CBP SOFTWARE TOOLBOX, VERSION 1.0 USER GUIDE

Cementitious Barriers Partnership

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CBP SOFTWARE TOOLBOX, VERSION 1.0
USER GUIDE

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ACKNOWLEDGEMENTS

DISCLAIMER

FOREWORD

The Cementitious Barriers Partnership (CBP) Project is a multi-disciplinary, multi-institutional collaboration supported by the United States Department of Energy (US DOE) Office of Tank Waste Management. The objective of the CBP project is to develop a set of tools to improve understanding and prediction of the long-term structural, hydraulic, and chemical performance of cementitious barriers used in nuclear applications.

A multi-disciplinary partnership of federal, academic, private sector, and international expertise has been formed to accomplish the project objective. In addition to the US DOE, the CBP partners are the Savannah River National Laboratory (SRNL), Vanderbilt University (VU) / Consortium for Risk Evaluation with Stakeholder Participation (CRESP), Energy Research Center of the Netherlands (ECN), and SIMCO Technologies, Inc. The Nuclear Regulatory Commission (NRC) is providing support under a Memorandum of Understanding. The National Institute of Standards and Technology (NIST) is providing research under an Interagency Agreement. Neither the NRC nor NIST are signatories to the Cooperative Research and Development Agreement (CRADA).

The periods of cementitious performance being evaluated are up to or longer than 100 years for operating facilities and longer than 1000 years for waste management. The set of simulation tools and data developed under this project will be used to evaluate and predict the behavior of cementitious barriers used in near-surface engineered waste disposal systems, e.g., waste forms, containment structures, entombments, and environmental remediation, including decontamination and decommissioning analysis of structural concrete components of nuclear facilities (spent-fuel pools, dry spent-fuel storage units, and recycling facilities such as fuel fabrication, separations processes). Simulation parameters will be obtained from prior literature and will be experimentally measured under this project, as necessary, to demonstrate application of the simulation tools for three prototype applications (waste form in concrete vault, high-level waste tank grouting, and spent-fuel pool). Test methods and data needs to support use of the simulation tools for future applications will be defined.

The CBP project is a five-year effort focused on reducing the uncertainties of current methodologies for assessing cementitious barrier performance and increasing the consistency and transparency of the assessment process. The results of this project will enable improved risk-informed, performance-based decision-making and support several of the strategic initiatives in the DOE Office of Environmental Management Engineering & Technology Roadmap. Those strategic initiatives include 1) enhanced tank closure processes; 2) enhanced stabilization technologies; 3) advanced predictive capabilities; 4) enhanced remediation methods; 5) adapted technologies for site-specific and complex-wide Decontamination and Decommissioning (D&D) applications; 6) improved Spent Nuclear Fuel (SNF) storage, stabilization and disposal preparation; 7) enhanced storage, monitoring and stabilization systems; and 8) enhanced long-term performance evaluation and monitoring.

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LIST OF ACRONYMS AND ABBREVIATIONS

CBP	Cementitious Barriers Partnership
CoV	Coefficient of Variation
CRESP	Consortium for Risk Evaluation with Stakeholder Participation
D&D	Decommissioning and Decontamination
DLL	Dynamic-link library
DOE	Department of Energy
ECN	Energy Research Centre of the Netherlands
GTG	GoldSim Technology Group
GUI	Graphical User Interface
LeachXS™	Leaching eXpert System
LXO	LeachXS™/ORCHESTRA
NIST	National Institute of Standards and Technology
NRC	Nuclear Regulatory Commission
ORCHESTRA	Objects Representing CHEmical Speciation and TRAnsport
SNF	Spent Nuclear Fuel
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
STADIUM®	Software for Transport and Degradation in Unsaturated Materials
THAMES	Thermodynamic Hydration And Microstructure Evolution Simulator
VTK	Visualization ToolKit

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1 INTRODUCTION

The Cementitious Barriers Partnership (CBP) has developed a set of software tools, namely the **CBP Software ToolBox**, to predict the structural, hydraulic, and chemical performance of cement barriers used in nuclear applications over extended time frames. These tools can be used to evaluate the behavior of cementitious barriers used in near surface engineered waste disposal systems including waste forms, containment structures, entombments, and environmental remediation. Cementitious materials can be exposed to various dynamic environmental conditions that cause changes in material properties; the current CBP Software ToolBox models (i) sulfate attack, (ii) carbonation, (iii) oxidation and (iv) primary constituent leaching.

Two state-of-the-art software tools were selected as a starting point to capture important phenomena:

- LeachXS™/ORCHESTRA developed by the Energy Research Centre of the Netherlands (ECN) (ECN 2007, Meeussen 2003) and

- STADIUM® developed by SIMCO Technologies, Inc. (SIMCO 2008).

The GoldSim Monte Carlo simulation program (GTG 2010d, GTG 2010e) was chosen as the code integration platform to allow LeachXS™/ORCHESTRA and STADIUM® to be run probabilistically (Brown & Flach 2009b). GoldSim (current Version 10.5) is a Windows based graphical object-oriented computer program that provides a flexible environment for model development (Brown & Flach 2009b).

A general Dynamic-link Library (DLL) interface was developed by the CBP that links GoldSim with the external codes (Smith III et al. 2010a). The DLL uses an instructions file, updated by GoldSim for each realization, to create an input file for the external application, runs the external code, and returns a list of outputs (read from files created by the external application) back to GoldSim. GoldSim provides: 1) a consistent user interface to the selected external applications, 2) the capability of performing probabilistic analysis with individual codes, and 3) the capability of ultimately coupling selected codes in a synergistic manner.

A GoldSim Player version is made available by the GoldSim Technology Group that allows running but not editing GoldSim models (GTG 2010c). The Player version makes the software readily available to a wider community of users that would wish to use the CBP application but do not have a license for GoldSim.

This user guide describes use of the CBP Software ToolBox in detail and discusses the following topics:

- What is the CBP Software ToolBox?
- How does the CBP Software ToolBox work?
- What Partner Codes are in the CBP Software ToolBox?
- CBP Software ToolBox File Structure
- Basic CBP Software ToolBox Concepts including model elements, navigating, and running
- Tutorials for both STADIUM® and LeachXS™/ORCHESTRA

The information provided in this user guide supersedes previous information.

2   WHAT IS THE CBP SOFTWARE TOOLBOX?

The CBP Software ToolBox is an integrated system that allows state-of-the-art partner codes (namely, STADIUM® and LeachXS™/ORCHESTRA) to be evaluated under a GoldSim probabilistic framework. The GoldSim framework provides a consistent interface to selected external applications allowing probabilistic analysis of individual codes that were generally designed for the deterministic analysis of reactive transport in cementitious materials for important aging and degradation phenomena. The degradation phenomenon involved in the current revision of the CBP Software ToolBox is sulfate ingress and attack (via cracking) of cementitious materials used in nuclear applications.

2.1   How is the CBP Software ToolBox Installed?

Installation of the CBP Software ToolBox requires that the user be registered with the CBP to obtain the appropriate installers and instructions.

A request for registration can be made by emailing the **ToolBox Administrator** (lbliss@cresp.org). The request will be processed and, upon approval, download and installation instructions will be provided to the registrant.

2.2   What is in the CBP Software ToolBox?

The CBP Software ToolBox consists of:

- A GoldSim model (in this instance saved in a GoldSim Player file, `CBPsoftwareToolbox.gsp`) including a series of Dashboards and external interface elements that control partner code evaluation.

- A CBP custom Dynamic-link Library (DLL) that is called from the GoldSim external interface element to link to the selected CBP partner code.

- CBP partner codes including

  o LeachXS™/ORCHESTRA – LeachXS™ is a database coupled with an expert system for material characterization and environmental impact assessment based on estimated contaminant release rates derived from leaching tests. Geochemical speciation and chemical reaction/transport modeling capabilities are integrated into LeachXS™ using ORCHESTRA.

  o STADIUM® – A numerical model used to predict the transport of ions and liquids in reactive porous media that has been used to estimate service life of concrete under attack from chloride and sulfate ions. Results have been validated through laboratory test results and field exposure observations.

- A custom CBP Mesh2D program (called from a GoldSim external interface) that creates the finite element mesh that is used in the STADIUM® partner code.

- A text editor to modify the model input files, including the finite element mesh file, needed to run a STADIUM® simulation.

- Gnuplot to view the finite element mesh created to run a STADIUM® simulation.

