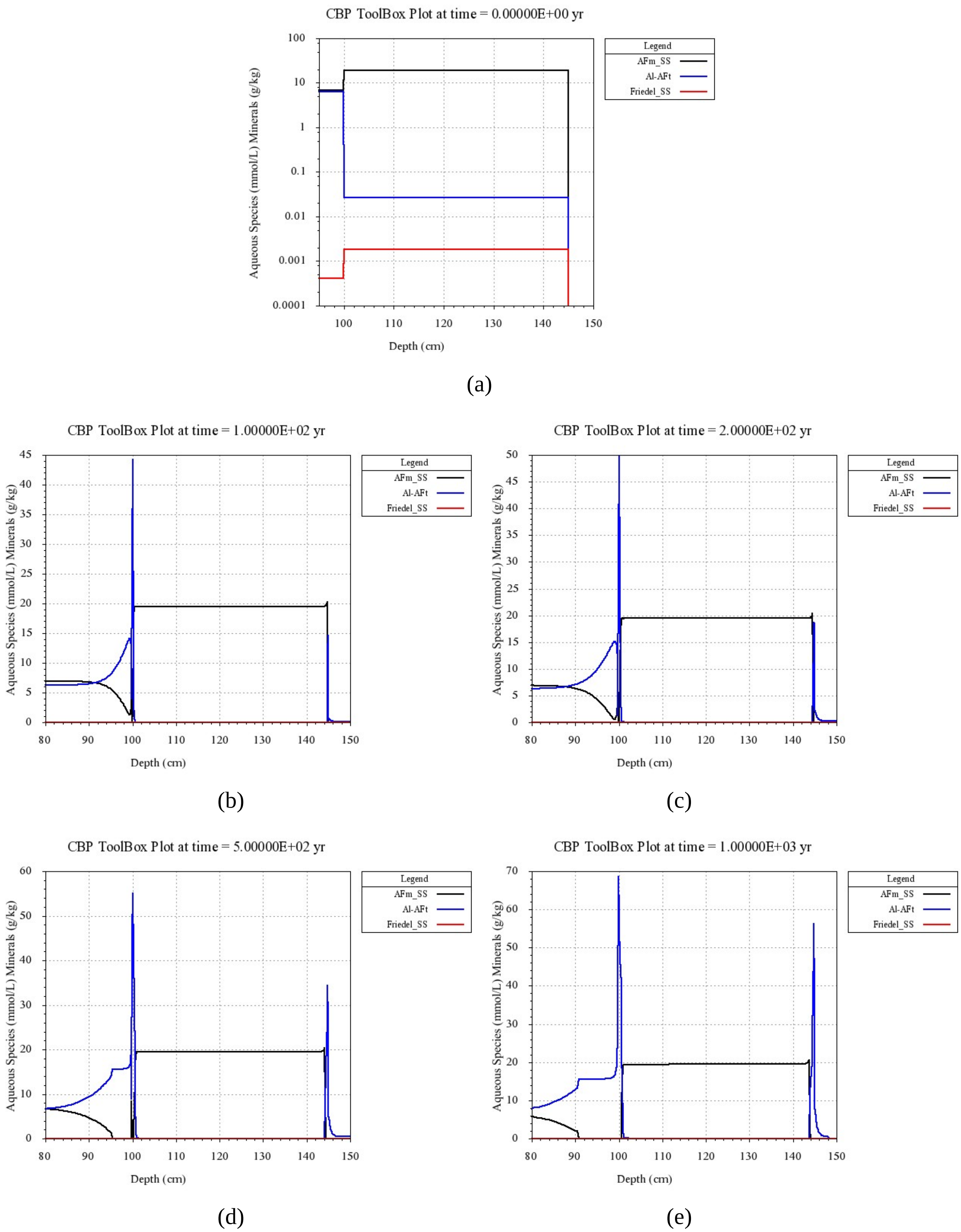


Figure 3-5. Progression of sulfate attack on 45 cm of Vault 1/4 concrete over 1000 years predicted by STADIUM@ CBP Toolbox executable.

3.3 LeachXS/ORCHESTRA

As noted previously, a new version of LeachXS/ORCHESTRA (LXO) for use in the CBP Toolbox is currently under development but was not available at the time the performance testing was performed. Therefore, the sulfate attack testing for LXO was limited to using the latest available version of the LXO model (ORCHESTRA-LXS 2013) to reproduce simulations similar to those performed previously by Flach and Smith (2013) using the initial version of LXO (ORCHESTRA-LXS 2008).

Two examples of sulfate attack were run using the LeachXS/ORCHESTRA Toolbox application:

1. A 500 yr simulation of 20 cm of Vault 2 concrete contacted with Saltstone pore solution having 0.124 M SO_4^{-2}.
2. A 500 yr simulation of 45 cm of Vault 1/4 concrete contacted with Saltstone pore solution having 0.124 M SO_4^{-2}.

Previous results (Flach and Smith, 2013) covered a range of sulfate concentration in the pore solution (0.1 M, 0.3 M and 0.5 M) and a range of concrete fractional porosity (0.30, 0.45 and 0.60). Fractional porosity, which has no direct equivalent in STADIUM$^{@}$ input, was identified as an important parameter in the LXO simulations and the testing performed here used the intermediate fractional porosity of 0.45 from the previous calculations. Results of the modeling are shown in Figures 3-7 and 3-8. The LXO simulations were run for 500 years; however, through an error in the output specification, results at 450 years were the last values output. LXO outputs results at approximately the specified times. Therefore to be certain that a result at or near 500 years is available; the simulation must be run for some time beyond 500 years.

Previous results closest to the evaluation runs for Vault 2 concrete made in this performance testing were from a simulation with 0.1 M SO_4^{-2} using a fractional porosity of 0.45. At 200 years, that simulation showed Al-Ettringite penetration of 2.7 cm. Figure 3-7(c) with slightly higher SO_4^{-2} at a simulation time of 200 years shows a smaller Al-Ettringite penetration of about 2.0 cm. For this analysis, the LXO damage parameter (omega) closely tracks the Al-Ettringite peak. Loss of Portlandite in the Vault 2 concrete also tracks with the formation of Al-Ettringite and the damage parameter. Previous results closest to the evaluation run for Vault 1/4 concrete were from a simulation with 0.1 M SO_4^{-2} using a fractional porosity of 0.45. At 450 years, that simulation showed Al-Ettringite penetration of approximately 16 cm. Figure 3-7(d) with slightly higher SO_4^{-2} shows Al-Ettringite penetration of about 5 cm. Loss of Portlandite in the Vault 1/4 concrete closely tracks the formation of Al-Ettringite in the concrete and the damage parameter.

Initial testing with CBP Toolbox LXO(ORCHESTRA-LXS 2008) showed a significant difference in performance between the Saltstone Vault 1/4 and Vault 2 concrete with Vault 1/4 more susceptible to degradation. CPB Toolbox LXO (ORCHESTRA-LXS 2013) shows the two concrete formulations behaving very similarly. In both cases, the first 5 cm of concrete has degraded within 450 years.

The LXO damage parameter (omega) was found to track with the loss of Portlandite and the ingrowth of Al-Ettringite. The damage parameter is related to the density of cracks forming in the concrete which is a function of strain. Strain is related to the change in solid volume from the dissolution and formation of different mineral phases in the concrete.

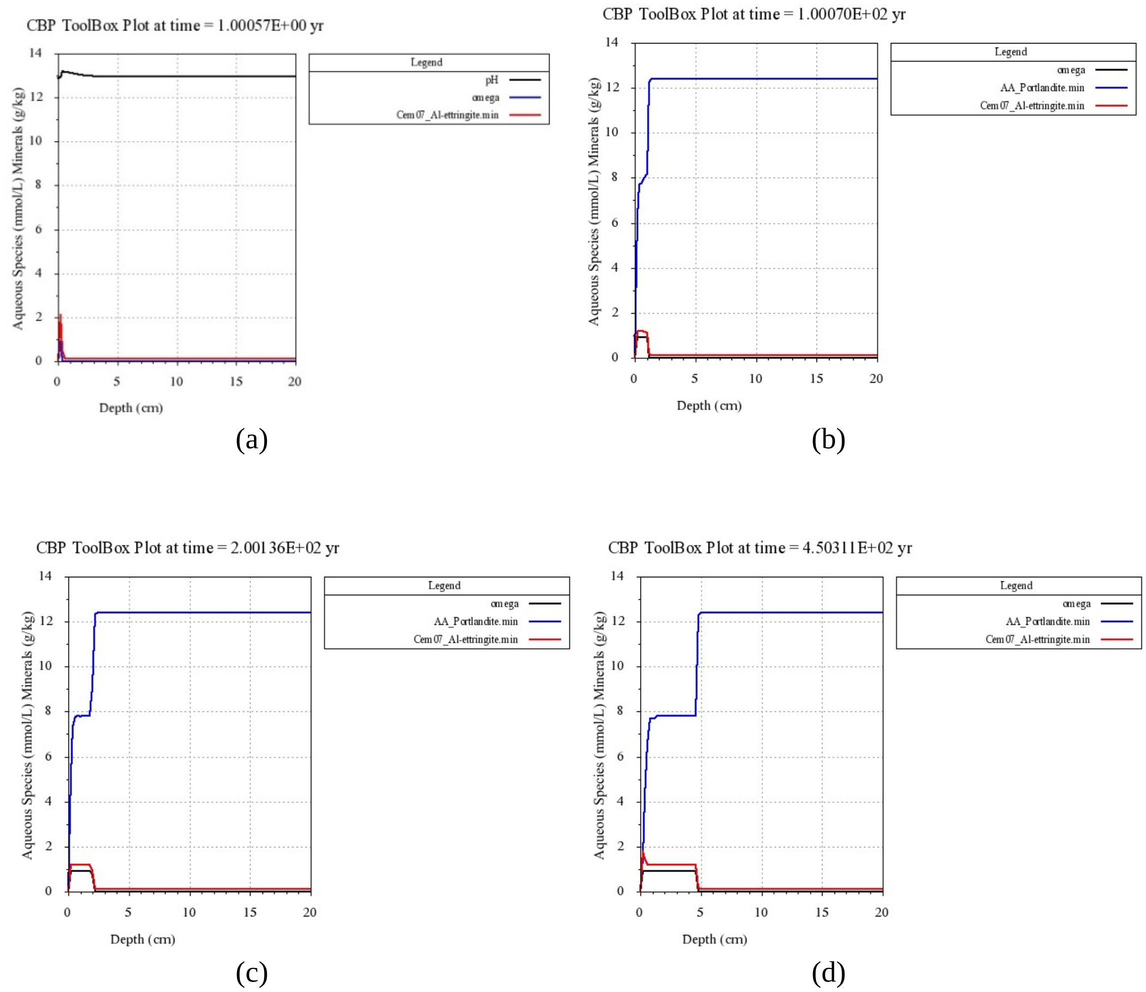


Figure 3-6. Progression of sulfate attack on 20 cm of Vault 2 concrete over 450 years predicted by LeachXS/ORCHESTRA Toolbox application.

