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A MODULE FOR GRAPHICAL DISPLAY OF MODEL RESULTS WITH THE CBP TOOLBOX

F. G. Smith, III

March 2015

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EXECUTIVE SUMMARY

This report describes work performed by the Savannah River National Laboratory (SRNL) in fiscal year 2014 to add enhanced graphical capabilities to display model results in the Cementitious Barriers Project (CBP) Toolbox. Because Version 2.0 of the CBP Toolbox has just been released, the graphing enhancements described in this report have not yet been integrated into a new version of the Toolbox. Instead they have been tested using a standalone GoldSim model and, while they are substantially complete, may undergo further refinement before full implementation. Nevertheless, this report is issued to document the FY14 development efforts which will provide a basis for further development of the CBP Toolbox.

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LIST OF ABBREVIATIONS

CBP	Cementitious Barriers Partnership
DLL	Dynamic Link Library
DOE	Department of Energy
GTG	GoldSim Technology Group
LXO	LeachXS/Orchestra
SRNL	Savannah River National Laboratory
STADIUM	Software for Transport and Degradation in Unsaturated Materials

1.0 Introduction

Modifications to the CBP Toolbox documented in this report involved improvements to the code integration functionality. The current version of the CBP Toolbox (Version 2.0) allows the user to run either a version of the STADIUM® code (SIMCO, 2010) to model sulfate attack or chloride ingress on cementitious materials or a version of the LeachXS/Orchestra code (ECN, 2007; Meeussen, 2009) to model sulfate attack, carbonation, or percolation with radial diffusion in cementitious materials. A user interface to these CBP partner codes was developed using the GoldSim software (Brown and Flach, 2009; Smith et al. 2010a; Smith et al. 2013).

GoldSim provides a graphical programming environment with features amenable to integrating individual modules into a cohesive framework. Connections between the GoldSim interface and CBP partner codes were created using a general Dynamic Link Library (DLL) interface developed as part of the CBP modeling effort. The overall concept behind this development was to use GoldSim as the top level software with interfaces to external partner codes for specific calculations. The DLL that accomplishes the code linking performs the following functions:

1) Collection of code inputs such as initial mineral and chemical concentrations within GoldSim.
2) Creation of input files to be used by the external application.
3) Execution of the modeling code external to GoldSim.
4) Returning output of model results read from files created by the external applications back to GoldSim for further processing.

Instructions for creating the input file, running the external code, and reading the output are contained within a user created file that is read and interpreted at runtime by the DLL. The design and functionality of the DLL interface has been described in detail by Smith et al. (2010a).

2.0 Results and Discussion

Version 1.0 of the CBP Toolbox used GoldSim plotting options to display results of model calculations. While STADIUM and LeachXS/Orchestra save results at multiple times during a simulation, the CBP Toolbox assumed that the user passes results at only one time (usually, but not necessarily, the last time in the calculation) back to GoldSim. Within GoldSim, aqueous and mineral concentrations are stored in vector arrays dimensioned by the maximum allowed nodes in the mesh. Therefore, the GoldSim plots of model data showed concentration as a function of computational node at one simulation time. Computational nodes are not necessarily evenly spaced so, with uneven node spacing, the GoldSim plots gave a distorted view of the spatial concentration distribution. It was also frequently difficult to read the node numbers along the x-axis without editing the plot. GoldSim plots were only available following completion of a simulation when GoldSim was in result mode and were lost when the CBP Toolbox was returned to edit mode to perform another set of calculations.

To enhance the display of model results, Version 2.0 of the CBP Toolbox used a Fortran application that employed the Gnuplot open source software to plot results from STADIUM and LeachXS/Orchestra calculations. The Fortran program read data directly from output files created by the partner codes. Therefore, if there were either pre-existing STADIUM or LeachXS/Orchestra output files in the Runs/realization_0 directory, the revised Toolbox could display plots of these results without performing new model calculations. Two types of plots were available, a two-dimensional plot (x-y plot) of model results from the last calculation time and a three-dimensional plot (surface plot) of model results at each saved time. This enhancement provided modest improvement over the initial GoldSim based plotting.

While the plots created with Gnuplot were better formatted and easier to read the two-dimensional plotting was limited by only displaying results for the last time step and the plotting could not display results from stochastic runs.

An enhanced interface to the CBP Toolbox has now been developed that allows the user much greater flexibility to plot results from Stadium and LeachXS/Orchestra model calculations. A schematic representation of the plotting interface is shown in Figure 2-1. Running the CBP partner codes using the CBP Toolbox generates output files which are placed in the **Runs** directory. The plotting interface is currently a separate GoldSim model named **CBP_Plotting** that can either be run from within the Toolbox or externally to the CBP Toolbox to plot data from preexisting model runs. The interface contains four dashboards which are described below and a DLL link to a set of Fortran codes. The dashboards allow the user to specify the type of plot to be created and to choose various plotting options. This information is passed from the GoldSim plotting application to the Fortran programs through the DLL. The Fortran programs read data files created by the CBP partner models, write instruction files for plotting the data using the Gnuplot open source software, and call Gnuplot which then creates the plots. The standalone graphics program could be distributed for use with Version 2.0 of the CBP Toolbox and will be incorporated into the next release of the Toolbox.

The GoldSim CBP Plotting Interface is described in Section 2.1 and several examples plots are presented in Section 2.2.

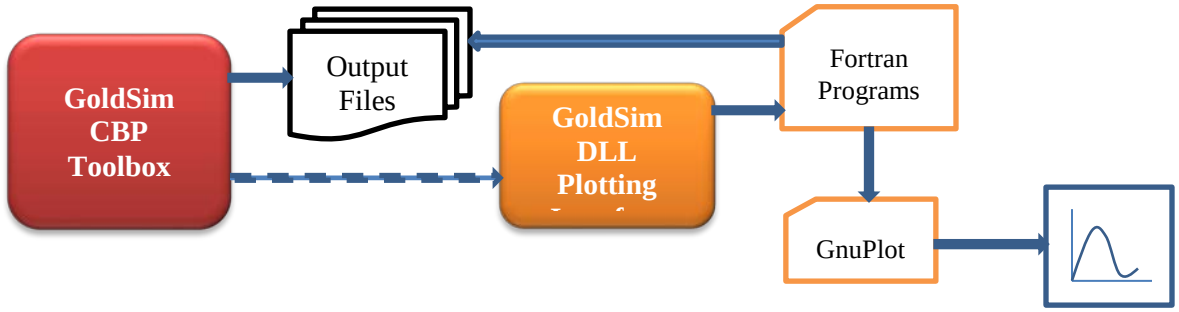

Figure 2-1. Schematic representation of CBP plotting.