2.3   What can I do with the CBP Software ToolBox?

Although partner codes can be run in standalone mode, the CBP Software ToolBox can be used to simulate the selected, state-of-the-art partner codes (namely STADIUM® and LeachXS™/ORCHESTRA) either deterministically or probabilistically for a predefined set of scenarios and conditions. The primary scenario involved in the current version of the CBP Software ToolBox is sulfate ingress and attack (via cracking) of cementitious materials.

For the STADIUM® code, contaminant (sulfate) ingress, ionic leaching in the pore solution, and modifications to microstructure of cementitious material are simulated for one-dimensional transport for 1-, 2-, and 3-layer models as illustrated in Figure 2-1.
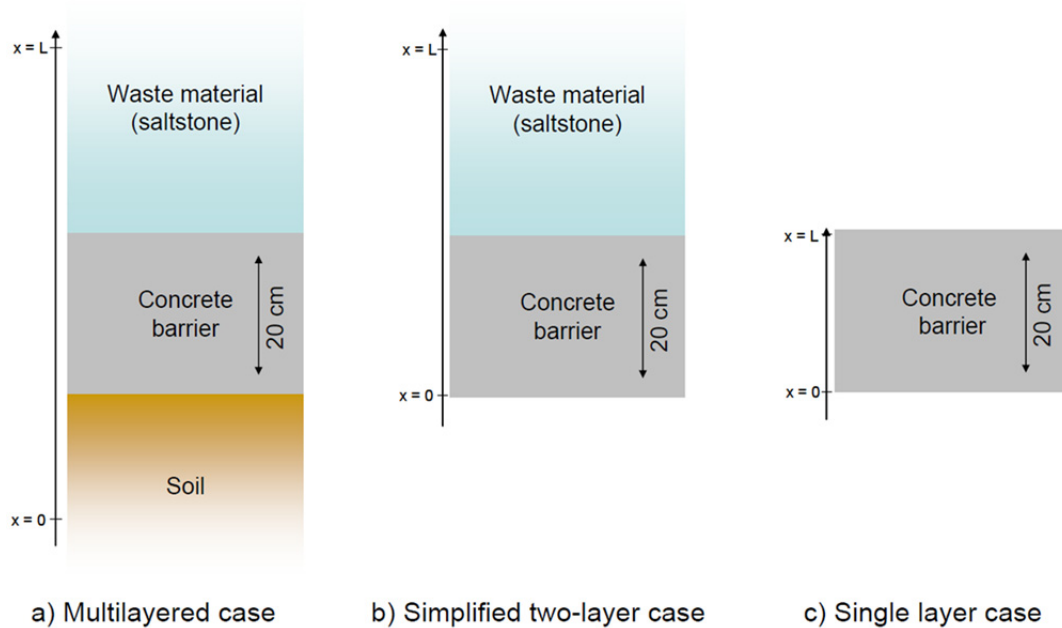
Figure 2-1.   Schematic representation of STADIUM® demonstration cases (SIMCO 2010)

For LeachXS™/ORCHESTRA, external sulfate attack is simulated for a one-dimensional, one-layer model analogous to that shown in Figure 2-1(c).

3   HOW DOES THE CBP SOFTWARE TOOLBOX WORK?

The CBP code integration work has produced a GoldSim model linked to the STADIUM® and LeachXS™/ORCHESTRA partner codes using a custom Dynamic-link Library (DLL) interface developed by the CBP. The DLL interface passes input augments from GoldSim to the selected code and then extracts output from the code-generated result files. The two partner codes are run independently from GoldSim with no coupling between the codes. Figure 3-1 shows a schematic diagram of the code integration structure.
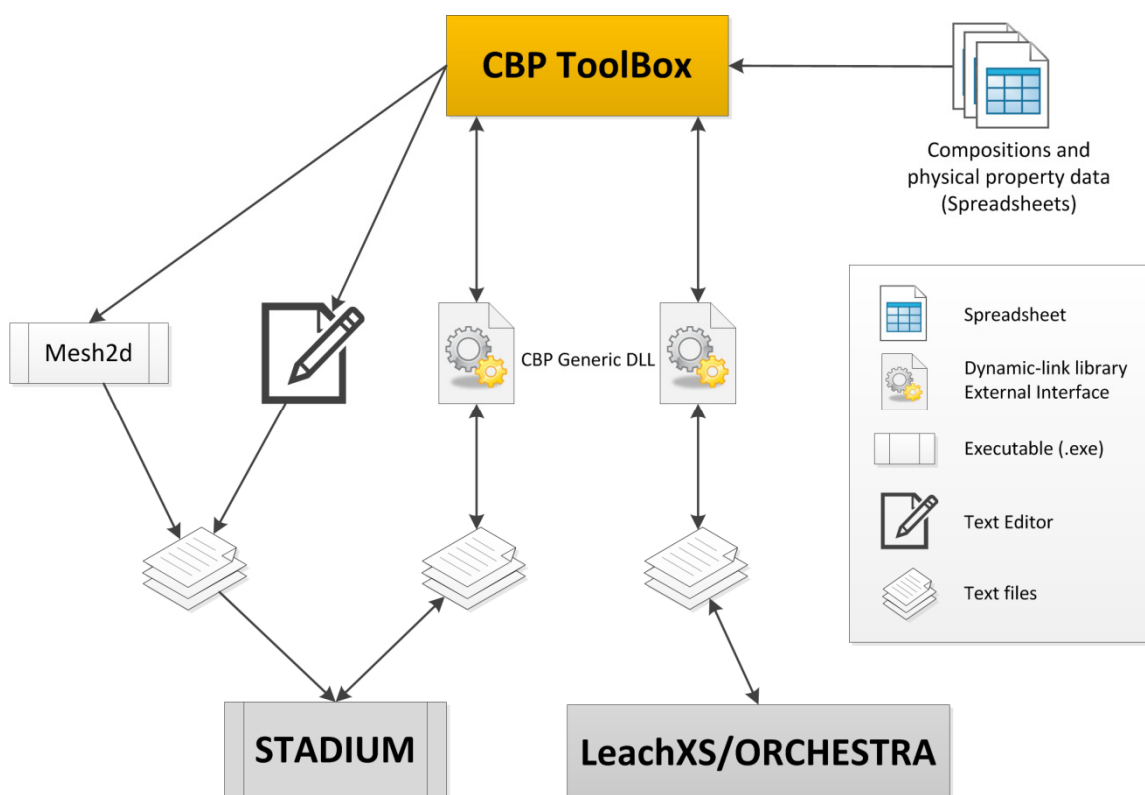
Figure 3-1.   Schematic representation of CBP code integration framework

GoldSim provides a framework for performing probabilistic analysis with partner codes by sampling stochastic distributions of selected model parameters within GoldSim. The analysis is accomplished by utilizing built-in GoldSim capabilities to create and sample stochastic distributions and to make repeated model runs (realizations) in conjunction with the code interface's ability to send random values from the distributions as input to the selected code.

The approach is demonstrated by the example calculations in the tutorials provided in Section 7. The standard version of GoldSim allows the user to run up to four realizations simultaneously. If the GTG distributed processing module is licensed (GTG 2010b), an essentially unlimited number of realizations can be run simultaneously to enhance productivity. Please refer to the *GoldSim Distributed Processing Module User's Guide* (GTG 2010b) for details on setting up and using the distributed processing module.

4   WHAT PARTNER CODES ARE IN THE CBP SOFTWARE TOOLBOX?

Brief descriptions of the partner codes (STADIUM® and LeachXS™/ORCHESTRA) that have been selected for the CBP Software ToolBox are provided in this section. This material was summarized from the CBP Task 3 report where detailed code descriptions are available (Brown & Flach 2009a).

4.1   What is the STADIUM® Partner Code?

SIMCO Technologies, Inc. has developed a numerical model called Software for Transport and Degradation in Unsaturated Materials (STADIUM®) that can be used to predict the transport of ions and liquids in reactive porous media (SIMCO 2008) including degradation of unsaturated concrete structures exposed to chemically aggressive environments. In particular, the model has been used to estimate the service life of concrete structures under attack from chloride and sulfate ions. STADIUM® results have been validated through laboratory test results and field exposure observations.