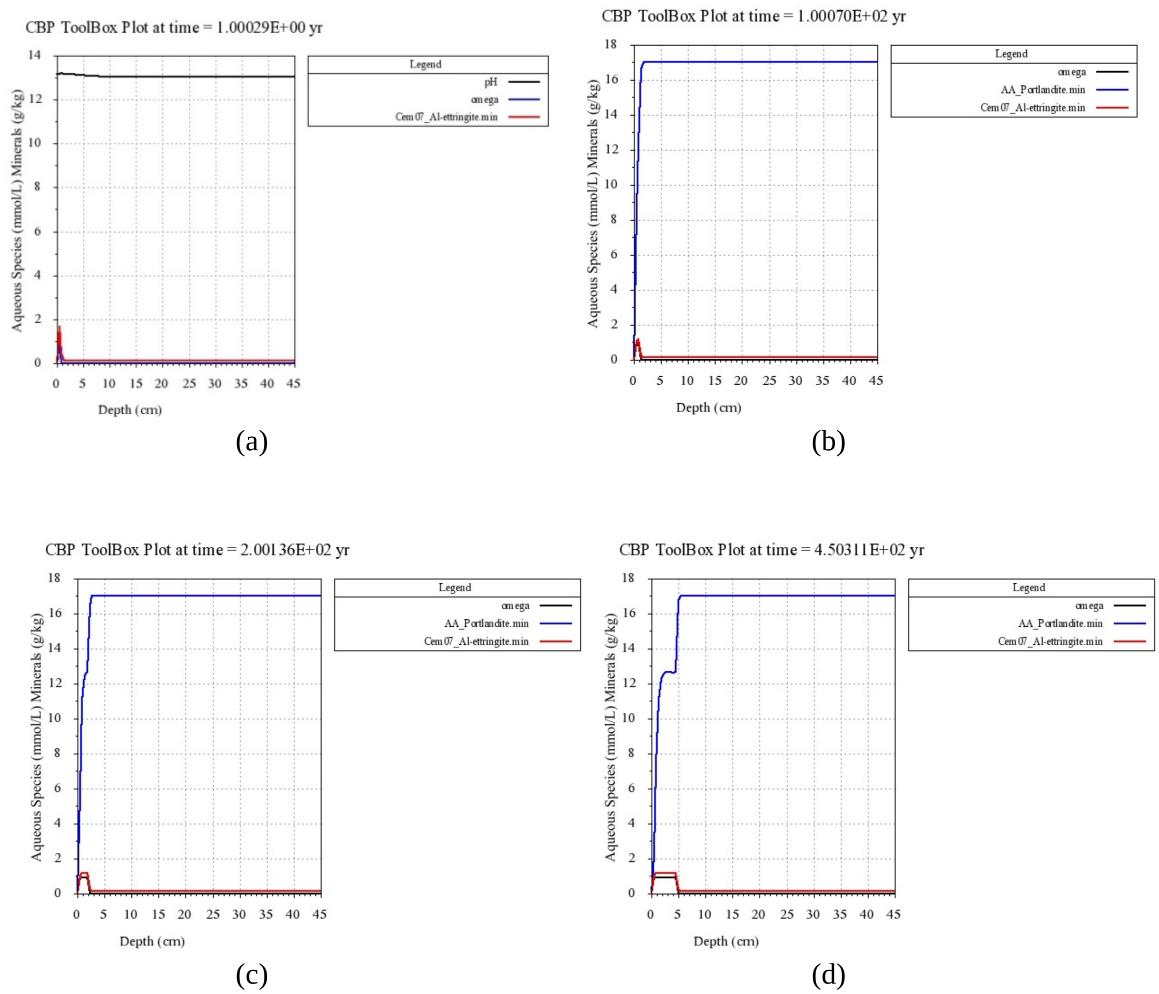


Figure 3-7. Progression of sulfate attack on 45 cm of Vault 1/4 concrete over 450 years predicted by LeachXS/ORCHESTRA Toolbox application.

3.4 Summary of Sulfate Attack Results

Results from the performance testing for sulfate attack on the two SRS Saltstone Vault concretes are summarized in Table 3-4. Penetration is the distance the mineral phase marker used to indicate sulfate attack has progressed into the concrete. For Stadium CBP Version 1, Al-Ettringite was used as a marker of sulfate attack while for Stadium[@] CBP Version 3 Al-Aft was used. In all cases, Al-Etrringite was used as a marker of sulfate attack for LXO. The results obtained with Stadium[@] CBP Version 3 for Vault 1/4 concrete do not appear to be reasonable. Assuming that penetration depth is proportional to the square root of time (Flach and Smith, 2013), the LXO models would predict penetration depths at 1000 years shown in the right hand columns of Table 3-4. With this approximation LXO Version 1, LXO Version 2 and Stadium Version 3 results for Vault 2 concrete fall within approximately a factor of two which would be considered good agreement.

Table 3-4. Summary of Model Results for Sulfate Attack

	Model Results		**Model Results**		**Extrapolated LXO**	
	Stadium[@] CBP Version 1		**LXO Version 1**		**LXO Version 1**	
Concrete	**Penetration (cm)**	**Time (Years)**	**Penetration (cm)**	**Time (Years)**	**Penetration (cm)**	**Time (Years)**
Vault 1/4	**5.5**	**1000**	**18.9**	**500**	**26.7**	**1000**
Vault 2	**0.5**	**1000**	**7.4**	**350**	**12.5**	**1000**
	Stadium[@] CBP Version 3		**LXO Version 2**		**LXO Version 2**	
Concrete	**Penetration (cm)**	**Time (Years)**	**Penetration (cm)**	**Time (Years)**	**Penetration (cm)**	**Time (Years)**
Vault 1/4	**< 1**	**1000**	**5**	**450**	**7.5**	**1000**
Vault 2	**16**	**1000**	**5**	**450**	**7.5**	**1000**

4.0 Code Performance Modeling Chloride Ingress

4.1 STADIUM@ CBP Web Application

Two examples of chloride ingress were run using the STADIUM@ CBP Web application:

1. A 1000 yr simulation of 100 cm of Saltstone waste material in contact with 20 cm of Vault 2 concrete with 100 cm of soil against the outside surface.
2. A 1000 yr simulation of 100 cm of Saltstone waste material in contact with 45 cm of Vault 1/4 concrete with 100 cm of soil against the outside surface.

Chloride ingress into the concrete takes place at the concrete soil boundary. To test code performance at a high concentration of chloride, the soil chloride concentration was increased from its nominal value of 4 ppm in SRS backfill to 350 ppm for the simulations. Results of the modeling are shown in Figure 4-1 for Vault 2 concrete and Figure 4-2 for Vault 1/4 concrete. For Vault 2 concrete the chloride ingress occurs at 1200 mm and for Vault 1/4 concrete at 1450 mm. Chloride ingress was tracked by plotting the STADIUM@ damage factor (scaled 0 – 3), the concentration of Chloride (Cl^-) ions (mmol/L), the concentration of mineral Cl-Al-HT_SS (g/kg), and total chloride (ppm). As noted above, the STADIUM@ damage factor is related to the formation of microcracks in the concrete (SIMCO, 2015b).

Examining Figure 4-1, concentrations of total chloride and the mineral phase Cl-Al-HT_SS show a steady progression from the soil boundary into the concrete over time and after 1000 years the tail of the Cl-Al-HT_SS peak is approaching full penetration of the concrete layer. After 1000 years of exposure, the chloride ion concentration in the concrete appears to be approaching a uniform value equal to the chloride concentration in the Saltstone waste (21.5 mmol/L). Because total chloride also responds to the presence of chloride in the Saltstone, it appears that using the concentration of Cl-Al-HT_SS provides the best indicator of chloride ingress into the concrete. For corrosion initiation, total chloride is usually tracked. In low chloride exposure cases, the ratio [Cl]/[OH] in pore solution is also a good parameter to track at the rebar location. The initial concentration of Cl-Al-HT_SS in the concrete was 0.014 g/kg. After 1000 years of exposure to a ground water concentration of 350 ppm chloride, the model predicts mineral concentrations of 14.2 g/kg at the soil boundary, 0.12 g/kg 10 cm into the concrete, and 0.033 g/kg at the concrete-Saltstone interface. Table 4-1 summarizes model predicted concentrations over time. It is apparent that chloride quickly penetrates the immediate surface layer and slowly migrates into the concrete. Note that the mineral phase Cl_Al-HT_SS may not indicate chloride attack on reinforced concrete but the simulation results appear to show it is a marker of chloride ingress.