2.1 Plotting Interface

Figure 2-2 shows the main dashboard that appears when the plotting application is started. As noted above, the CBP plotting interface is specifically designed to plot results from Stadium and LeachXS/Orchestra model calculations. Each code has its own data formatting and the Fortran programs have specific coding to read output files from either application. Therefore, the first plotting option is to specify the model that generated the data to be plotted.

Following model selection, the user specifies the type of plot to be made. Five types of plots are available:

1. An x-y plot for multiple variables where x is the model material distance and y is the variable being plotted at a user specified simulation time and for a user specified realization.
2. An x-y plot for multiple variables where x is the simulation time and y is the variable being plotted at a user specified model material distance and for a user specified realization.

3. A three-dimensional surface plot for a single variable where x is the material distance, y is the simulation time, and z is the variable being plotted for a user specified realization.
4. An x-y plot of multiple realizations for a single variable where x is the material distance and y is the variable being plotted at a user specified simulation time.
5. An x-y plot of multiple realizations for a single variable where x is the simulation time and y is the variable being plotted at a user specified material distance.

While the user must enter a plot time for the first and fourth type of plot and a plot material distance for the second and fifth type these values do not need to be exactly the same as times or distances appearing in the model output. The application will select the time or distance in the output nearest to the requested value for plotting. If the entered value is greater than the last output value the last output will be plotted.

After specifying the plot type, the user selects the output species (and/or properties for LeachXS) to plot. Figure 2-3 shows the dashboard display for Stadium plotting. Two lists appear on the Stadium dashboard. The list on the left contains the 11 Stadium aqueous species available for plotting and the list on the right contains the 10 Stadium mineral species. The use can select up to a total of 20 species for plotting by clicking check boxes from either list. The limit of 20 plots on one graph is arbitrary and can be increased if desired. Figure 2-4 shows the dashboard display for LeachXS/Orchestra plotting. In this case six lists appear. The list in the upper left contains 11 LeachXS aqueous species available for plotting, the list in the top middle contains 10 LeachXS minerals, and list in the upper right contains 26 Cem07 minerals. The list in the lower left contains 7 LeachXS properties, the lower middle list contains 19 LeachXS solids, and the list in the lower right contains 14 Cem07 solids. Up to a total of 20 items can be selected from any of the lists for plotting on a single graph.

If more than 20 items are selected for plotting the error message “too many materials selected” will appear and the GoldSim plotting application will stop. Similarly if no materials are selected or if all of the materials selected do not appear in the output file the error message “no material was selected” will appear and the GoldSim plotting application will stop. The last error is primarily applicable to LeachXS/Orchestra which is very flexible such that the species list for a model run can be easily changed. However, a fixed list of species had to be used for the selection and plotting process. Therefore, some species in the selection lists may not appear in the model output. In this case, the plotting code eliminates the missing species from the plotting list and does not report an error unless there are no species left to plot. A complete list of the Stadium and LeachXS/Orchestra species include in the plotting routines is provided in the Appendix.

As shown in Figures 2-3 and 2-4, both species selection dashboards include a “**Reset**” button that can be used to clear existing selections.

Next, as shown in Figure 2-2, the user specifies the GoldSim realization(s) to be plotted. When either of the first two types of plots is selected, the realization number entered into the “First” box determines the data that will be plotted. For deterministic calculations Realization Number 0 must be used. The last two types of x-y plots allow the user to plot results for a single variable from multiple realizations created by probabilistic simulations. In this case the plotted realizations will start with the realization entered into the “First” box and end with the realization number entered into the “Last” box. If more than 20 realizations are specified, the error message “too many realizations selected” will appear and the GoldSim plotting application will stop. Because many more than 20 realizations may have been run, multiple plots may be required to show all of the results or the maximum number of plots appearing on a single graph may need to be increased. Alternatively, the application could be programmed to plot summary results from the probabilistic runs such as the mean, median, maximum, minimum, and ±95% and ±50% confidence interval values. This option is not currently available.

After these basic plotting selections have been made, the user has some limited control on the format of the plot. Pressing the "**Plot Options**" button displays the dashboard shown in Figure 2-5. Figure 2-5 shows the configuration for 3-D plots when all of the controls are active. The "Default" button in the upper right can be used to reset plot options to the default values shown in the figure. Using this dashboard, the user can specify the following plotting options:

1. Minimum and maximum values for the plot axes and use of a logarithmic scale on the axis. If zero (0) is entered in both boxes, Gnuplot will automatically select plotting limits. The best use of this feature is to first view an unrestricted plot and then set axes limits and recreate the plot to better view details in a specific region of the output. A logarithmic scale is particularly useful for long simulation times and if variables with significantly different values are to be displayed. The user can also enter the plot rotation in degrees about the x and z axes for 3-D plots.
2. Plotting styles:
    a. Use of lines, points, or both lines and points to display x-y data.
    b. Use of surfaces (lines), solid surfaces, or surfaces with contours to display three-dimensional data.
3. The user can enter integer values of the line width.
4. The user can check a box to save the plot as a JPEG image. Images are saved in the folder where the plotting application has been run (*Template* folder) and are given a unique name using the date and time and may be renamed by the user with more meaningful descriptors.

After entering plotting arguments through the dashboards the user clicks on the "**Display Plot"** button to initiate a screen display of the plot. After the "**Display Plot**" button is pressed, the user must also perform the following steps:

1. If the plot does not appear, click the "**Run**" button in the GoldSim Run Controller box. Note that Gnuplot displays x and y coordinates as the mouse is moved over x-y plots and surface plots can be rotated by holding down the left mouse button and moving the mouse. The rotation values appear in the lower left hand corner of the plot.
2. When finished viewing the plot, close the plot by clicking on the command window that appears behind the plot and pressing the enter key.
3. Acknowledge the "Simulation Complete!" message.
4. Click the "**Edit**" button in the GoldSim Run Controller box to allow changing values for another plot.
5. Acknowledge the "Exit Result Mode" dialog box by clicking on the "**OK**" button.

To exit the plotting model, close the GoldSim application.