Calculations in STADIUM® are divided into two primary modules as shown in Figure 4-1. The first module accounts for coupled transport of ions and water omitting chemical reactions using a volume-averaged version of the extended Nernst-Planck equation. Transport equations are coupled to Poisson's equation that gives the electrical potential in the material as a function of the ionic distribution and including equations for moisture conservation and heat conduction. The second module is a chemical equilibrium code. After each transport step, this module equilibrates concentrations at each node with the phases present. Solid phases form as a result of species penetrating into the pores of the material. Variation of solid phases leads to local variations in porosity, which affects the local transport properties of the material (in the transport module).
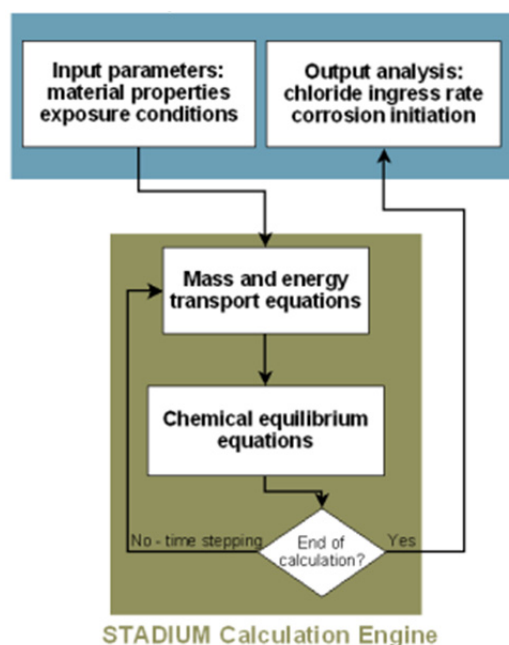
Figure 4-1.   STADIUM® Overview

The input information needed to run STADIUM® consists of information entered into a text file (SIMCO 2008, Brown & Flach 2009a):

- **Geometry and Time** – the user provides the space and time discretization parameters needed for the underlying numerical algorithm.

- **Material Properties** – the user provides the characteristics of the material to be modeled including: mixture proportions, transport properties, binder chemical composition, and initial state.

- **Exposure Conditions (Boundary Conditions)** – the user enters the exposure conditions including information describing the ionic species and temperature and humidity boundary conditions (e.g., average temperature and relative humidity of the environment, the salinity of seawater, or the concentration of the ionic contaminant).

- **Initial Values** – the user provides initial values for each variable in the model including data on the initial composition of the hydrated cement paste.

- **Corrosion and Printing Options** – the user defines the output frequency (step), how and when corrosion results are computed, and the frequency and number of rebar positions to be analyzed.

At the end of a simulation, output text files are created containing three series of results (SIMCO 2008, Brown & Flach 2009a):

- **Content versus depth** – species concentrations over the material thickness as a function of time,

- **Content versus time** – corrosion related quantities, in total chloride or chloride/hydroxide ratio at specific locations as a function of time, and

- **Corrosion initiation** results.

4.2 What is LeachXS™/ORCHESTRA?

The Leaching eXpert System (LeachXS™) is a database coupled with an expert system for material characterization and environmental impact assessment based on estimated contaminant release rates derived from leaching tests. Databases used by LeachXS™ include data for over 600 materials, scenarios, and regulations to allow comparisons of test data against specific utilization or disposal conditions. The expert system assists in evaluation and laboratory guidance, data management and evaluation, source term description, impact evaluation, and decision analysis.

Geochemical speciation and chemical reaction/transport modeling capabilities are integrated into LeachXS™ using the Objects Representing CHEmical Speciation and TRAnsport (ORCHESTRA) modeling environment. ORCHESTRA is a modeling framework for defining geochemical equilibrium models and combining these models with mass transport (diffusion, convection, etc.) for user defined processes (Meeussen 2003). The ORCHESTRA chemical module calculates chemical thermodynamic equilibrium in a similar way to other speciation codes but is internally organized very differently. Instead of defining all model equations within the source code, equations are defined in a user accessible text file in ORCHESTRA. ORCHESTRA has been used in practice for a wide range of applications that include aqueous speciation, precipitation, ion exchange, surface complexation, diffusion, convection, solid solutions, colloid adsorption, and biota uptake.
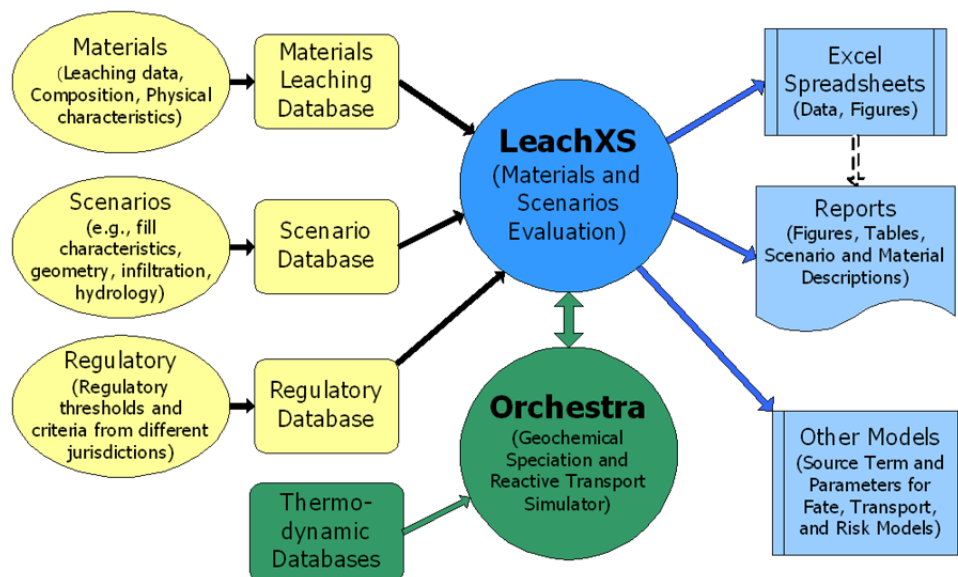
Figure 4-2.   LeachXS™/ORCHESTRA Overview

All ORCHESTRA models contain chemical equilibrium modules describing the chemical reactions and distribution of elements over different physical-chemical forms in a material. These models require:

- A set of chemical equilibrium reactions representative for the material under consideration.

- A set of element concentrations that can be estimated from total composition measurements or from pH dependent leaching test results.

- A set of parameters describing adsorbing surfaces; the necessary parameters can be estimated by determining extractable Fe and Al.

- Liquid to solid ratio.

The main result of a chemical equilibrium calculation is the distribution of elements over the different physical and chemical forms according to the set of thermodynamic equilibrium reactions provided as input. For each element, the distribution over the possible forms is calculated. Other generated outputs include: pH, REDOX potential, ionic strength, and electrical conductivity. The set of results from the LeachXS™/ORCHESTRA chemical equilibrium module is described by Brown & Flach (2009a). The LeachXS™ User guide also provides more detailed information about running the program and the results obtained (ECN 2012).

ORCHESTRA transport modules calculate mass transport and maintain mass balance using information provided by the chemical modules on the mobility of elements. The transport model needs a set of physical input parameters including:

- Physical dimensions of the system,

- Porosity, density and effective tortuosity of the material(s),

- Flow rates (for column simulation),

- Refresh rates (for tank test),

- Water saturation/gas volume, and

- Chemical composition of each solid material and each solution that is used in the simulation, including the parameters describing adsorbing surfaces.

The ORCHESTRA reactive transport model generates a chemical composition that provides basically the same output as that for a single chemical equilibrium reaction, but as a function of time and space. Outputs include:

- Chemical composition of the system as a function of time and space (i.e., concentration profiles) including distribution of elements (over mineral, aqueous, gaseous, and other phases), pH, and REDOX conditions.

- Total fluxes of elements over chosen internal or external system boundaries.

The set of results from the LeachXS™/ORCHESTRA transport module is described by Brown & Flach (2009a). Additional, detailed information is available in the LeachXS User Guides (ECN 2007, ECN 2012).

5   CBP SOFTWARE TOOLBOX FILE STRUCTURE

The code integration application is supplied with the top level file structure shown in Figure 5-1. The folders **Codes** and **Template** contain executable versions (subject to user licensing) of the CBP partner codes used for the code integration software. **Template** is a local folder that contains the information that the user needs to perform a simulation. The **Codes** folder and the other four auxiliary folders, briefly described below, would normally be of secondary interest to a user.