The damage factor is essentially a peak at the concrete soil boundary and close to 1.0 throughout most of the concrete layer. Typically, chloride attack on concrete leads to corrosion of reinforcement bars which degrades the material. Reinforced concrete was not modeled in this test so it is not surprising that the damage factor did not indicate degradation in the concrete.

In Figure 4-2, similar trends are seen for the Vault 1/4 concrete as were observed for the Vault 2 concrete. The concentrations of total chloride, chloride ion and the mineral phase Cl-Al-HT_SS steadily increase in the concrete layer over time. As was seen for Vault 2, the concentration of chloride ion in the concrete is strongly influenced by the high concentration in the Saltstone. For Vault 1/4 concrete the damage factor appears to follow the Cl-Al-HT_SS concentration more closely than observed for Vault 2 concrete. Table 4-1 gives a summary of model predicted concentrations of the mineral phase Cl-Al-HT_SS at selected times for both concretes.

Table 4-1. STADIUM@ Web based model predictions of mineral phase Al-Cl-HT_SS concentration over time in Saltstone vault concretes.

Time (Years)	Depth of Concrete from Soil Boundary (cm)	Vault 2 Concentration of Al-Cl-HT_SS (g/kg)	Vault 1/4 Concentration of Al-Cl-HT_SS (g/kg)
0	0	0.014	0.005
	10	0.014	0.005
	20	0.014	0.005
	30		0.005
	45		0.005
100	0	13.5	6.5
	10	0.016	0.008
	20	0.016	0.005
	30		0.007
	45		0.011
300	0	13.7	10.8
	10	0.021	0.055
	20	0.018	0.014
	30		0.011
	45		0.013
500	0	13.8	12.9
	10	0.044	0.113
	20	0.020	0.027
	30		0.017
	45		0.015
1000	0	14.2	15.2
	10	0.118	0.228
	20	0.033	0.062
	30		0.033
	45		0.020

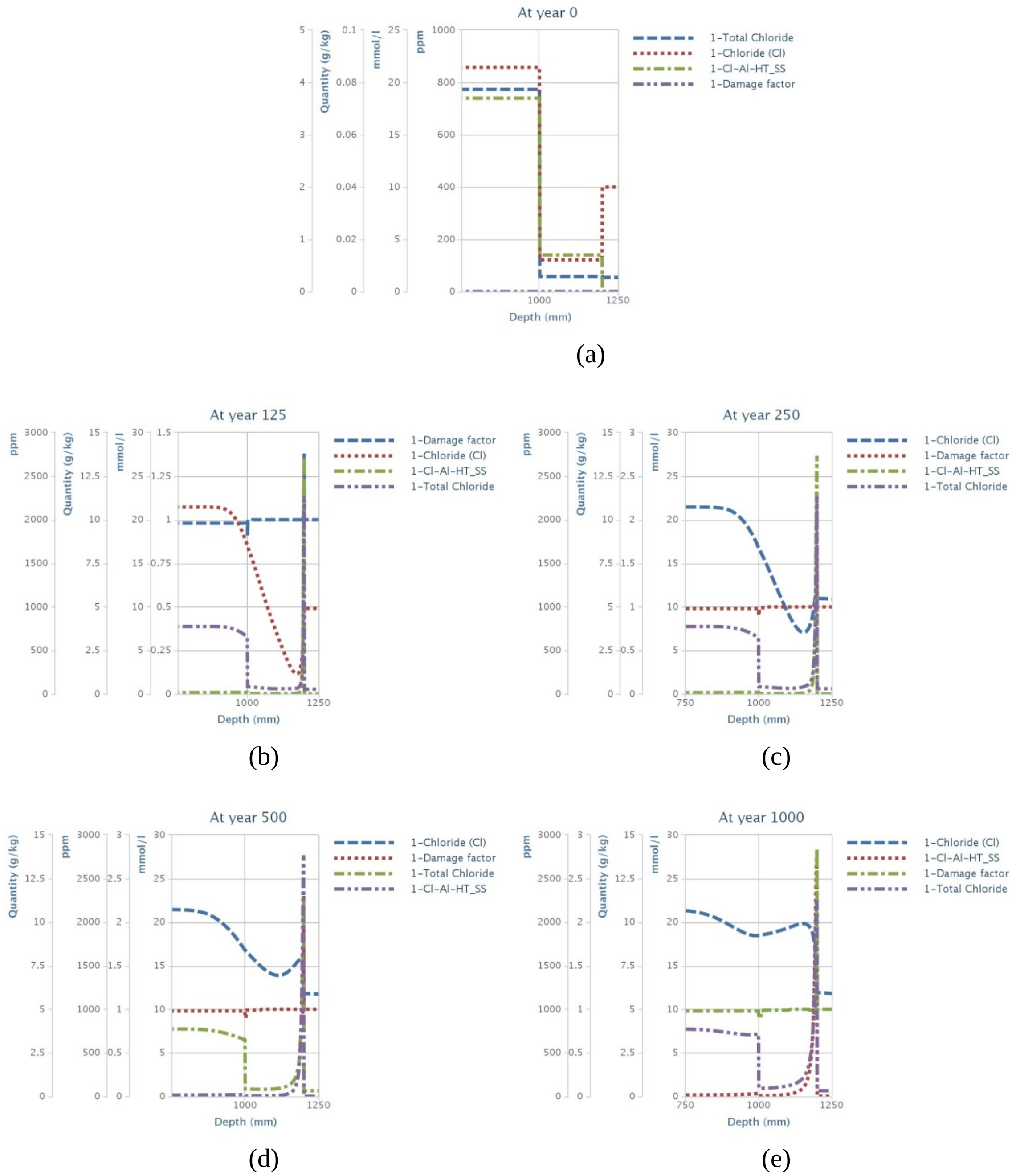
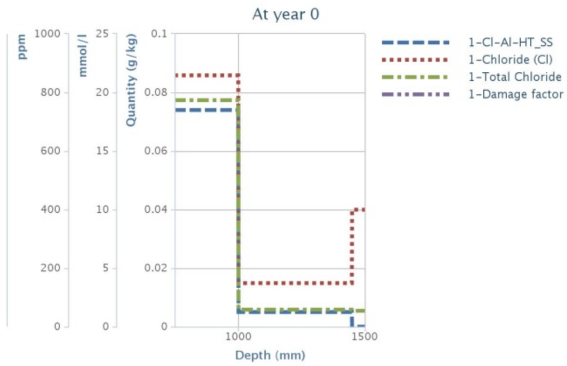
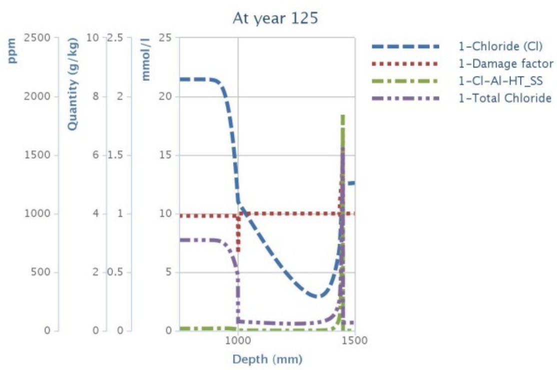


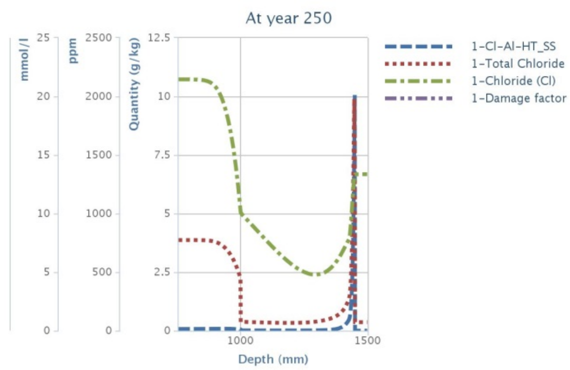
Figure 4-1. Progression of chloride ingress into 20 cm Vault 2 concrete over 1000 years predicted by STADIUM@ CBP Web application.



(a)



(b)



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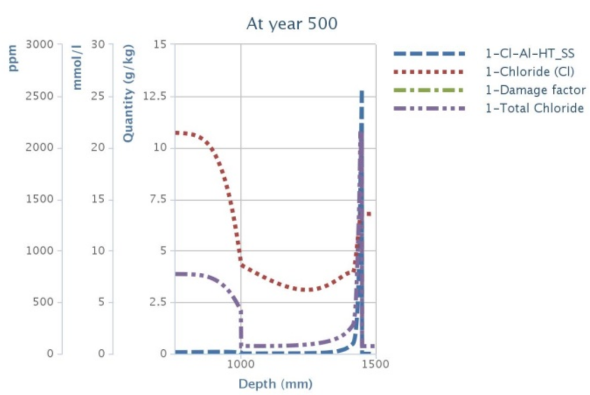

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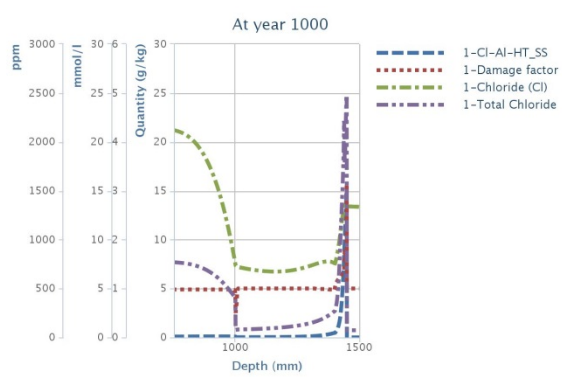


(e)

Figure 4-2. Progression of chloride ingress into 45 cm Vault 1/4 concrete over 1000 years predicted by STADIUM@ CBP Web application.