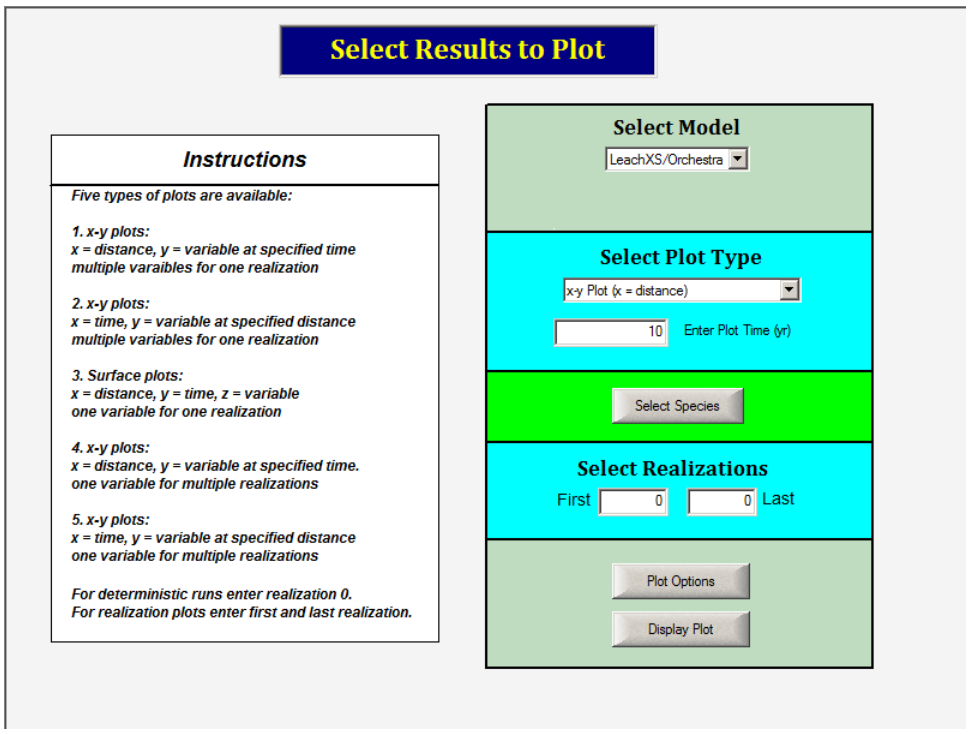

Figure 2-2. Dashboard display for Stadium plotting.

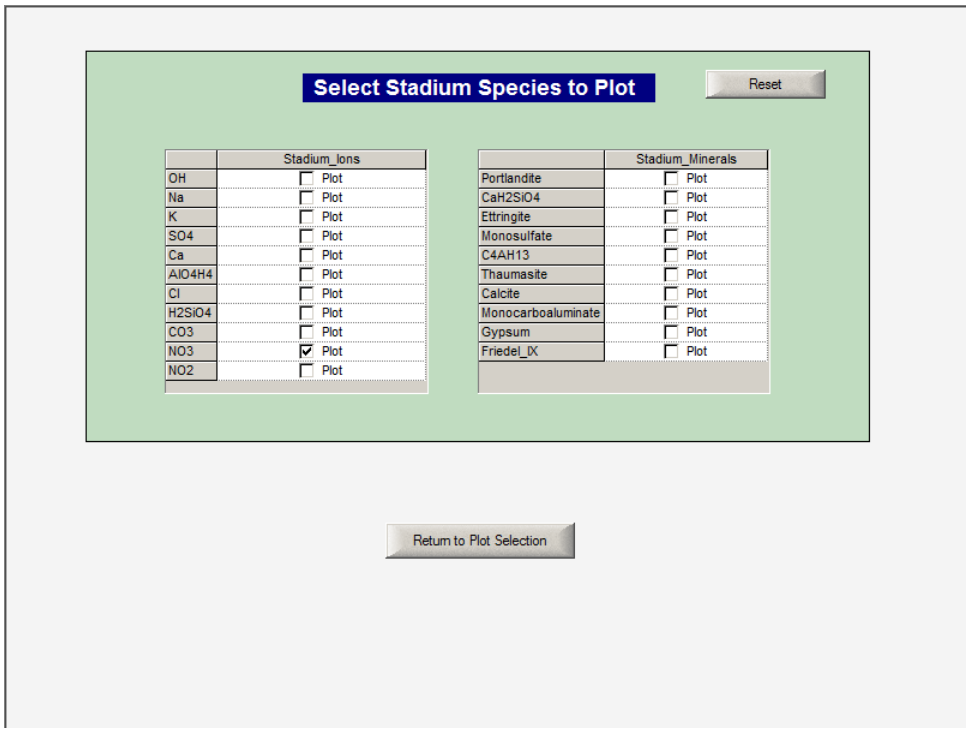

Figure 2-3. Dashboard display for selecting Stadium species to plot.

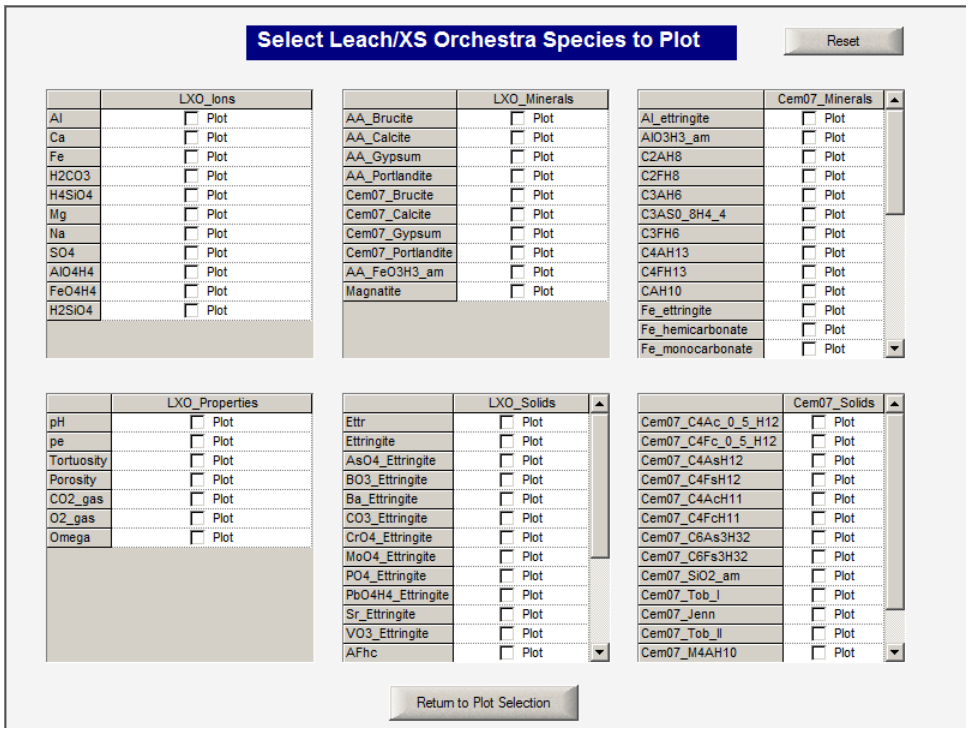

Figure 2-4. Dashboard display for selecting LeachXS/Orchestra species to plot.