As indicated in the ToolBox Installation Guide (Brown et al. 2012), it is recommended that the user create a copy of the **Template** *folder to run their simulations; this operation is performed, for example, to run the tutorials presented in this Guide (Section 7) .*
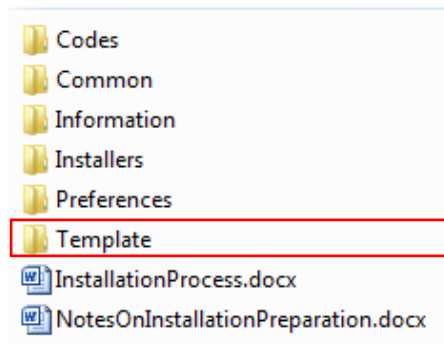
Figure 5-1.   Top-level file structure for CBP code integration application. The Template folder contains the information needed to perform a simulation.

5.1   Codes Folder and Files

The substructure of the **Codes** folder, which contains the various software programs that may be needed to run a simulation, is shown in Figure 5-2.
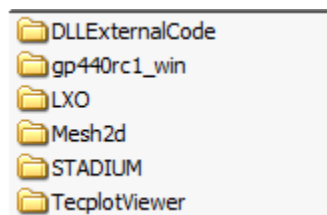
Figure 5-2.   Contents of Codes folder

Subfolders in the **Codes** folder contain the software that can be run using the GoldSim code integration interface. The subfolder names are largely self-explanatory:

1. **DLLExternalCode** contains the source code and compiled DLL files for the DLL interface. Details of the DLL interface and instructions for its use are described by Smith, et al. (2010a).

2. **gp440rc1_win** and its subfolders contain files for the open source plotting software Gnuplot (http://www.gnuplot.info/).

3. **LXO** contains subfolders that perform LeachXS™/ORCHESTRA calculations for cement carbonation for a 1-layer system and external sulfate attack for 1-, 2- and 3-layer models. The two- and three-layer sulfate attack models are not currently available from the GoldSim model; the model structure serves as a placeholder for these subsequent options.

4. **Mesh2d** contains the source code and executable for the grid generation software used in the code interface application. A complete description of the functionality of the grid generation software is provided by Flach and Smith III (2012). The user can access this software and associated files through the GoldSim interface.

5. **STADIUM** contains an evaluation version of the STADIUM® executable program (provided by SIMCO Technologies as described in the CBP Software ToolBox Installation Guide (Brown et al. 2012)) and the input files: `PITZER-STADIUM-V3.dat,` `CHM-DB-STADIUM-V3.txt` and `SOLUTES-DB-STADIUM-V3.dat` that are required by STADIUM®. A fully functional version of STADIUM® must be licensed from SIMCO Technologies, Inc. (http://www.stadium-software.com/).

The free software contained in these subfolders is neither supported nor promoted by the CBP.

5.2 Auxiliary Folders and Files

The auxiliary folders shown in Figure 5-1 perform the following functions:

1. **Common** is currently unused and is intended for future use as a folder to store data common to all CBP partner codes (e.g., common databases called by the GoldSim interface).

2. **Information** contains:

   a. Copies of the DLL documentation (in the **CBP_DLL** subfolder)

   b. Copies of relevant CBP reports (in the **CBPreports** subfolder),

   c. Relevant **LeachXS-ORCHESTRA** documentation,

   d. Relevant documentation and example of the **Mesh2d** program used to generate the finite element mesh for STADIUM® execution, and

   e. Relevant **STADIUM®** documentation.

3. **Installers** contain the installation files for:

   a. **GNUplot** used to view the finite element mesh for STADIUM® execution

   b. **GoldSim** Player

   c. Java Runtime Environment (**JavaRE)** needed to run LeachXS™/ORCHESTRA

   d. **LeachXS-ORCHESTRA** that includes the LeachXS Lite installer

   e. **STADIUM** is currently empty as an evaluation version of the necessary executable file is provided separately by SIMCO Technologies, Inc. as described in the CBP Software ToolBox Installation Guide (Brown et al. 2012)

4. **Preferences** contains shortcuts to text editors and plotting programs that the user can modify for use as desired as described in the ToolBox Installation Guide (Brown et al. 2012). For example, the shortcut MyTextEditor points to the default text editor currently specified as WordPad.

While source code is available for the CBP generic DLL interface and the Mesh2d software, it is expected that the user would not normally modify this code.

*It is recommended that the user work entirely <u>in a copy of the</u> **Template** <u>folder</u> as described both below and in the ToolBox Installation Guide (Brown et al. 2012).*

5.3 Template Working Folder and Files

The expectation is that the CBP Software ToolBox user would work exclusively *in a copy of the* **Template** *folder* (Brown et al. 2012). The contents of the **Template** folder are shown in Figure 5-3. The full GoldSim model used to link to partner codes is in `CBPsoftwareToolbox.gsm`; a GoldSim Player version (GTG 2010c) of the same model is provided for users that do not have a GoldSim license in `CBPsoftwareToolbox.gsp`. The free Player version of GoldSim allows users to view and run but not edit GoldSim models. Using the dashboards explained in Section 6, the Player version can be used to modify code inputs and run CBP simulations.

📁 LXO	📄 DLL_LXO_CO3.dat
📁 Materials	📄 DLL_STADIUM_2Layers.dat
📁 Mesh	📄 DLL_STADIUM_3Layers.dat
📁 STADIUM	📄 DllDel.dll
📁 THAMES	📄 DllExternalCode_LXO_1Layer.dll
📄 CBPsoftwareToolbox.gsp	📄 DllExternalCode_LXO_2Layers.dll
📄 Default_depth_1Layer.xlsx	📄 DllExternalCode_LXO_3Layers.dll
📄 Default_depth_2Layers.xlsx	📄 DllExternalCode_LXO_CO3.dll
📄 Default_depth_3Layers.xlsx	📄 DllExternalCode_STADIUM_2Layers.dll
📄 Default_depth_CO3.xlsx	📄 DllExternalCode_STADIUM_3Layers.dll
📄 DLL_LXO_1Layer.dat	📄 DllTie.dll
📄 DLL_LXO_2Layers.dat	📄 eps.xls
📄 DLL_LXO_3Layers.dat	

Figure 5-3.   Example contents of Template folder

The **Template** folder currently contains multiple versions of the DLL code interface for 2- and 3-layer STADIUM® modeling of sulfate ingress, 1-, 2- and 3-layer LeachXS™/ORCHESTRA (LXO) modeling of external sulfate attack, and a 1-layer LXO modeling cement carbonation. The primary difference among these DLLs is the dimensioning of the input and output arrays used to exchange data between the GoldSim model and the DLLs. The corresponding data specification (`*.dat`) and log (`*.log`) files and other support files are also contained in this folder.

The subfolders in the **Template** directory perform the following functions:

1. The **LXO** folder (Figure 5-4) contains an input file (`leachxs_parameters.txt`) that is updated by the CBP DLL at run time and copied to the appropriate realization folder (described below) for execution. The line and column numbers referenced in the `DLL.dat` input instructions file (Smith III et al. 2010a) must conform to the data locations in the template file. The **LXO** folder also contains the batch files (`*.bat`) used to run LeachXS™/ORCHESTRA (LXO) and duplicates of the folders containing the corresponding models.

   Typically, basic LXO models are generated and edited using LeachXS™ (ECN 2012); however, the LXO models in the ToolBox for sulfate attack and carbonation have been tested and should not be edited by the user. These models should be used in their pre-configured modes; additional models will be added to the ToolBox for other scenarios (multiple layers, different geometries and/or additional phenomena) that will also be defined using LeachXS™ advanced modeling capabilities.

   The batch files `bincopy1.bat` and `bincopyCO3.bat` are called from the DLL to copy the files needed for execution of the 1-layer sulfate attack and cement carbonation, respectively. The corresponding files for the 2- and 3-layer sulfate attack models are included as placeholders. The batch files `noscreen1.bat` and `noscreenCO3.bat` are called from the DLL interface to make LXO calculations; these batch files run models without opening the normal, interactive LXO GUI. The **CBPSulfateAttack_1Layer** and **CBPCarbonation** folders contain copies of the LXO model files for the 1-layer sulfate attack and carbonation models, respectively. The results files (e.g., `output_profiles.dat`) are also copied to the **Runs** directory (described below) for subsequent processing by the DLL. This folder also contains the Excel workbooks that are linked to the GoldSim model. Based on the model run, GoldSim writes summaries of the LXO input used for each realization to separate spreadsheets in the workbook. The workbook saves the input values used for later analysis and is particularly valuable for stochastic runs where the input values are randomly assigned.