4.2 STADIUM@ CBP Toolbox Executable

Two examples of chloride ingress were run using the STADIUM@ CBP Toolbox executable (stadium_win_v2016a.exe):

1. A 1000 yr simulation of 100 cm of Saltstone waste material in contact with 20 cm of Vault 2 concrete with 100 cm of soil against the outside surface.
2. A 1000 yr simulation of 100 cm of Saltstone waste material in contact with 45 cm of Vault 1/4 concrete with 100 cm of soil against the outside surface.

The chloride concentration in the soil water was increased from the nominal concentration of 4 ppm to 350 ppm for the simulations to test code performance with a high chloride concentration. Input files used to make these simulations are provided in in a separate file that will be archived with this report and made available on request.

The CBP Toolbox Version 3.0 has been set up to plot calculated results for chemical species and minerals. STADIUM output contains other variables including: temperature, water content, pH, damage factor and total chloride. However, plots of these other parameters are not available in the current version of the Toolbox. Other plotting options will be included in future releases of the Toolbox. For purposes of this evaluation only a comparison of chloride and Al-Cl-HT_SS can be made. Results of the STADIUM@ modeling for these two variables using the executable version of the code and the CBP Toolbox plotting features are shown for Vault 2 concrete in Figure 4-3 and for Vault 1/4 concrete in Figure 4-4.

Visual comparison of the results plotted in Figures 4-3 and 4-4 with the results obtained using the STADIUM@ web application that are plotted in Figures 4-1 and 4-2 immediately indicates that the two sets of results are essentially the same. Table 4-2 provides a comparison of numerical values for selected results obtained using the executable version of STADIUM@ for the two types of concrete simulated. Comparison of Table 4-2 with the results shown in Table 4-1 confirms that results from both sets of simulations are essentially the same. This met the expected behavior that the two versions of the STADIUM@ code would produce the same result.

Table 4-2. STADIUM@ toolbox executable model predictions of mineral phase Al-Cl-HT_SS concentration over time in Saltstone vault concretes.

Time (Years)	Depth of Concrete from Soil Boundary (cm)	Vault 2 Concentration of Al-Cl-HT_SS (g/kg)	Vault 1/4 Concentration of Al-Cl-HT_SS (g/kg)
0	0	0.014	0.005
	10	0.014	0.005
	20	0.014	0.005
	30		0.005
	45		0.005
100	0	13.5	6.6
	10	0.016	0.008
	20	0.017	0.005
	30		0.007
	45		0.011
300	0	13.7	10.9
	10	0.022	0.049
	20	0.018	0.014
	30		0.011
	45		0.013
500	0	13.8	12.9
	10	0.045	0.116
	20	0.021	0.028
	30		0.017
	45		0.016
1000	0	14.2	15.2
	10	0.119	0.225
	20	0.033	0.064
	30		0.033
	45		0.021

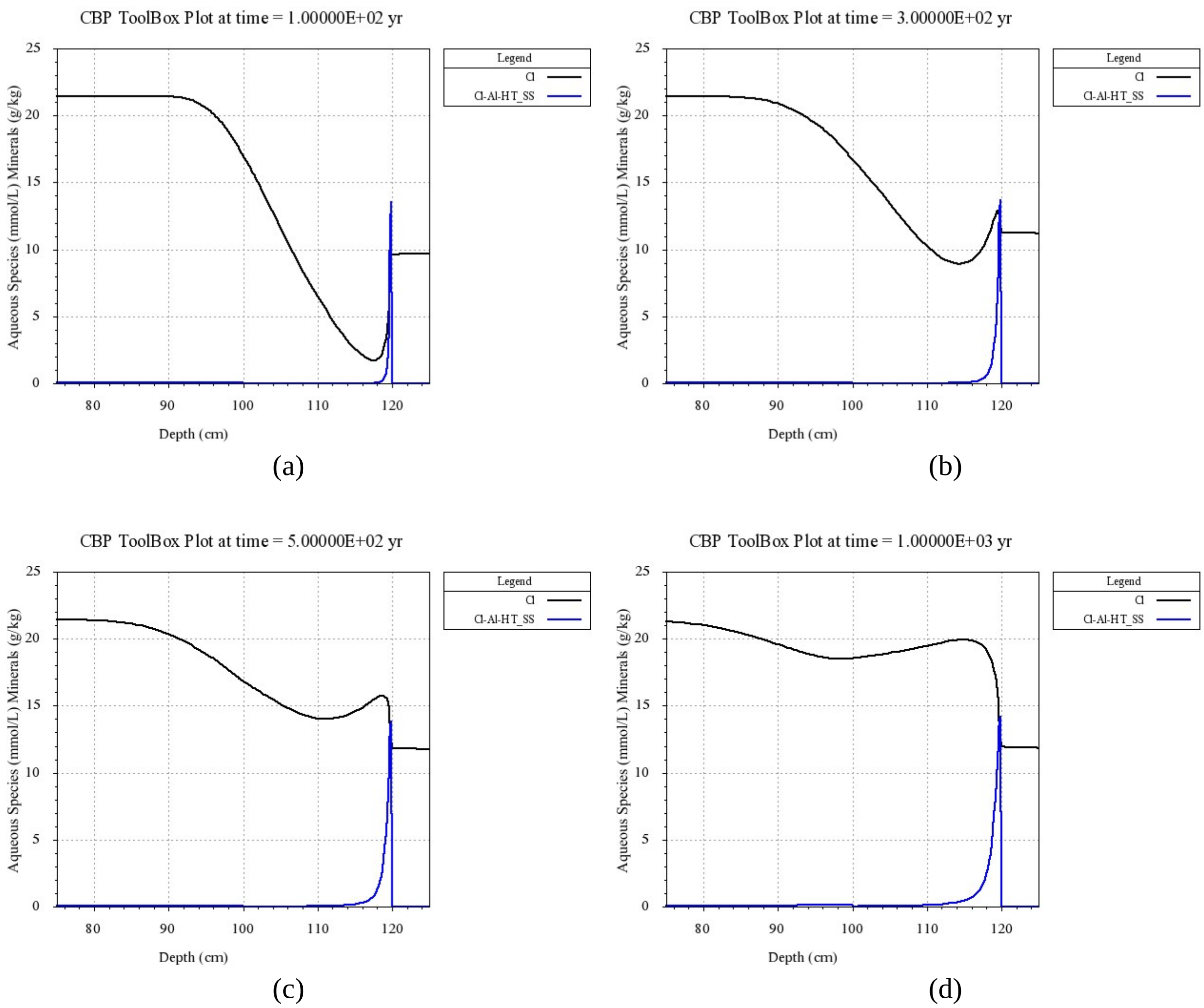


Figure 4-3. Progression of chloride ingress into 20 cm of Vault 2 concrete over 1000 years predicted by STADIUM[@] CBP Toolbox executable.

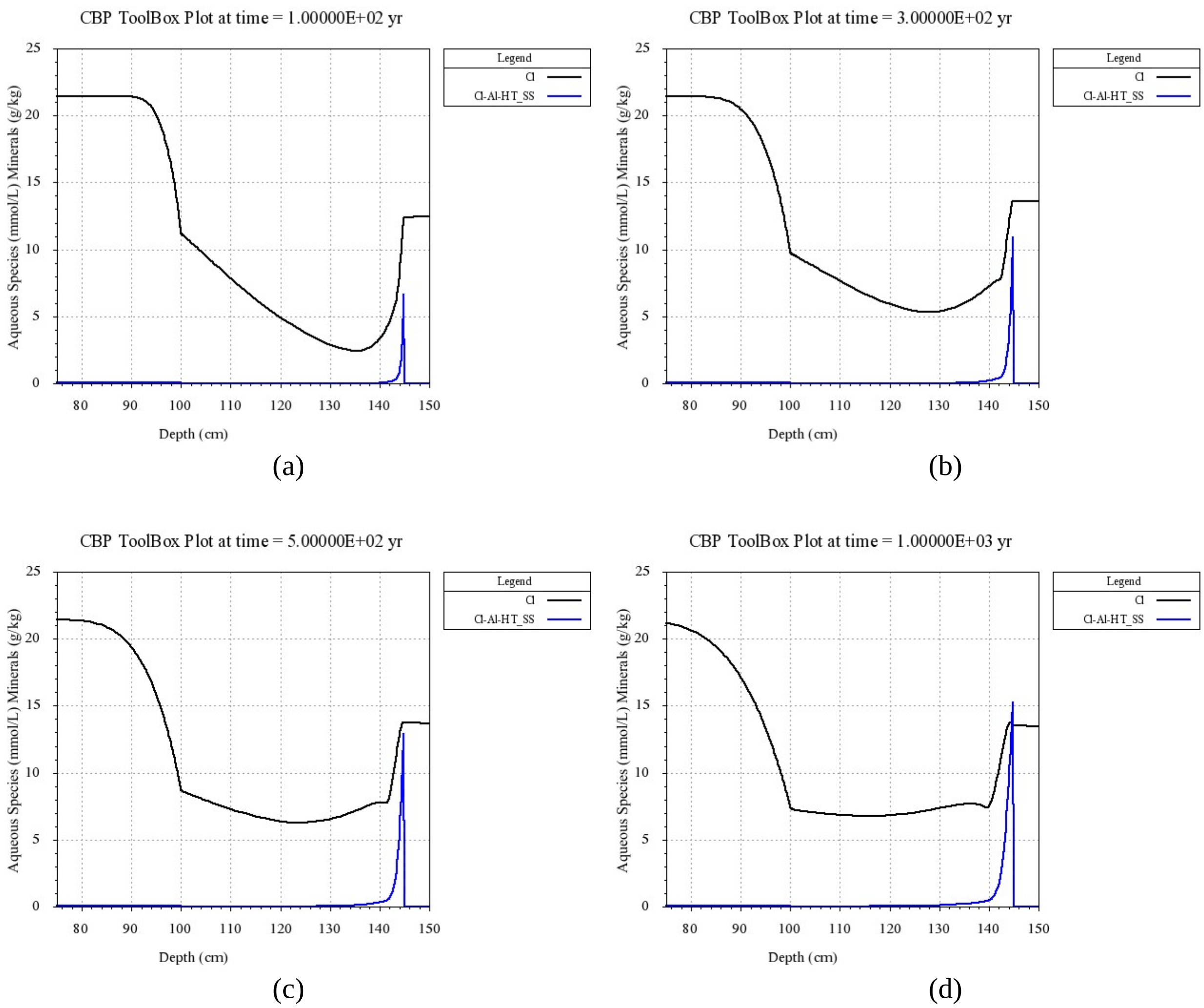


Figure 4-4. Progression of chloride ingress into 45 cm of Vault 1/4 concrete over 1000 years predicted by STADIUM[@] CBP Toolbox executable.