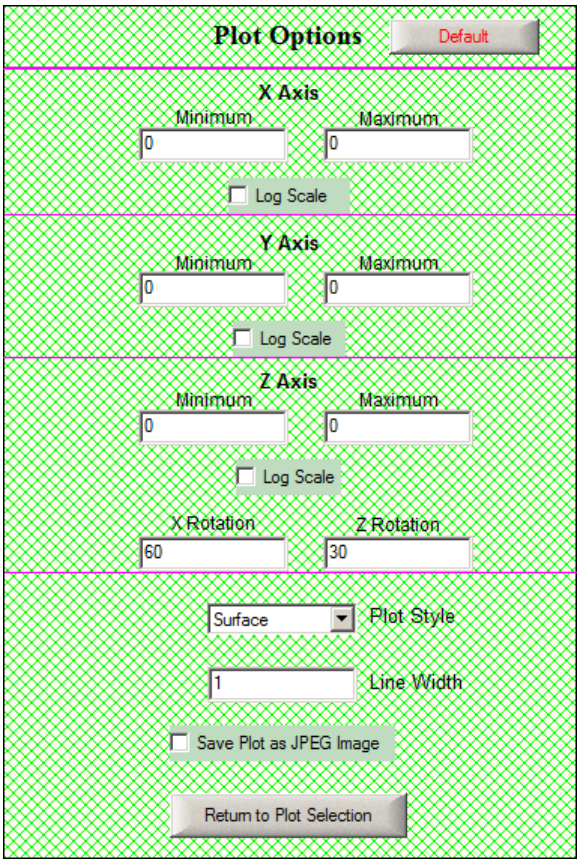

Figure 2-5. Dashboard display for selection of plotting options.

2.2 Example Plots

A few examples demonstrating the improved plotting capabilities are shown in Figures 2-6 through 2-12. Figure 2-6 shows a surface plot of results from a Stadium run. A short 10 year simulation was used to quickly create these model results. The model domain was 120 cm of Saltstone interfacing with a 20 cm concrete wall. The results show transport of nitrate from the Saltstone into the concrete over the 10 year simulation. Figure 2-7 shows a plot of five aqueous species and five mineral concentrations over the model domain after 10 years of simulation. Because the change in composition is confined to the Saltstone-concrete interface and there are large differences in the magnitude between the concentrations, the data is replotted in Figure 2-8 using the plot settings:

$X_{min} = 100$, $X_{max} = 140$
$Y_{min} = 0.0001$, $Y_{max} = 10000$
Log Scale Y axis

Similar plots of LeachXS/Orchestra results are shown in Figures 2-9 and 2-10. In Figure 2-9, one item has been selected for plotting from four of the LeachXS/Orchestra lists shown in Figure 2-4. Since it is again difficult to see some details of the results, the data is replotted in Figure 2-10 using a log scale on the Y axis, setting the maximum X axes range to 4 cm and plotting points and lines to indicate the simulation nodes.

Figure 2-11 shows an example of plotting dissolved Al^{+3} concentration from three realizations calculated with the LeachXS/Orchestra model.

Figure 2-12 shows six example plots demonstrating different 3-diemsnional views of data generated from a trial run of LeachXS/Orchestra. The six plots in Figure 2-12 are:

a) A surface plot of the LeachXS/Orchestra data as it originally appears without user formatting.
b) A plot of the data with the maximum x-axis value set to four.
c) A plot of the data using a logarithmic x-axis with minimum and maximum values set to 0.1 and 10, respectively.
d) Shows a 3-dimensional solid representation of the data.
e) Rotates Figure 2-12 (b) from the default (60°, 30°) to (70°, 20°).
f) Changes the minimum z-axis value to -1.5 (note that a maximum z-axis value of 2.5 must also be specified when the minimum value is set) and adds a contour of the surface which appears on the lowest z plane.

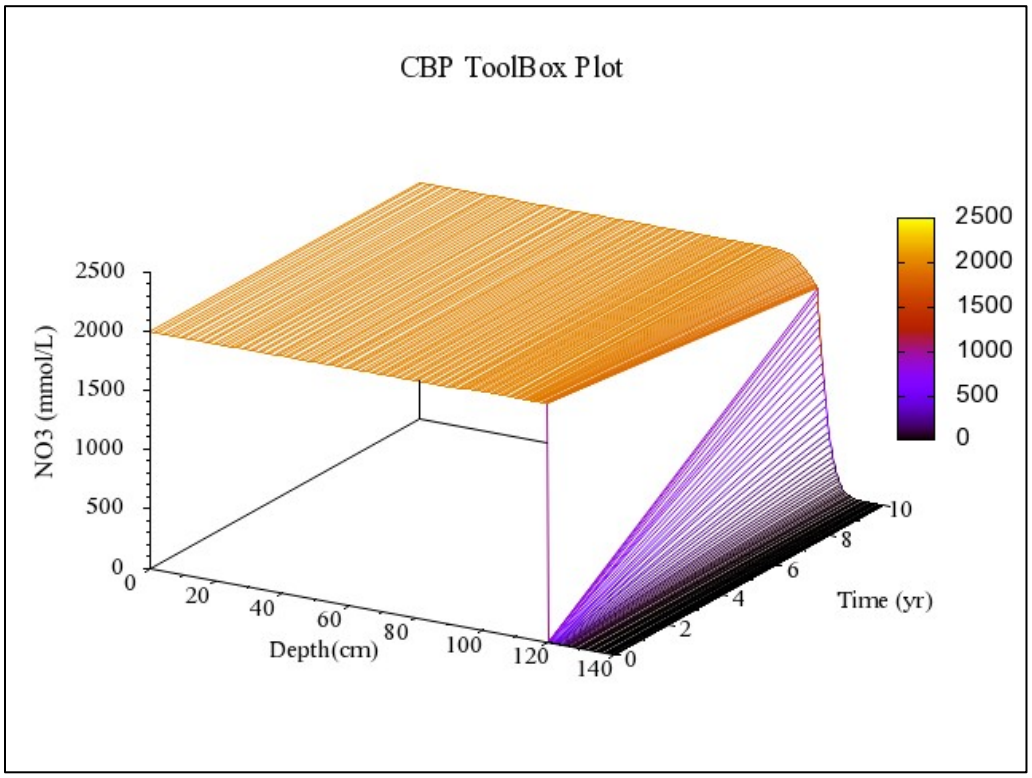

Figure 2-6. Example surface plot of Stadium output.