   Blank worksheets should already exist for each realization in the `LXO_Summary.xls` *and* `LXO_Summary_CO3.xls` *workbooks. (The information in* `LXO_Summary_CO3_by_rows.xls` *workbook is added by rows, which has a minimum of 65,536 in supported versions of Microsoft Excel. The maximum number of worksheets in a workbook is limited by available memory.) If a realization is run corresponding to a non-existent worksheet, then GoldSim will add worksheets as described in Section 8.3. Worksheets can be added to a workbook as described in Microsoft Excel Help.*
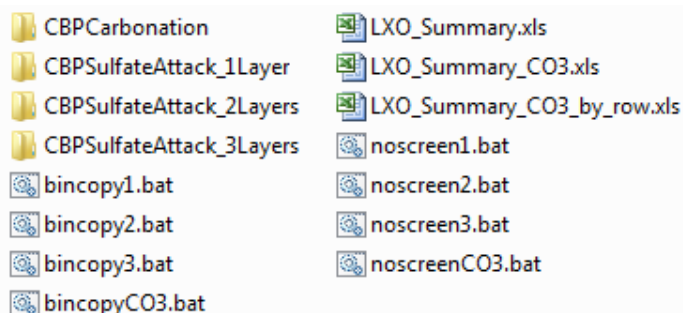
Figure 5-4.   Example contents of the LXO folder

2. The **Materials** folder (Figure 5-5) currently contains three Microsoft Excel spreadsheets containing composition and physical property data for concrete, salt waste, and soil. The spreadsheets, at a

minimum, hold data for Type 1 and Type 2 concrete, Type 1 and Type 2 Saltstone (i.e., SRS salt waste), and Type 1 soil. Type 1 concrete composition and properties are representative of the concrete used to make SRS Saltstone Vault 2 while the Type 2 concrete properties are representative of the concrete used to make SRS Saltstone Vaults 1 and 4. The Type 1 and Type 2 Saltstone differ only in the initial composition of chemicals and minerals. The properties used for these materials were taken from the SIMCO Technologies, Inc. CBP Task 7 report (SIMCO 2010).
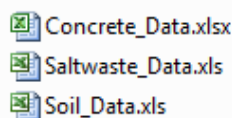
Figure 5-5.   Contents of Materials folder

3. The **Mesh** folder **(**Figure 5-6**)** contains the data files used to define the STADIUM® computational grid and output files created from running the Mesh2d finite element mesh generation program (Flach & Smith III 2012) using the GoldSim interface as shown in Section 6.4.1. Creating the grid also generates files that can be used to view the grid formatted for Tecplot Viewer, Gnuplot, and as a Visualization Tool Kit (VTK) graphics file suitable for viewing with the VisIt and Paraview plotting software. Mesh files formatted for use by STADIUM® and PORFLOW are also created.
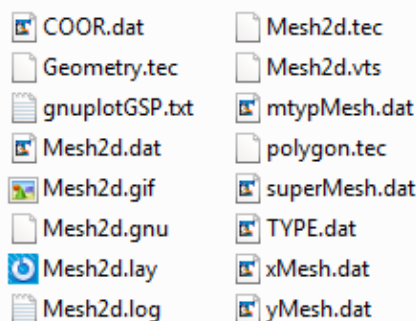
Figure 5-6.   Contents of Mesh folder

4. The **Runs** folder contains subfolders where simulation results are stored. The DLL interface automatically creates subfolders in **Runs** for each realization when the **Save Output** option is selected. For a deterministic calculation, a subfolder named **realization_0** is created as shown in Figure 5-7. The contents of this folder with input and output files from an example deterministic 3-layer STADIUM® run are shown in Figure 5-7.
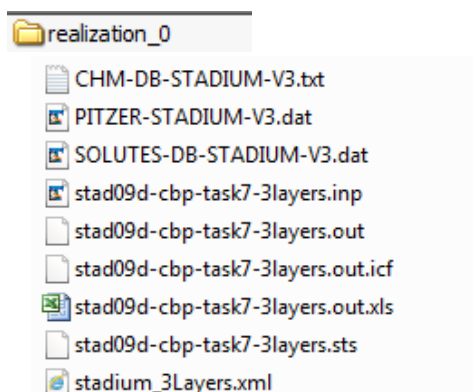
Figure 5-7.   Example contents of Runs folder for a STADIUM® simulation

5. The **STADIUM** folder contains an input template file (`stad09d-cbp-task7-template.inp`) used by the DLL interface as shown in Figure 5-8. The line and column numbers referenced in the `DLL.dat` input instructions file (Smith III et al. 2010a) must conform to the data locations in this template file. The DLL interface uses this template and the instructions in the appropriate `DLL.dat` file to create a STADIUM® input file that will be placed in the corresponding realization folder in **Runs** (Figure 5-8). The **STADIUM** folder also contains the appropriate mesh coordinate and element files (e.g., `20cm-50cm-mesh.cor` and `20cm-50cm-mesh.ele`, respectively, as illustrated in Figure 5-8) that are required as input to STADIUM®. This folder also contains the Excel workbook `STADIUM_Summary.xls` that is linked to the GoldSim model. GoldSim writes a summary of the STADIUM® input used for each realization to separate spreadsheets in this workbook. This workbook saves the input values used for later analysis and is particularly valuable for stochastic runs where the input values are randomly assigned.

    Blank worksheets should already exist in the `STADIUM_Summary.xls` *workbook for each realization. If a realization is run corresponding to a non-existent worksheet, then GoldSim will add worksheets as described in Section 8.3. (The maximum number of worksheets in a workbook is limited by available memory.) Additional worksheets corresponding to increased realizations can be added to the summary workbook as described in Microsoft Excel Help.*
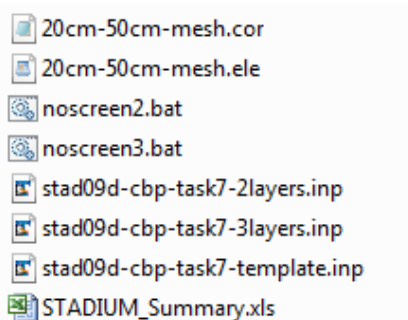
Figure 5-8.   Example contents of the STADIUM folder

6. The **THAMES** folder is currently not used but is included as a placeholder for planned NIST development work that will, in part, create an interface to this additional CBP partner code.