5.0 Code Performance Modeling Carbonation

5.1 STADIUM@ CBP Web Application

Two examples of cement carbonation under saturated conditions were run using the STADIUM@ CBP Web application:

1. A 1000 yr simulation of 100 cm of Saltstone waste material in contact with 20 cm of Vault 2 concrete with 100 cm of soil having a bicarbonate concentration of 250 ppm against the outside surface.
2. A 1000 yr simulation of 100 cm of Saltstone waste material in contact with 45 cm of Vault 1/4 concrete with 100 cm of soil having a bicarbonate concentration of 250 ppm against the outside surface.

Results from the simulations are shown in Figures 5-1 and 5-2. The Vault 2 concrete material is located from 1000 mm to 1200 mm in the simulation mesh and the surface in contact with soil where carbonation occurs is located at 1200 mm. The Vault 1/4 concrete material is located from 1000 cm to 1450 mm in the simulation mesh and the surface in contact with soil where carbonation occurs is located at 1450 mm. The soil layer with groundwater at the specified bicarbonate concentration is to the right of the concrete surface in both cases.

Examination of the numerical simulation output indicated that formation of calcite would be an indicator of carbonation in the concrete. Figure 5-1 shows that calcite in Vault 2 concrete quickly rose to a peak concentration of approximately 53 (mmol/L) at 125 years into the simulation then slowly increased to about 66 mmol/L at 1000 years while penetrating less than 2 cm into the concrete. These results would suggest that, after an initial reaction at the surface exposed to carbonate, carbonation in the Vault 2 concrete is a relatively slow process under the conditions assumed for the test case.

Figure 5-2 shows that Vault 1/4 concrete is more resistant to carbonation than Vault 2 concrete. At 250 years the calcite peak is about 0.47 (mmol/L) with little or no penetration into the concrete. At 500 years, the calcite peak in the concrete has decreased to about 0.1 (mmol/L). At 1000 years, the peak has increased to 35 (mmol/L) but the peak is still confined to within about one cm of the surface. The numerical results showed that while the calcite peak occurs within the concrete some calcite is in the soil immediately in contact with the concrete as well. This is likely from either calcite or calcite forming minerals leaching out of the concrete into the soil. No calcite was found in the soil during the Vault 2 test. For this case, the damage factor appeared to indicate concrete damage because it peaked at the same location as the calcite although the difference between the baseline and peak value of the damage factor was small. As noted previously, the STADIUM@ damage factor is related to the formation of micro cracks in the concrete (SIMCO, 2015a). The small damage factor may relate to a change in the concrete volume either through calcite formation or the dissolution of other mineral phases.

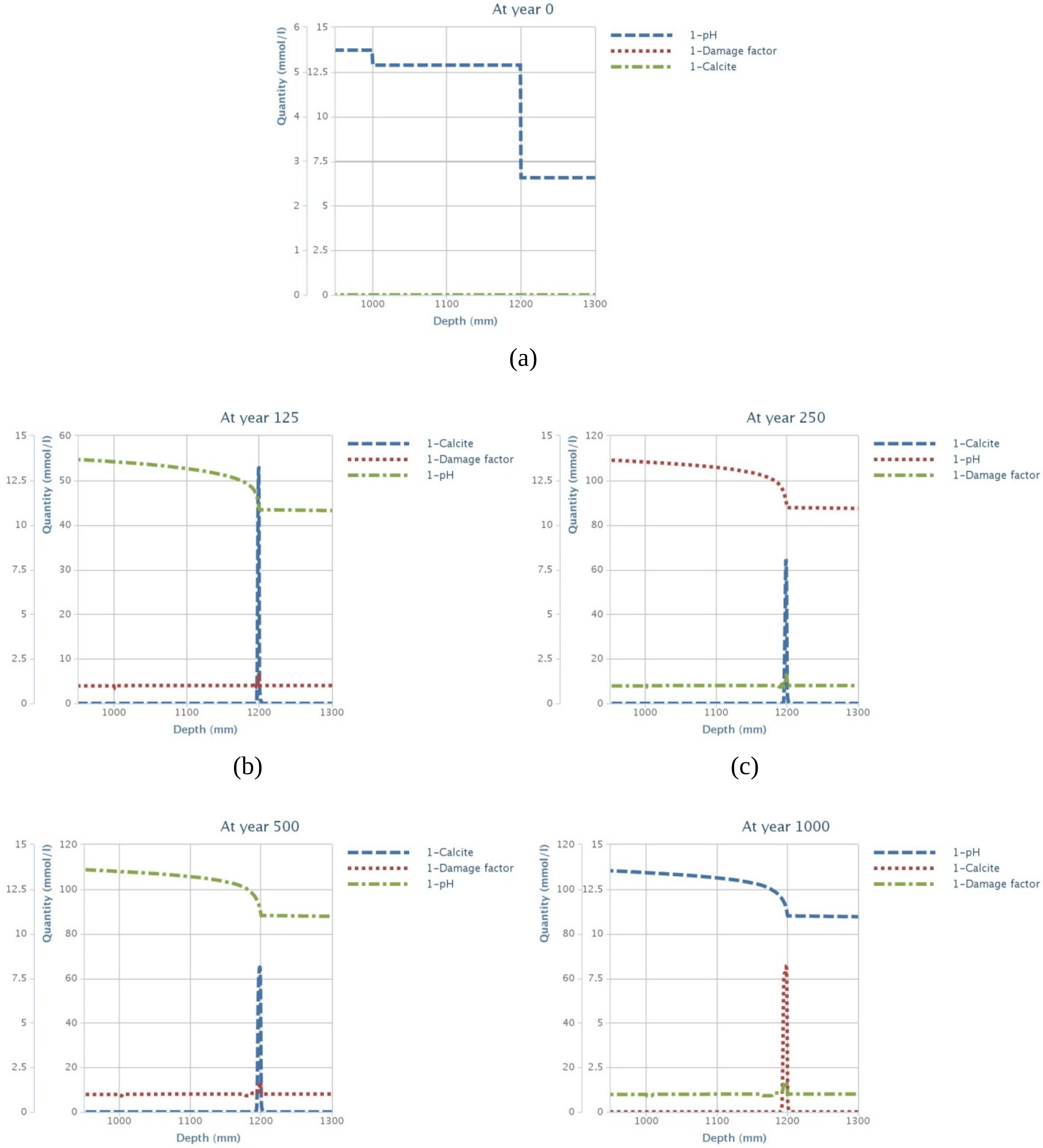


Figure 5-1. Carbonation progression in Vault 2 concrete over 1000 years predicted by STADIUM@ Web application.