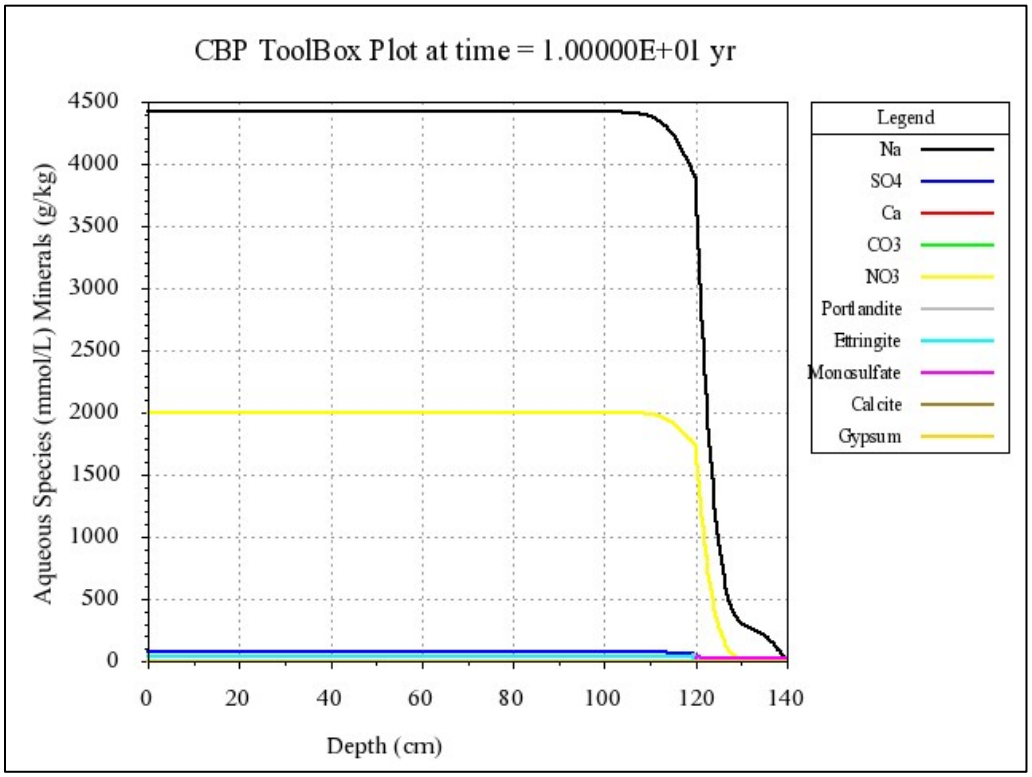

Figure 2-7. Example x-y plot of Stadium aqueous and mineral concentrations.

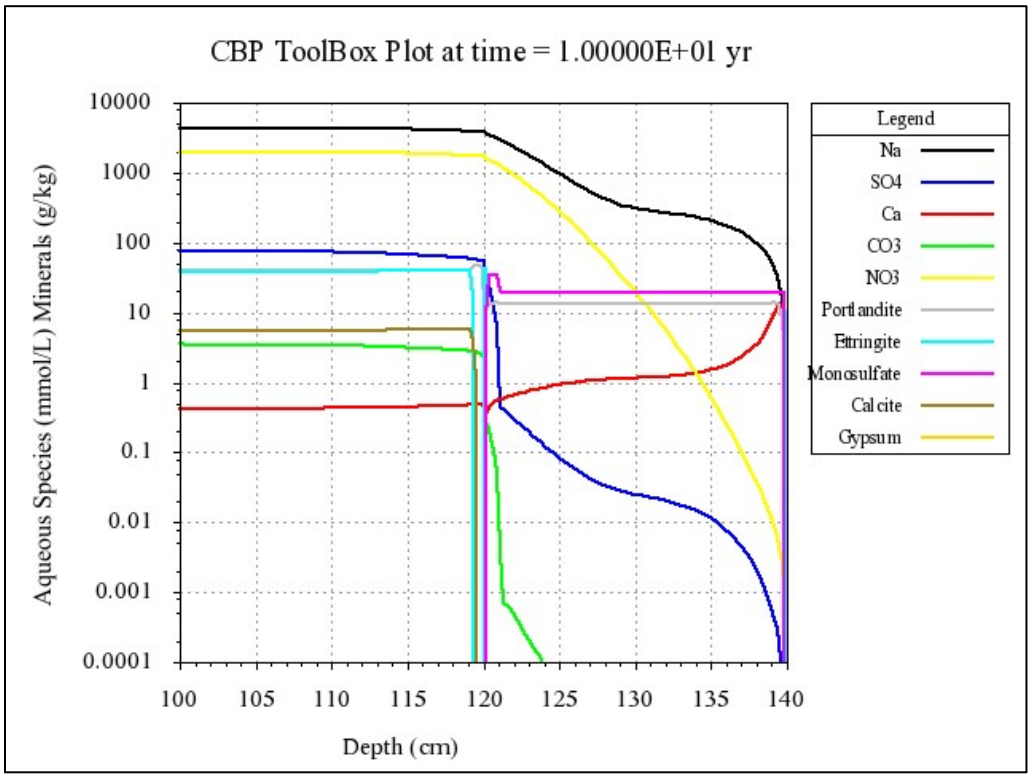

Figure 2-8. Rescaled example x-y plot of Stadium aqueous and mineral concentrations.