6   BASIC CBP SOFTWARE TOOLBOX CONCEPTS

The CBP Software ToolBox provides a bridge to the STADIUM® and LeachXS™/ORCHESTRA partner codes. Operation of the interface is controlled through a series of GoldSim Dashboard elements (i.e., "control panels" with simulation control and display functions) that have been created within the GoldSim software (GTG 2010d). When the user first opens the CBP ToolBox, the top level container shown in Figure 6-1 appears. (If the ToolBox does not open as shown in Figure 6-1, the user can select the "**Go**" button on the **GoldSim Run Controller** and select "**Go to Model Root ...**" from the resulting list.) Dashboards (accessible from the Top-Level or Root container) have been created so that the user can set up and run a simulation and view the results without having to interact directly with the underlying GoldSim model or linked codes (which would require a fully-licensed version of GoldSim). The Dashboard functions will be explained in the following sections.
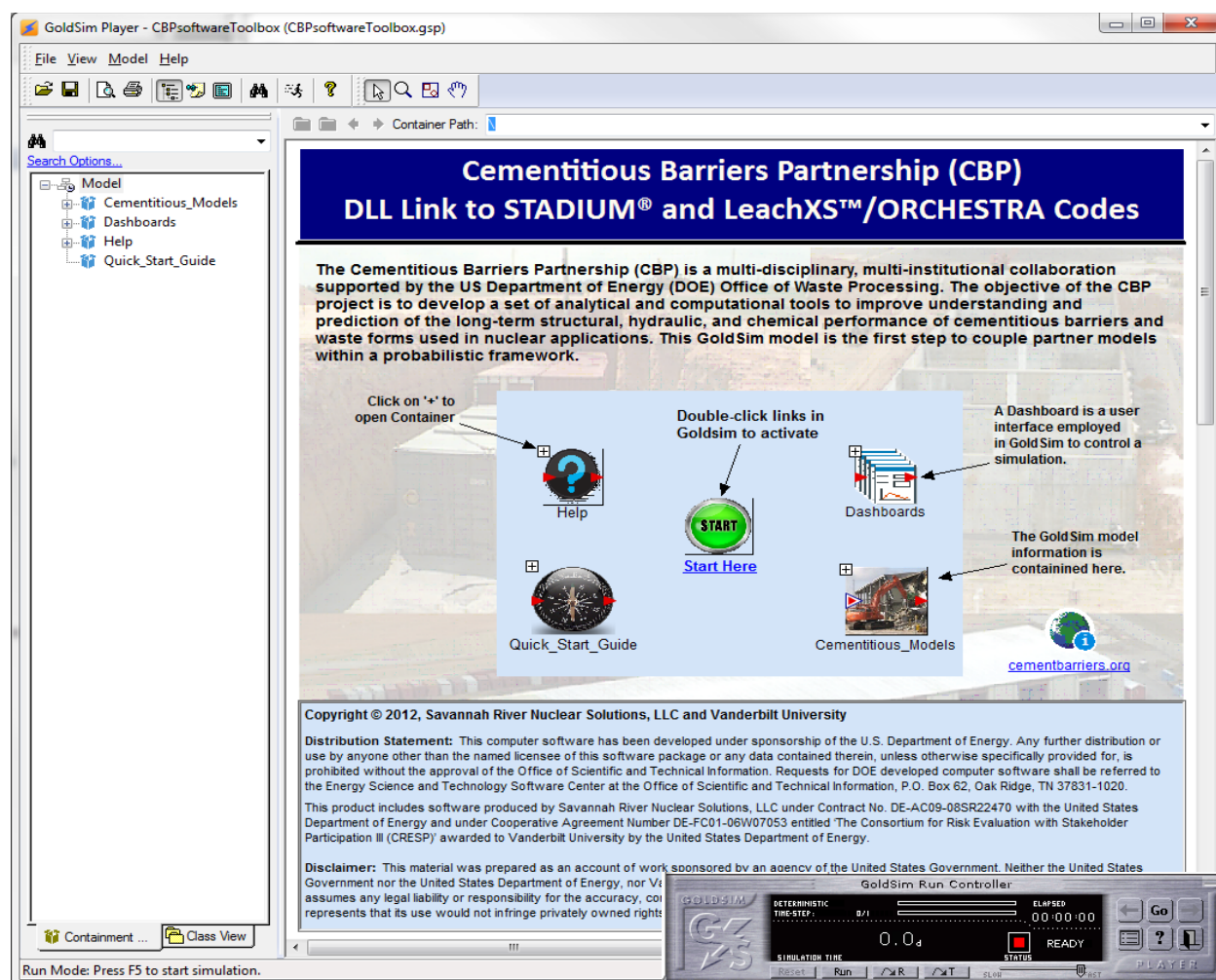
Figure 6-1.   Top-Level or Root Container in CBP Software ToolBox and the GoldSim Run Controller

6.1 GoldSim Model Elements

The various objects with which a GoldSim model is constructed are referred to as elements. Each element represents a basic building block of the simulation and has a particular symbol or graphical image (that can be customized) representing it on the GoldSim model browser (Figure 6-1). Most elements accept inputs and, in turn, produce outputs. Typically, elements are given unique name by which they are referenced in the model. Elements provide mechanisms for entering data into the model and for sampling from distributions for probabilistic analysis. However, because the CBP Software ToolBox is primarily acting as a "whiteboard" for information obtained from running partner codes, only a subset of the GoldSim elements are used—and fewer are critical to ToolBox operation. The primary elements used in the ToolBox are described in Table 6-1.

Table 6-1.   Overview of GoldSim Model Elements used in the ToolBox (GTG 2010d)

| Element	Default Symbol	Browser Icon	Function
Data			Defines scalar, vector, or matrix data.
Stochastic			Defines uncertain data using probability distributions.
Expression			Defines mathematical or logical expressions.
Lookup Table			Defines a one-, two-, or three-dimensional lookup table (e.g., representing a response surface).
External (DLL)			Dynamically links to a user-specified external function (compiled as a Microsoft Windows Dynamic-link Library or DLL).
Spreadsheet			Dynamically links to an Excel spreadsheet.
Array View			Displays vectors and matrices of results.

A special set of function elements (e.g., Spreadsheet and External) can be used to link GoldSim models to external applications. Because much of the functionality needed for the CBP tools is available in existing partner codes, the External elements that use the generic Dynamic-link Library (DLL) developed by CBP to link the GoldSim model to external codes are the most critical to ToolBox operation.

GoldSim elements are grouped in Containers; these are easily identified in the model as they all have a small ⊞ in their upper left-hand corner. Selecting the ⊞ (or Crtl+double-clicking on the element) opens the container. Containers can be nested, and the picture associated with the Container can be changed.

Container1
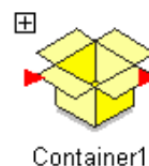
6.2   Navigating through the CBP Software ToolBox

There are a variety of ways to navigate through a GoldSim model based on the situation. For example, when the user is examining the model using the browser window (e.g., Figure 6-1), the easiest way to navigate is to use the controls at the top of the browser window as shown in Figure 6-2. These controls remain available as one drills down into the Containers that organize the ToolBox. There is also an optional browser view of the model in the pane on the left-hand side of the window that displays the containment hierarchy in a manner similar to how a Microsoft Windows directory structure is shown.
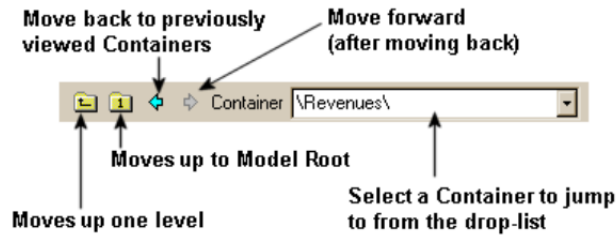
Figure 6-2.   The GoldSim Navigation Bar (GTG 2010d)

When a Dashboard element is being displayed in the GoldSim Player, neither the navigation bar (Figure 6-2) nor the optional browser view are available to the user. However, many Dashboard elements in the ToolBox contain control buttons that allow the user to navigate to other Dashboards or to browse the model (by returning to the Root level shown in Figure 6-1).

In general, the user can navigate through the various Dashboard elements in a GoldSim Player model by selecting the **Go** *button on the* **GoldSim Run Controller** *(Figure 6-1) and then selecting the name of the desired Dashboard from the resulting list as shown in Figure 6-3.*

Figure 6-3.   Selecting a Dashboard from the GoldSim Run Controller

6.3   Starting Up and Controlling a Simulation using the CBP ToolBox

Double clicking on the START button shown in Figure 6-1 opens the Simulation Controls Dashboard shown in Figure 6-4, where the user can access simulation controls for selected partner codes. These top level controls, consisting of a GoldSim Combo Box to select the partner code and scenario and buttons that are activated based on the selection to open dashboards to create a simulation mesh and setup and run STADIUM® or to set up and run LeachXS™/ORCHESTRA for either sulfate attack or cement carbonation. In general, the color blue corresponds to STADIUM® information and the color green to LeachXS™/ORCHESTRA.
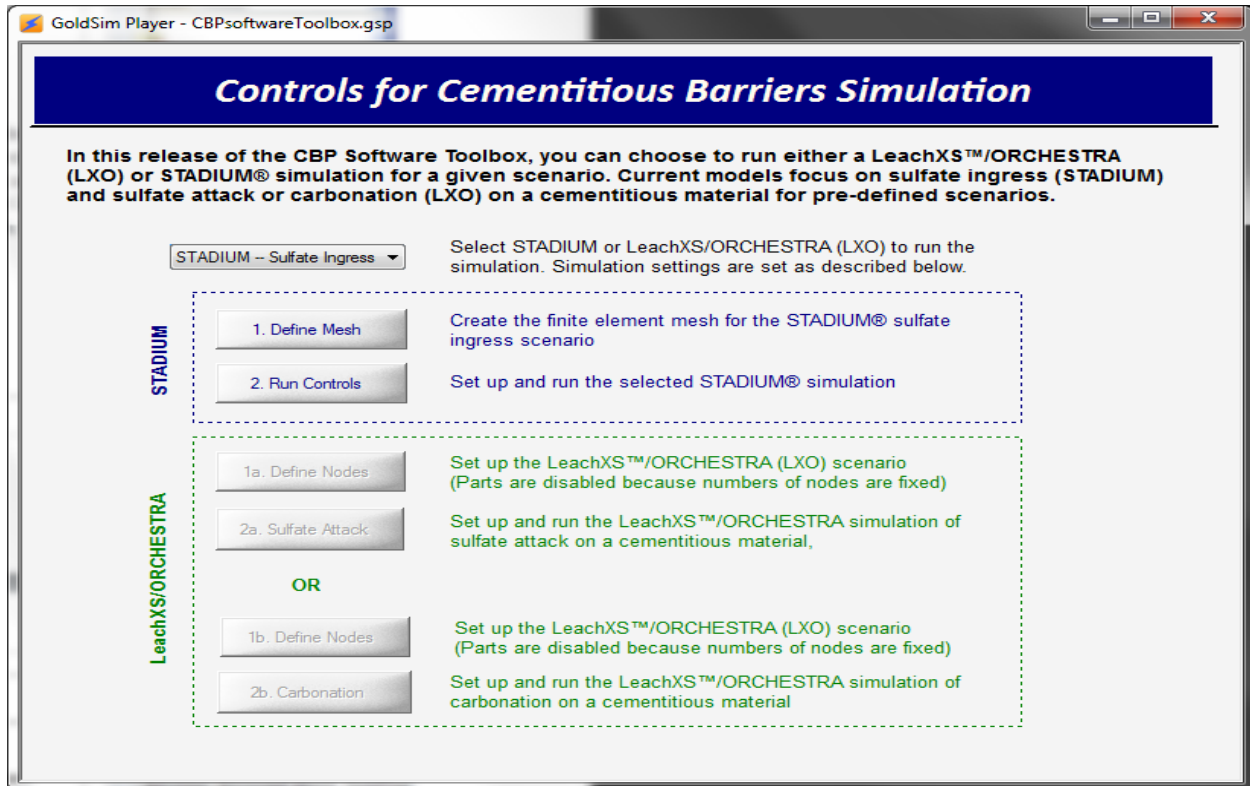
Figure 6-4.   Controls Dashboard to Select Partner Code and Scenario