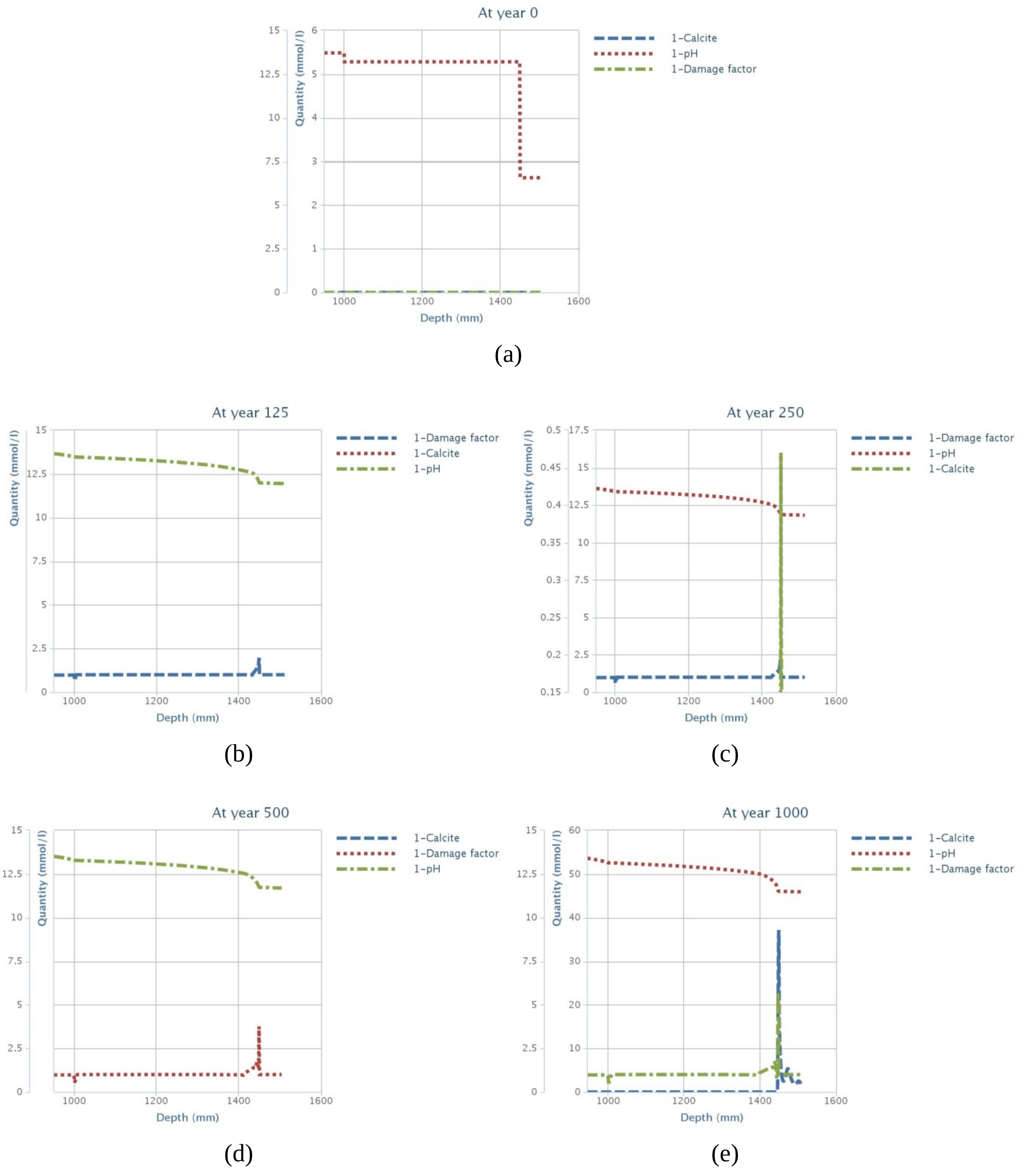


Figure 5-2. Carbonation progression in Vault 1/4 concrete over 1000 years predicted by STADIUM@ Web application.

5.2 STADIUM@ CBP Toolbox Executable

Two examples of carbonation under saturated conditions were run using the STADIUM@ CBP Toolbox executable code (stadium_win_v2016a.exe):

1. A 1000 yr simulation of 100 cm of Saltstone waste material in contact with 20 cm of Vault 2 concrete with 100 cm of soil having a bicarbonate concentration of 250 ppm against the outside surface.
2. A 1000 yr simulation of 100 cm of Saltstone waste material in contact with 45 cm of Vault 1/4 concrete with 100 cm of soil having a bicarbonate concentration of 250 ppm against the outside surface.

These tests are identical to the simulations run with the web application. Results from the simulations are shown in Figures 5-3 and 5-4. The Vault 2 concrete material shown in Figure 5-3 is located from 100 cm to 120 cm in the simulation mesh and the surface in contact with soil where carbonation occurs is located at 120 cm. The Vault 1/4 concrete material shown in Figure 5-4 is located from 100 cm to 145 cm in the simulation mesh and the surface in contact with soil where carbonation occurs is located at 145 cm. The soil with groundwater at the specified bicarbonate concentration is to the right of the concrete surfaces. For the Toolbox application it was only possible to plot the calcite concentration. The damage factor and other mineral phases will be included in the retrieved output in future revisions to the CBP Toolbox.

Figure 5-3 shows that, as expected, the calcite peak in Vault 2 concrete is very close to the solution obtained with the STADIUM@ Web application shown in Figure 5-2. The model predicts that the calcite mineral phase reaches a maximum concentration of about 70 g/kg around 300 years and then slowly grows into the concrete. After 1000 years of exposure, the calcite extends approximately one cm into the concrete. At 100 years and 300 years a Thaumasite peak is present slightly further into the concrete than the calcite. However, by 500 years this peak has disappeared.

An initial plot of the Vault 1/4 results showed a small calcite peak (<0.1 g/kg at 500 years) within the soil layer with no appreciable concentration in the concrete. Concentrations of several other minerals were then plotted as shown in Figure 5-4. From these plots, it can be seen that a relatively small Thaumasite peak grows in the concrete near the surface exposed to soil which may be an indicator of carbonation. While carbonation results from the two versions of the STADIUM@ model were in good agreement for Vault 2 concrete, the results were significantly different for Vault 1/4 concrete. SIMCO was able to trace the difference to the management of mineral phases in the chemical equilibrium module. They concluded that for carbonation results obtained with the GoldSim Toolbox interface are more reliable.

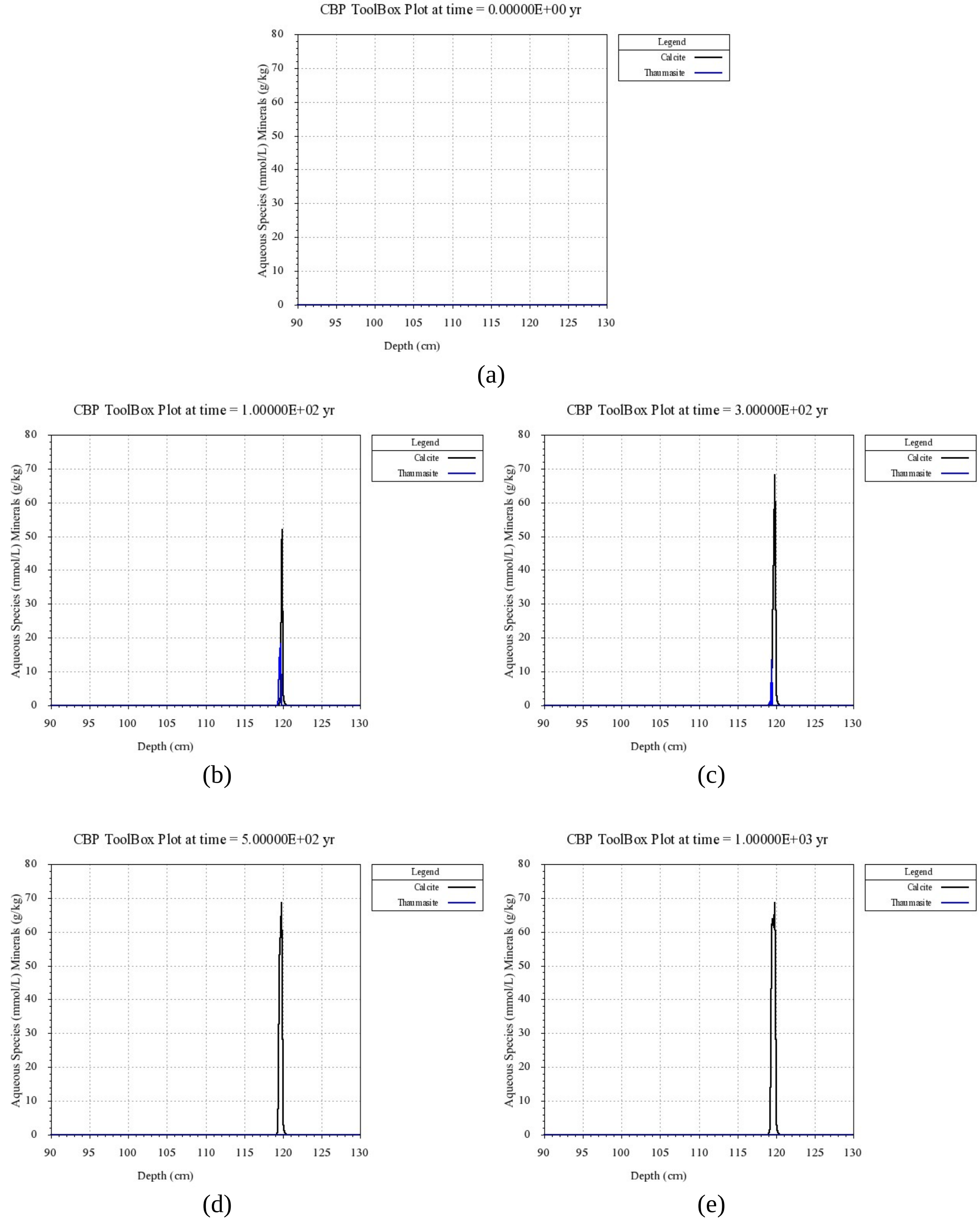
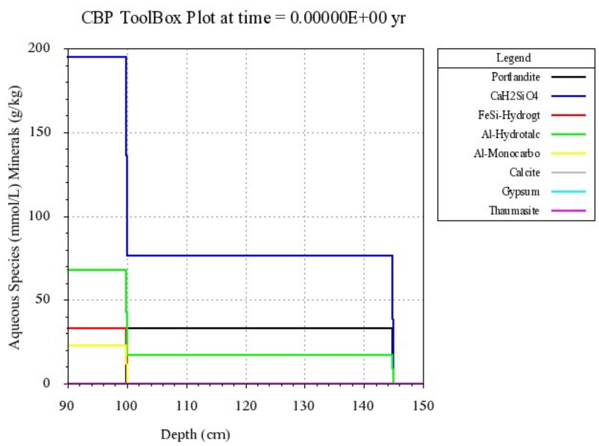
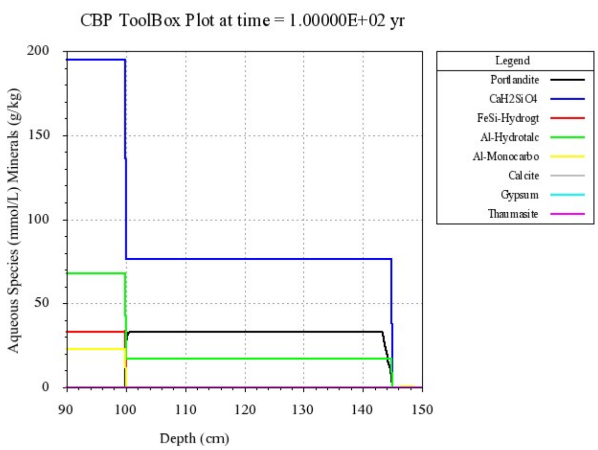


Figure 5-3. Carbonation progression in Vault 2 concrete over 1000 years predicted by STADIUM@ Toolbox application.