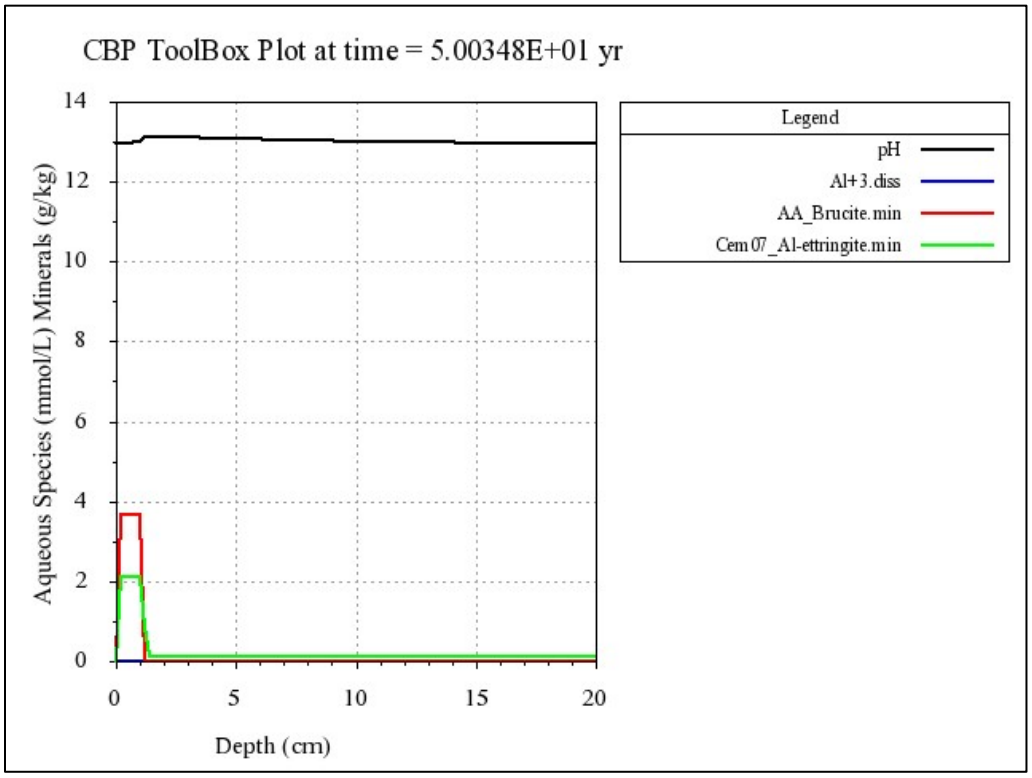

Figure 2-9. Example x-y plot of LeachXS/Orchestra output.

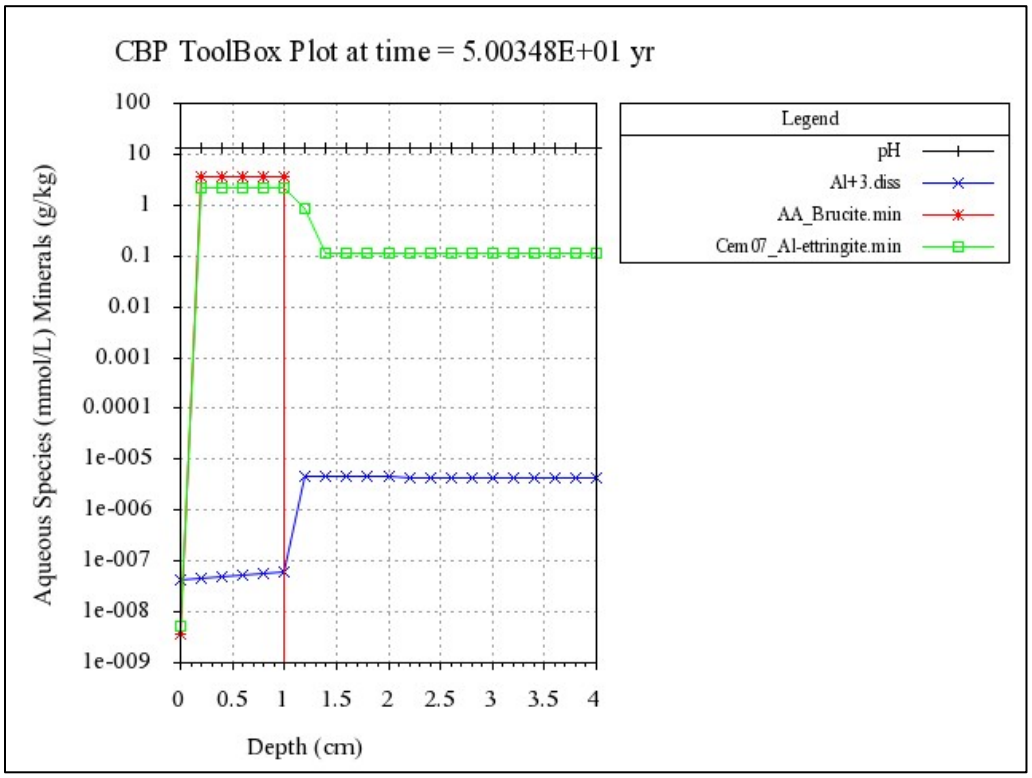

Figure 2-10. Rescaled example x-y plot with lines and points of LeachXS/Orchestra output.