6.4   Running the STADIUM® Partner Code

The STADIUM® partner code can be used to simulate sulfate ingress and damage from the CBP Software ToolBox by selecting the **STADIUM – Sulfate Ingress** calculation option from the Combo Box shown in Figure 6-4. When this option is selected, the "**1. Define Mesh**" and "**2. Run Controls**" control buttons become active (i.e., are not grayed out) and the buttons for the other scenario options are inactive (i.e., grayed out).

6.4.1 Generating the STADIUM® Finite Element Mesh using the CBP Mesh2d Program

The CBP Software ToolBox can be used to simulation sulfate ingress (and corresponding damage) using the STADIUM® partner code; the code requires a finite element mesh to run. For the **STADIUM – Sulfate Ingress** option, the finite element mesh is defined by selecting the "**1. Define Mesh**" button (Figure 6-4); the Controls dashboard takes the user to the simulation mesh dashboard shown in Figure 6-5. The simulation mesh dashboard allows the user to create input files for the Mesh2d program that builds the finite element mesh for STADIUM®, run the Mesh2d program, and view the resulting grid.
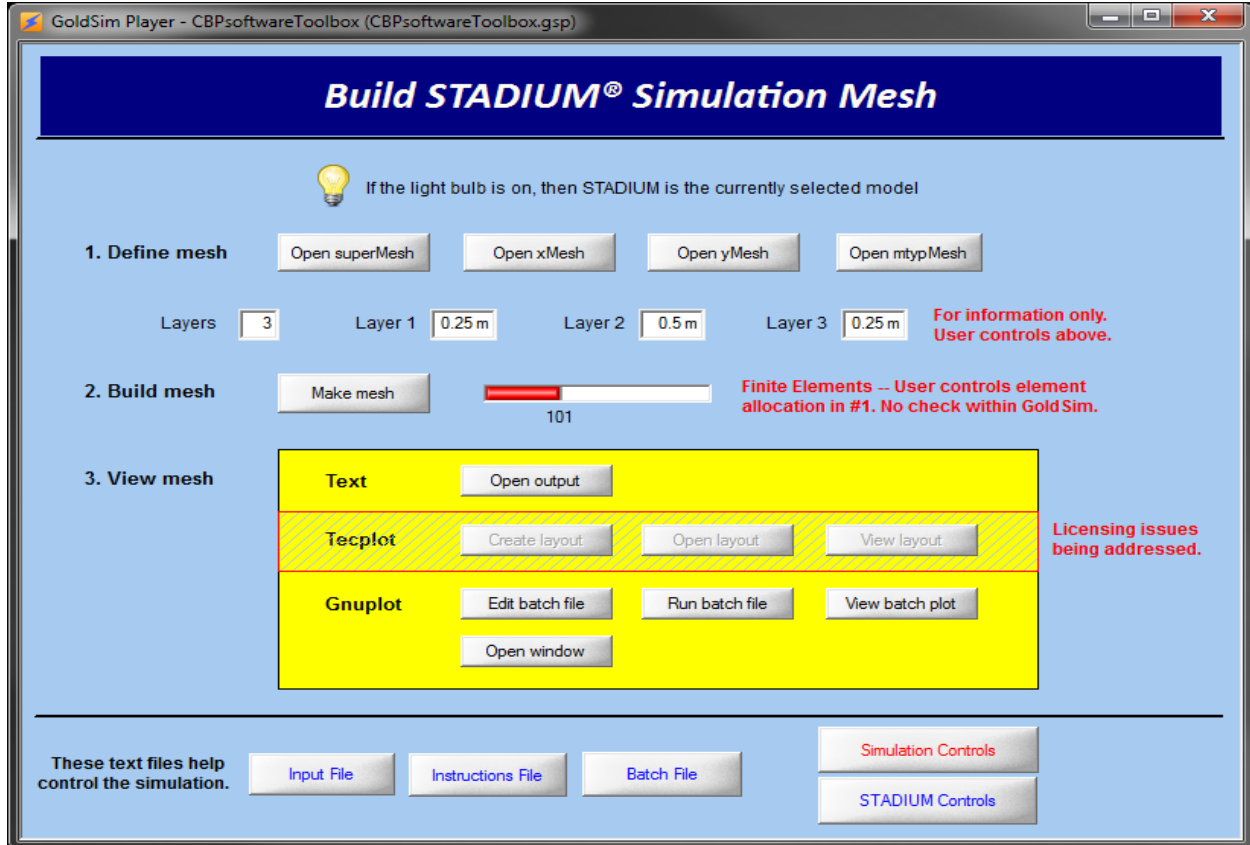
Figure 6-5.   Simulation mesh generation dashboard

Mesh2d is a Fortran90 program developed by SRNL to generate two-dimensional structured grids of the form [x(i),y(i,j)] where [x,y] are grid coordinates identified by indices (i,j). The x(i) coordinates generated from the Mesh2d program can be used to specify a one-dimensional grid, such as for STADIUM®. *Because all the models linked to from the ToolBox are one-dimensional in nature, only the x(i) coordinates are considered in detail in this guide.* A full explanation of the Mesh2d software is provided by Flach & Smith III (2012). Mesh2d also assigns an integer (representing the material type) to each grid cell, mtyp(i,j), in a user-specified manner where the complete grid is specified through three separate input files defining variations in x(i), y(i,j), and mtyp(i,j).

The overall mesh is constructed from grid zones (usually corresponding to distinct materials or larger geometric shapes) that are typically subdivided into a collection of smaller grid cells. The structured grid zones are identified through uppercase indices (I,J). Subdivision of zonal regions into grid cells can be done uniformly, or non-uniformly using either a polynomial or geometric skewing algorithm. Grid cells may be concentrated backward, forward, or toward both ends.

The four control buttons on the line labeled "**1. Define mesh**" (Figure 6-5) are used to define the finite element mesh needed to run STADIUM®. Each button opens the corresponding text file (`superMesh.dat`, `xMesh.dat`, `yMesh.dat` or `mtypMesh.dat`) that resides in the **Mesh** folder in **Template** using the default text editor specified in the top level **Preferences** folder; the preferred editor can be changed as described in the ToolBox Installation Guide (Brown et al. 2012). These four text files contain instructions that are read by the Mesh2d program to create the computational grid for STADIUM®.

The top-tier input to Mesh2d is a *superfile* containing filenames and high-level option specifications, in the order indicated by Table 6-2. The input file containing the x(i) grid specifications (Table 6-3) can be assigned an arbitrary name, but is conventionally denoted *xMesh.dat*. Similarly, *yMesh.dat* (Table 6-4) and *mtypMesh.dat* (Table 6-5) are the traditional names for the y(i,j) and mtyp(i,j) specifications. *The contents of the* `yMesh.dat` *file can be changed by the user, but this operation is not recommended because all models will be one-dimensional for the current implementation, and the default* `yMesh.dat` *file provided with the ToolBox installation will be appropriate for these models.* The conventional names will be used for convenience in the remaining discussion.