(a)



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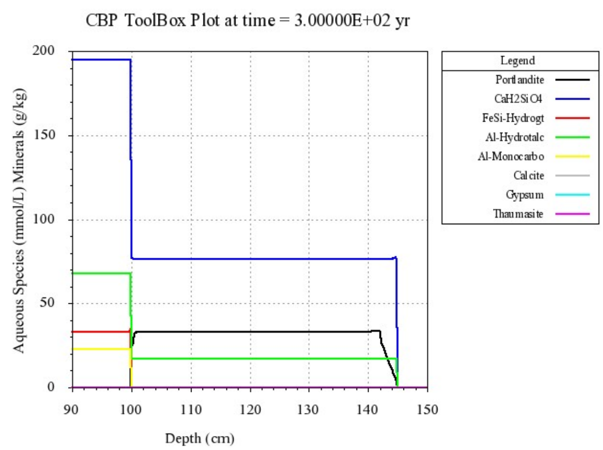

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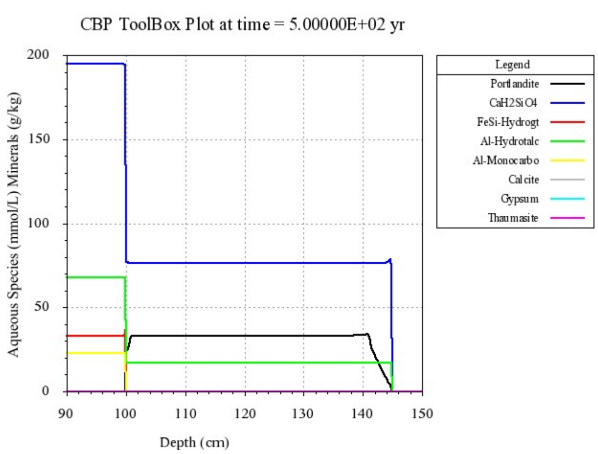

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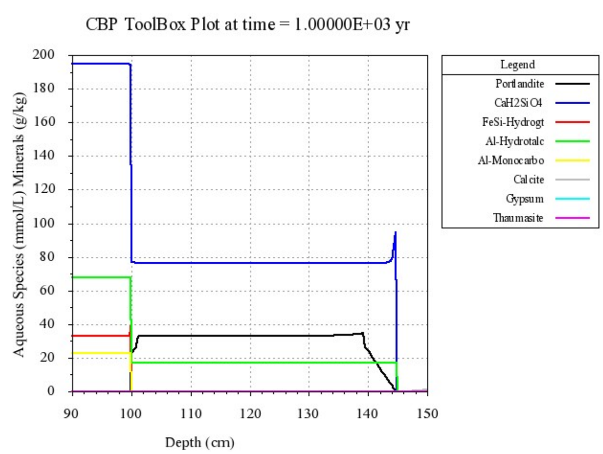


(e)

Figure 5-4. Carbonation progression in Vault 1/4 concrete over 1000 years predicted by STADIUM@ Toolbox application.

5.3 LeachXS/ORCHESTRA

Two examples of carbonation were run using the CBP Toolbox LeachXS/ORCHESTRA (ORCHESTRA-LXS 2013):

1. A 500 yr simulation of 50 cm of Vault 2 concrete in contact with 100 cm of soil.
2. A 500 yr simulation of 50 cm of Vault 1/4 concrete in contact with 100 cm of soil.

For both LXO simulations, water in the soil was in equilibrium with gas having an oxygen partial pressure of 0.2 atm and CO_2 at a partial pressure of 0.02 atm which is a high soil-gas CO_2 concentration. An infiltration rate of 14 in/yr, typical of conditions at the Savannah River Site, was used and the concrete saturation was set to 80%. Unlike for the STADIUM@ runs, because CO_2 is only slightly soluble in water, gas phase reactions will dominate the LXO carbonation calculation. The LXO Toolbox application required a minimum concrete thickness of 50 cm which was used in both example calculations. The LXO simulations were run for 500 years; however, the results at 450 years were the last values output (the LXO simulation ran for just slightly less than 500 years and failed to print output at the specified time).

Results from the simulations are shown in Figures 5-5 and 5-6. In this case, the surface where carbonation starts is located on the left-hand side of the plot where the concrete depth is zero. With LXO, calcite formation in the concrete appears to a reasonable marker for carbonation. Changes in the pH, also plotted in Figures 5-5 and 5-6, de-passivate concrete reinforcing members leading to cracking and rebar corrosion. Therefore, pH is the parameter of interest. The LXO model differs significantly from the STADIUM@ model of carbonation where the water carbonate concentration is specified and dissolved carbonate reacts with the concrete. The STADIUM@ carbonation calculations were performed under saturated conditions while the LXO simulations assumed 80% saturation.

The LXO results for the two concretes, plotted in Figures 5-5 and 5-6, appear to be almost identical. Examination of the numerical output showed only small differences in results for the two concretes. For example at 450 years, the calcite in Vault 2 concrete varies from 6.70 g/kg at the surface to 1.21 g/kg in the bulk of the concrete. For Vault 1/4 the variation is from a surface value of 6.50 g/kg to bulk value of 1.04 g/kg. Because the concrete formulations were different, this small difference between the two is somewhat surprising. The results are in general agreement with the STADIUM@ simulation for Vault 2 which shows a sharp peak in calcite at the surface and essentially no concentration in the bulk. However, the quantitative results are different by approximately a factor of 10 with STADIUM@ predicting the larger amount of calcite formation. As noted above, the LXO and STADIUM@ carbonation models use different boundary conditions and are controlled by different reaction mechanisms which make the results not directly comparable.

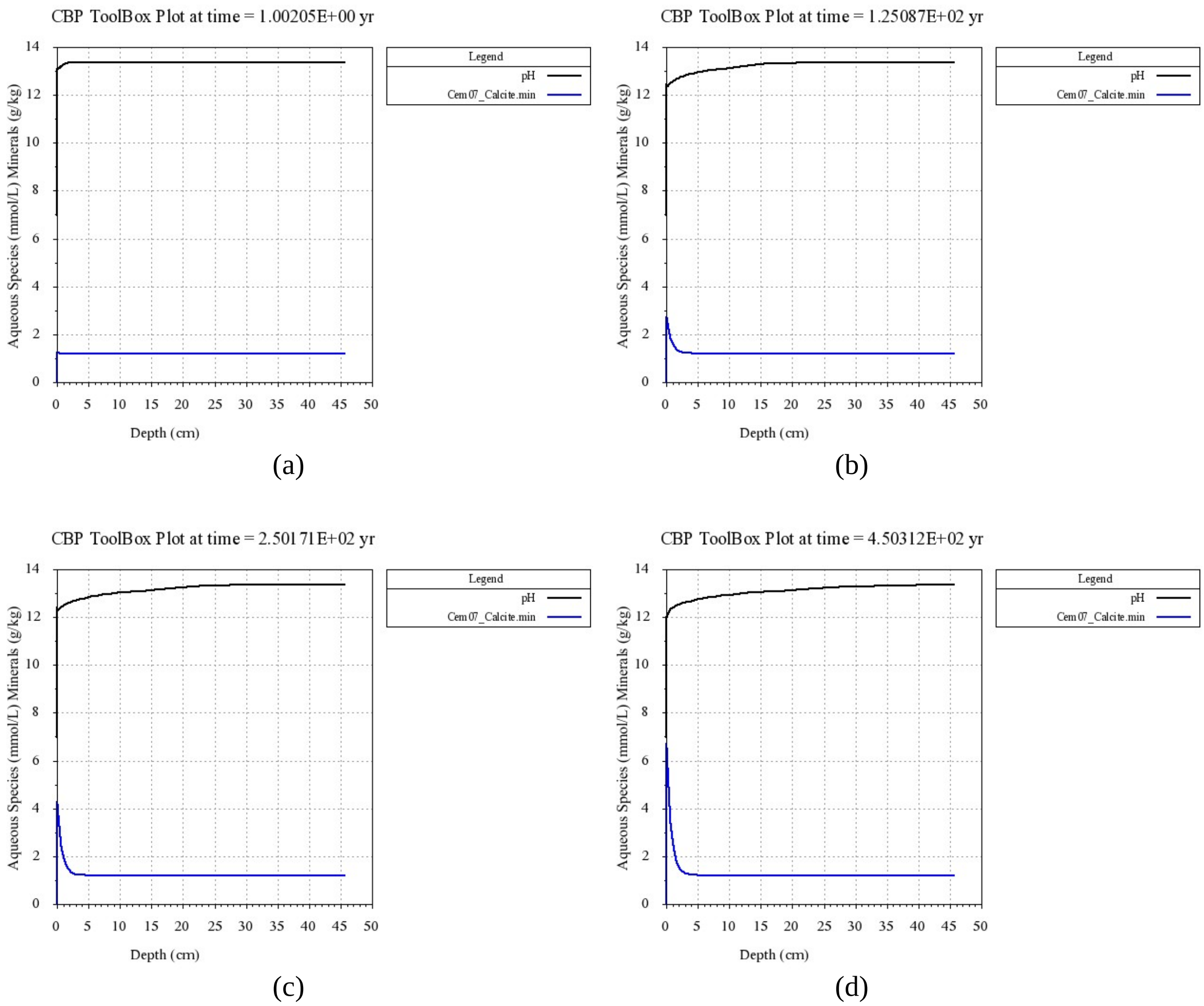
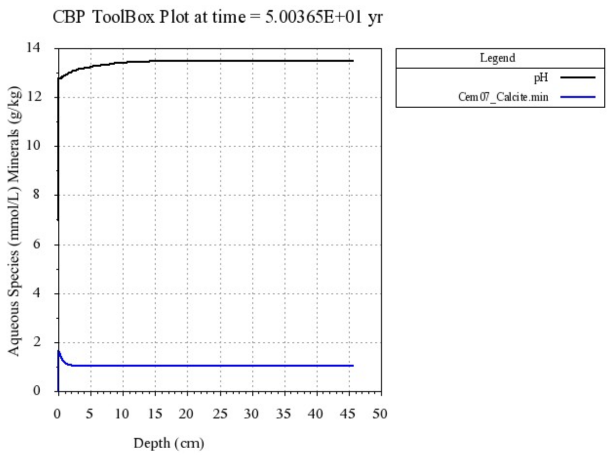
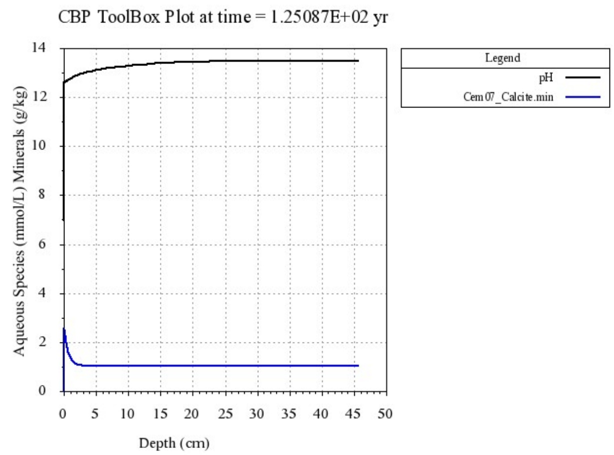