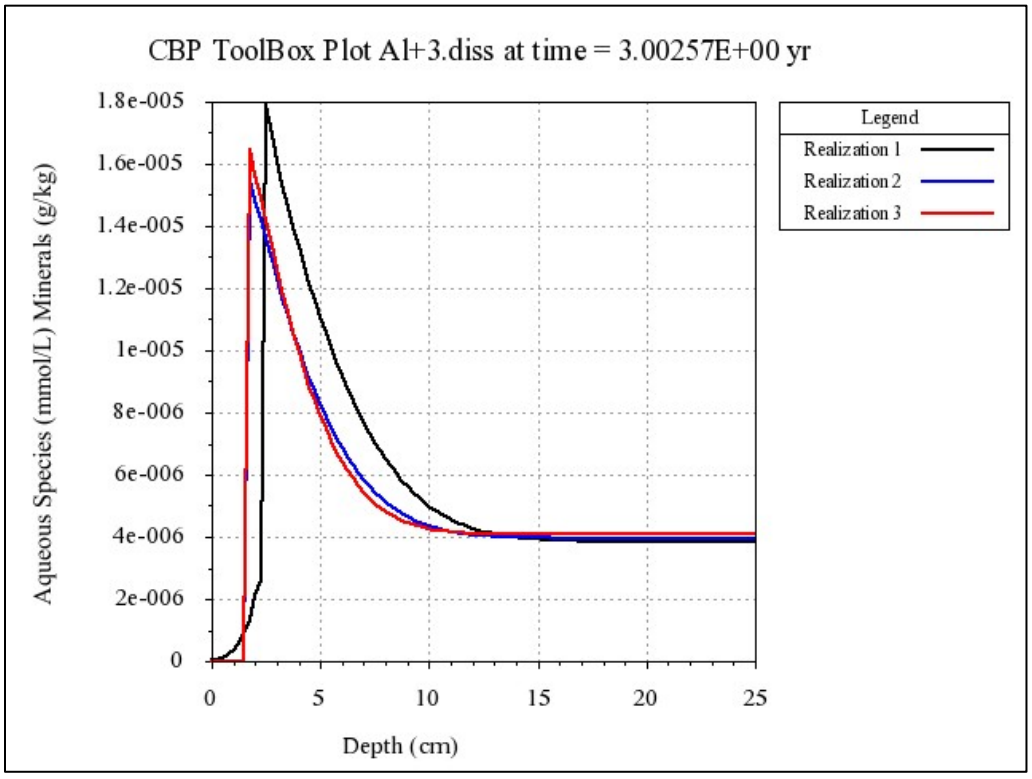

Figure 2-11. Example x-y plot of three realizations from LeachXS/Orchestra output.

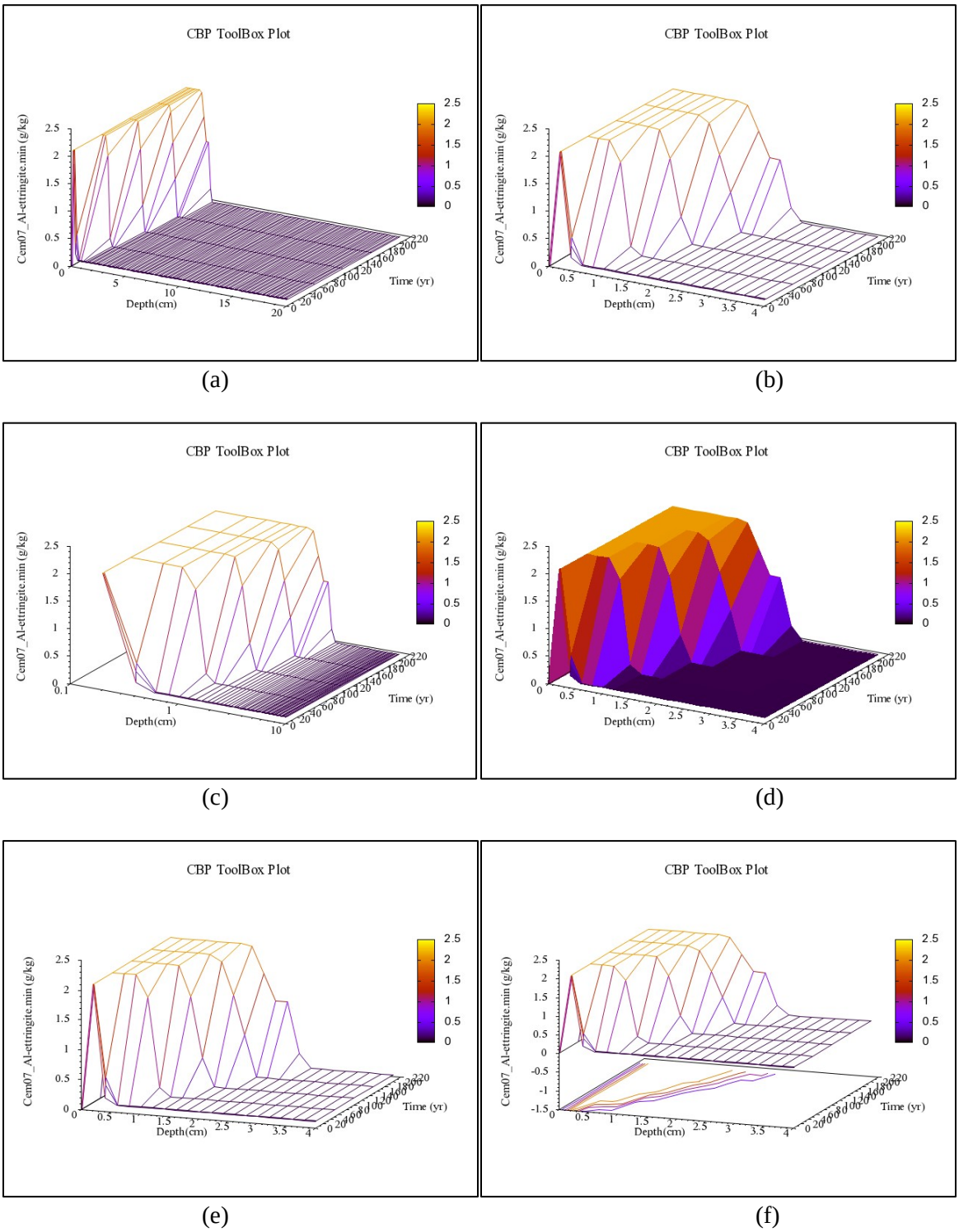

Figure 2-12. Example 3-dimensional plots of LeachXS/Orchestra output.

3.0 Conclusions

The development work described in this report can be summarized as the following suggested changes to the CBP Toolbox:

1) Include the dashboard based graphical display capability described in Section 3 of this report to display results from deterministic runs and selected realizations. This could be implemented as either a stand-alone GoldSim application or integrated directly into the toolbox as an option in the simulation control dashboard (shown below in Figure 3-1). Previously, plotting of model results has been available on the individual model control dashboards. However, once a model is chosen, the CBP Toolbox is designed to run the DLL launching the selected model. Using the GoldSim plotting application requires running GoldSim to access the plotting DLL so this action must be placed at the higher simulation control level.

2) Link the existing graphics Buttons in the toolbox to display GoldSim plots already created in the Cementitious_Models container. This would allow access to GoldSim visualization of results from stochastic model runs.

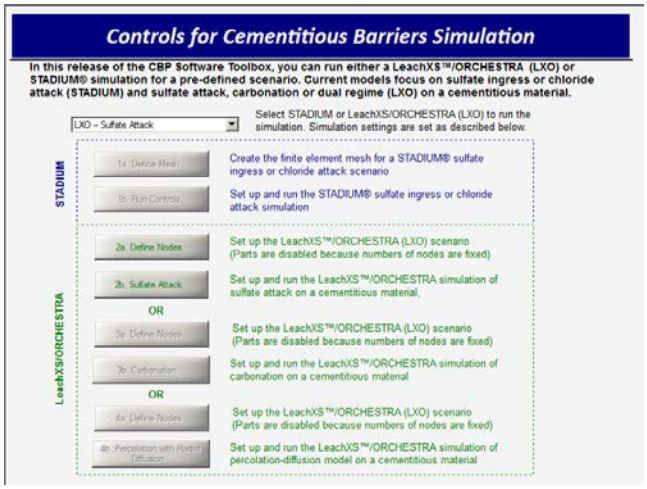

Figure 3-1. Simulation control dashboard in CBP Toolbox.