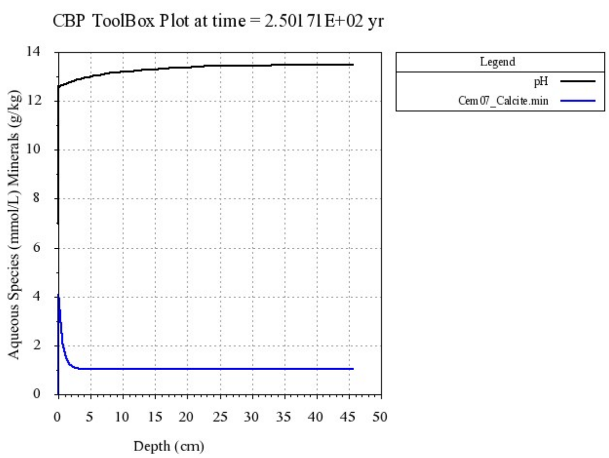
Figure 5-5. Carbonation progression in Vault 2 concrete over 450 years predicted by LeachXS/ORCHESTRA Toolbox application.



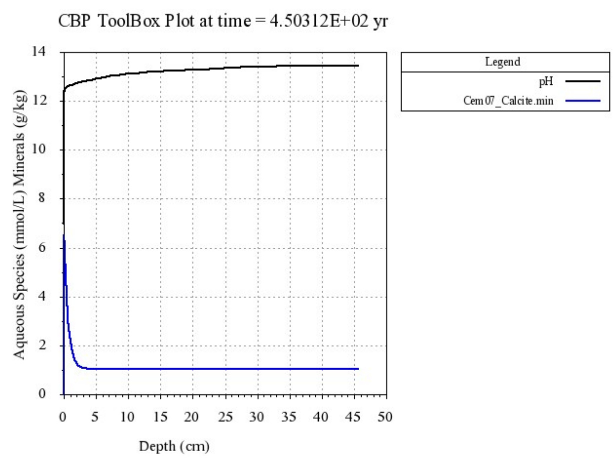
(a)



(b)



(c)



(d)

Figure 5-6. Carbonation progression in Vault 1/4 concrete over 450 years predicted by LeachXS/ORCHESTRA Toolbox application.

6.0 Conclusions

All of the planned tests on the CBP partner codes were successfully run. To give an estimate of the time required to make a simulation, run times obtained by SRNL are listed in Table 6-1. Of course, these times will depend on the computer used. The SRNL based STADIUM@ simulations were made on a high end Laptop capable of using eight threads (Dell Precision M6800 2.7 GHz 32 GB RAM). The LeachXS/ORCHESTRA runs were made on a Lenovo ThinkStation with Intel 2.0 GHz Xeon processors and 16 GB RAM. The STADIUM@ web application runs used the SIMCO Linux server. All of the run times were acceptable with the exception of the STADIUM@ Vault 2 pore solution test and the STADIUM@ Vault 2 carbonation run. The LXO run times were estimated from the simulation starting and ending times. Recording of this timing was missed for the Vault 2 sulfate attack run but was on the order of 16 hours like the other LXO simulations.

The STADIUM@ CBP web application was found to be easy to use with good documentation and good plotting capabilities. Using the web server has the obvious advantage that it does not tie up the user's personal computer to make extended runs thus facilitating long term simulations. Disadvantages to using the STADIUM@ CBP web application are the limited number of materials available, no direct link between the web application and the CBP Toolbox, and lack of the ability to perform uncertainty analysis. SIMCO is planning to include uncertainty analysis capabilities in the web application in the future. The remaining disadvantages are discussed further in the following paragraph.

The CBP Toolbox application uses Excel spreadsheets to define material compositions and properties with preset values for some materials. The user can modify these spreadsheet entries to simulate other materials as needed. In this respect, the CBP Toolbox is more flexible than the web application. Results from STADIUM@ web application runs can be downloaded as a Zip file to the Toolbox Template\Runs\Realization_0 folder. The user can then unzip the file and rename the Excel file containing simulation results into a name the Toolbox graphics function will recognize (e.g. stadium-3layers.xls). This file is in the same format as previous STADIUM@ CBP toolbox output and the Toolbox graphics have been modified to read the current list of chemicals and minerals and plot results. The extra steps involved to assessing the web based results are inconvenient and the results are not available within the GoldSim Toolbox itself for further analysis or uncertainty calculations.

Not all of the results obtained in this performance evaluation met expectations. In particular, results obtained with the STADIUM@ toolbox executable for sulfate attack and carbonation of Vault 1/4 concrete were different from those obtained using the STADIUM@ web application. In both cases, the web application appeared to give more reasonable results which were in general agreement with those obtained in previous simulations. Results of the testing have been shared with SIMCO but clearly their path forward is development of the web application and they understandably may not wish to divert resources to debugging the core executable used in the CBP Toolbox. Results for sulfate attack and carbonation of Vault 2 concrete and for chloride ingress into Vault 2 and Vault 1/4 concrete obtained with the STADIUM@ web application and core executable were in excellent agreement. This behavior may suggest a numerical problem with the Vault 1/4 sulfate attack and carbonation simulations using the executable; however, time was not available to pursue this further.

LeachXS/ORCHESTRA results for sulfate attack on Vault 1/4 concrete were different from those obtained in previous simulations. A new version of LXO is currently undergoing verification and validation testing and will be released soon. Until it is available, it is recommended that the original version of LXO (ORCHESTRA-LXS 2008) be used to model sulfate attack (Flach and Smith, 2013). Carbonation modeling in LXO is restricted to using at least 50 cm of concrete limiting the applicability of the results. For the evaluation testing, 50 cm of both Vault 2 and Vault 1/4 concrete were specified which did not match the true dimensions. Carbonation results for the two concretes were almost identical.

As noted previously, the code developers have provided validation testing of their codes in the respective QA documentation (SIMCO, 2015b and Meeussen and Brown, 2016). The validation results and the performance testing described in this report indicate that the codes can be used as a part of PA analyses. Further development of the STADIUM@ CBP web application and LXO are anticipated in the near future. The performance testing can be repeated when new versions are available. As was done by Flach and Smith (2013) to estimate Saltstone vault performance, best practice would be to run both models for the same degradation scenario and use the most conservative result in the PA.

Table 6-1. Simulation CPU Times

CBP Code	Simulation	Simulation Time (Years)	CPU Time (Hours)
STADIUM Web[1]	Vault 2 Sulfate Attack	1000	8.5
	Vault 1/4 Sulfate Attack	1000	46.1
	Vault 2 Chloride Ingress	1000	1.5
	Vault 1/4 Chloride Ingress	1000	44.8
	Vault 2 Carbonation	1000	176.1
	Vault 1/4 Carbonation	1000	50.9
	Vault 2 Pore Solution	250	128.6
STADIUM Toolbox Executable[2]	Vault 2 Sulfate Attack	1000	1.5
	Vault 1/4 Sulfate Attack	1000	18.6
	Vault 2 Chloride Ingress	1000	1.5
	Vault 1/4 Chloride Ingress	1000	18.8
	Vault 2 Carbonation	1000	51.4
	Vault 1/4 Carbonation	1000	14.6
LeachXS ORCHESTRA[3]	Vault 2 Sulfate Attack	500	~16.0
	Vault 1/4 Sulfate Attack	500	15.6
	Vault 2 Carbonation	500	16.0
	Vault 1/4 Carbonation	500	16.6

[1]SIMCO web based Linux server
[2]SRNL high end laptop
[3]SRNL Lenovo ThinkStation with Intel Xeon processors

All input and output files used in the testing described in this report are available in a separate file that will be archived with this report and available on request.

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