4.0 References

Brown, K.G. and G.P. Flach, 2009, *CBP Software Summaries for LeachXS™/ORCHESTRA, STADIUM®, THAMES, and GoldSim*, CBP-TR-2009-003, Rev. 0, in *Description of the Software and Integrating Platform*, Vanderbilt University/CRESP and Savannah River National Laboratory; Cementitious Barriers Partnership, Nashville, TN and Aiken, SC. Available from: http://cementbarriers.org/reports.html.

Brown, K.G., J. Arnold, S. Sarkar, G.P. Flach, H. van der Sloot, J.C.L. Meeussen and D.S. Kosson, 2012, *Modeling Carbonation of High-Level Waste Tank Integrity and Closure*, NUCPERF 2012 Conference, Cadarache, France, November 12-15, 2012.

Crawford, R., 2009, *Gnuplot 4.4 An Interactive Plotting Program*, November 25, 2009.

ECN, 2009, *LeachXS User Manual*, Energy Research Center of The Netherlands, Denmark. Available from: http://www.leaching.org, September 1, 2009.

Meeussen, J.C.L., 2003, *ORCHESTRA: An Object-Oriented Framework for Implementing Chemical Equilibrium Models*, Environmental Science & Technology, vol. 37, no. 6, pp. 1175-1182.

SIMCO, 2010, *CBP Task 7 Demonstration of STADIUM® for the Performance Assessment of Concrete LAW Storage Structures*, CBP-TR-2010-007-C3, Rev. 0, SIMCO Technologies Inc.; Cementitious Barriers Partnership, Quebec, Canada. Available from: http://cementbarriers.org/reports.html.

Smith III, F.G., G.P. Flach and K.G. Brown, 2010a, *CBP Code Integration GoldSim DLL Interface*, CBP-TR-2010-009-2, Rev. 0, Savannah River National Laboratory and Vanderbilt University/CRESP; Cementitious Barriers Partnership, Aiken, SC and Nashville, TN. Available from: http://cementbarriers.org/reports.html.

Smith III, F.G., G.P. Flach, K.G. Brown and S. Sarkar, 2010b, *CBP Phase I Code Integration*, CBP-TR-2011-009-1, Rev. 0, Savannah River National Laboratory and Vanderbilt University/CRESP; Cementitious Barriers Partnership, Aiken, SC and Nashville, TN. Available from: http://cementbarriers.org/reports.html.

Smith III, F.G., G.P. Flach and K.G. Brown, 2013, *CBP Toolbox Version 2.0: Code Integration Enhancements*, CBP-TR-2013-03, Rev. 0, Savannah River National Laboratory and Vanderbilt University/CRESP; Cementitious Barriers Partnership, Aiken, SC and Nashville, TN. Available from: http://cementbarriers.org/reports.html.

Appendix A. Stadium and LeachXS/Orchestra species

Table A-1Stadium Species.

Species	Aqueous	Minerals
1	OH	Portlandite
2	Na	CaH2SiO4
3	K	Ettringite
4	SO4	Monosulfate
5	Ca	C4AH13
6	Al(OH)4	Thaumasite
7	Cl	Calcite
8	H2SiO4	Monocarboaluminate
9	CO3	Gypsum
10	NO3	Friedel_IX
11	NO2	

Table A-2LeachXS/Orchestra Species.

Species	Aqueous	Minerals	Cem07 Minerals	Solid Species	Properties
1	Al+3	AA_Brucite	Al-ettringite	ettr_ss	pH
2	Ca+2	AA_Calcite	Al[OH]3[am]	Ettringite_ss	pe
3	Fe+3	AA_Gypsum	C2AH8	AsO4_Ettringite_ss	tortuosity
4	H2CO3	AA_Portlandite	C2FH8	BO3_Ettringite_ss	porosity
5	H4SiO4	Cem07_Brucite	C3AH6	Ba_Ettringite_ss	CO2[g].gas
6	Mg+2	Cem07_Calcite	C3AS0.8H4.4	CO3_Ettringite_ss	O2[g].gas
7	Na+	Cem07_Gypsum	C3FH6	CrO4_Ettringite_ss	omega
8	SO4-2	Cem07_Portlandite	C4AH13	MoO4_Ettringite_ss	
9	Al[OH]4-	AA_Fe[OH]3[am]	C4FH13	PO4_Ettringite_ss	
10	Fe[OH]4-	Manganite	CAH10	Pb[OH]4-2_Ettringite_ss	
11	H2SiO4-2		Fe-ettringite	Sr_Ettringite_ss	
12			Fe-hemicarbonate	VO3_Ettringite_ss	
13			Fe-monocarbonate	AFhc_ss	
14			Fe-monosulfate	AFm_ss	
15			Fe-stratlingite	AFmc_ss	
16			Fe[OH]3[mic]	AFt_ss	
17			M4ACH9	CSHi_ss	
18			M4AH10	CSHii_ss	
19			M4FH10	LDH_ss	
20			SiO2[min]	Cem07_C4Ac[0_5]H12_ss	
21			Thaumasite	Cem07_C4Fc[0_5]H12_ss	
22			tricarboaluminate	Cem07_C4AsH12_ss	
23			hemicarboaluminate	Cem07_C4FsH12_ss	
24			monocarboaluminate	Cem07_C4AcH11_ss	
25			monosulfoaluminate	Cem07_C4FcH11_ss	
26			Stratlingite	Cem07_C6As3H32_ss	
27				Cem07_C6Fs3H32_ss	
28				Cem07_SiO2[am]_ss	
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31				Cem07_Tob_II_ss	
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Distribution:

SRNL

H. H. Burns, 773-41A
D. A. Crowley, 773-43A
G. P. Flach, 773-42A
J. C. Griffin, 773-A
E. N. Hoffman, 999-W
K. M. Kostelnik, 773-42A
C. A. Langton, 773-43A
S. L. Marra, 773-A
F. G. Smith, III 703-41A
Records Administration (EDWS)

DOE

B. J. Gutierrez, 704-S
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