The formats of the `xMesh.dat`, `yMesh.dat` and `mtypMesh.dat` text files are defined in Table 6-3 through Table 6-5. All three text files may contain empty lines and/or comment lines denoted by an exclamation point in column 1, as any such lines will be discarded during input processing. Material type specifications in `mtypMesh.dat` overwrite any prior specifications.

Table 6-2.   Mesh2d Superfile format (Smith III et al. 2010b)

Input	Description
	Mesh2d inputs:
xMesh.dat	Input file containing x(i) grid specifications
yMesh.dat	Input file containing y(i,j) grid specifications
mtypMesh.dat	Input file containing mtyp(i,j) grid specifications
xyz or *xrt*	Cartesian (xyz) or cylindrical (xrt) coordinates for PORFLOW
	Mesh2d outputs:
Mesh2d.log	Log file
Mesh2d.dat	PORFLOW high-level grid specification statements
COOR.dat	PORFLOW coordinates file
TYPE.dat	PORFLOW material type file
Stadium.cor	Stadium coordinate file
Stadium.ele	Stadium element connectivity and material file
Mesh2d.tec	Tecplot graphics file containing grid data points
Geometry.tec	Tecplot graphics file containing "TextGeom" geometries outlining grid zones & material boundaries
polygon.tec	Tecplot graphics file containing "TextGeom" geometries for polygons (if used) to define materials
Mesh2d.vts	VTK graphics file suitable for VisIt and Paraview plotting software
Mesh2d.gnu	Gnuplot graphics file

Table 6-3.   File format for specifying the x(i) grid coordinates (Smith III et al. 2010b)

Line	Format
Line 0	scale x0
Line I, I=1→M	iFlag nx dir scheme skew scale dx|x
	(one line per each of M grid zones in the x-direction)

Input	Description

iFlag	Mode flag (integer = 0 or 1):
	    0 = Interval size specification for grid zone in field 7 (dx)
	    1 = End position of grid zone specification in field 7 (x)

nx	Number of grid cells within the grid zone (integer ≥ 1)
dir	Skewing direction (character): *n* = negative | *p* = positive | *c* = central | *d* = disabled (uniform gridding)

scheme	Skewing scheme (4 character string):
	    prev = (<u>prev</u>ious) polynomial skewing scheme
	    poly = <u>poly</u>nomial skewing scheme
	    geom = <u>geom</u>etric skewing scheme

skew	Skewing parameter, s (real < 2.0)
scale	Multiplier to dx|x typically used for units conversions (real > 0.0), e.g., scale = 30.48 to convert dx|x in feet to centimeters for grid coordinates.
x0	Line 0: The origin of the x coordinate system (x0) (real)
dx|x	Line I > 0: The size (dx) or ending position (x) of grid zone I (real, dx > 0.0)

Table 6-4.   File format for specifying the y(i,j) grid coordinates (Smith III et al. 2010b)

Line	Format
Line 0	iFlag scale y0|nPts
Line 0.1 … 0.nPts	x y (if iFlag = 1) … (nPts instances)
Line J, J=1→N	iFlag ny dir scheme skew scale dy|y|nPts (one line per each of N grid zones in the y-direction)
Line J.1 … J.nPts	x dy|y (if iFlag = 2|3) … (nPts instances)
Input	**Description**
iFlag	Mode flag (integer = 0 to 3): For Line 0, 0 = Fixed baseline for grid in field 3 (y0) 1 = Variable baseline for grid in field 3 (nPts) For Line J, 0 = Fixed interval size specification for grid zone in field 7 (dy) 1 = Fixed end position of grid zone specification in field 7 (y) 2 = Variable interval size specification for grid zone in field 7 (nPts) 3 = Variable end position of grid zone specification in field 7 (nPts)
ny	Number of grid cells within the grid zone (integer ≥ 1)
dir	Skewing direction (character): *n* = negative | *p* = positive | *c* = central | *d* = disabled (uniform gridding)
scheme	Skewing scheme (4 character string): *prev* = (<u>prev</u>ious) polynomial skewing scheme defined by Equation (1) *poly* = <u>poly</u>nomial skewing scheme defined by Equations (1) and (2) *geom* = <u>geom</u>etric skewing scheme defined by Equations (3) and (4)
skew	Skewing parameter, s, in Equations (1) through (4) (real < 2.0)
scale	Multiplier to dy|y typically used for units conversions (real > 0.0), e.g., scale = 30.48 to convert dy|y in feet to centimeters for grid coordinates. The scaling factor is also applied to any x values specified (e.g., iFlag = 2|3).
y0|nPts dy|y|nPts	Line 0: The origin of the y coordinate system (y0) (real) Line i > 0 and iFlag = 0|1: The size (dy) or ending position (y) of grid zone J (real, dy > 0.0) Line i > 0 and iFlag = 2|3: The number of (x,dy|y) pairs to follow (integer > 0)
x dy|y	For iFlag = 2|3, (x,dy|y) pairs, nPts in total, one pair per line

Table 6-5. **File format for specifying the mtyp(i,j) material assignments (Smith III et al. 2010b)**

Line	Format
Line K	iFlag im|xm ip|xp jm|ymm jp|ypm mZone
Line K.2 if iFlag = 2	ymp ypp
Line K.2 if iFlag = 3	polygon (filename)
repeat as needed	
Input	**Description**
iFlag	Mode flag (integer = 0 to 3): 0 = Material zone specified using grid zone indices (I,J) 1 = Material zone specified using grid element indices (i,j) 2 = Material zone specified by trapezoid with vertical sides using (x,y) points 3 = Material zone specified by general polygon using (x,y) points
im|xm	iFlag = 0, 1: starting zone (I) or element (i) index in x-direction (integer) iFlag = 2: left or x- coordinate of trapezoid (real) iFlag = 3: read but ignored
ip|xp	iFlag = 0, 1: ending zone (I) or element (i) index in x-direction (integer) iFlag = 2: right or x+ coordinate of trapezoid (real) iFlag = 3: read but ignored
jm|ymm	iFlag = 0, 1: starting zone (J) or element (j) index in y-direction (integer) iFlag = 2: lower left y coordinate of trapezoid (real) iFlag = 3: read but ignored
jp|ypm	iFlag = 0, 1: ending zone (J) or element (j) index in y-direction (integer) iFlag = 2: lower right y coordinate of trapezoid (real) iFlag = 3: read but ignored
mZone	Material type identification number (arbitrary integer)
ymp	iFlag = 2: upper left y coordinate of trapezoid (real)
ypp	iFlag = 2: upper right y coordinate of trapezoid (real)
polygon	iFlag = 3: filename of polygon with (x,y) vertices. Empty lines and lines with 'P', '#' or a blank in column 1 are ignored. The first vertex is repeated to close the polygon, e.g., (x1,y1) (x2,y2) … (x1,y1)

Examples of the `superfile.dat`, `xMesh.dat`, `yMesh.dat` and `mtypMesh.dat` text files are provided in Table 6-6 through Table 6-9, respectively, for an example one-dimensional, three-layer mesh. The user enters the number of layers for the model, and the layer dimensions in the input blocks on the STADIUM® Run Controls Dashboard (see Figure 6-6 in Section 6.4.2) so this information is available to both the GoldSim model and the Mesh Generation Dashboard (Figure 6-5). This information is reproduced on this Dashboard for reference. Similar controls have been developed to modify scenario geometry for LeachXS™/ORCHESTRA simulations and are discussed in Section 6.6.

Table 6-6.   superfile for example one-dimensional, three-layer mesh

```
xMesh.dat
yMesh.dat
mtypMesh.dat
xyz
Mesh2d.log
Mesh2d.dat
COOR.dat
TYPE.dat
..\STADIUM\25cm-50cm-25cm-mesh.cor
..\STADIUM\25cm-50cm-25cm-mesh.ele
Mesh2d.tec
Geometry.tec
polygon.tec
Mesh2d.vts
Mesh2d.gnu
```

Table 6-7.   xMesh.dat file for example one-dimensional, three-layer mesh

```
!iFlag key:
!       0=constant interval
!       1=constant position
!dir key:
!       p=positive
!       n=negative
!       c=center
!       d=disabled
!scheme key:
!       geom=geometric growth factor
!       poly=polynominal transformation
!       prev=previous polynomial transformation
!
!iFlag  nx      dir     scheme  skew    scale   dx|x
                                        1       0       !origin at x=0
0       25      c       poly    1.35    0.01    25      !25cm w/1cm spacing
0       50      n       poly    1.56    0.01    50      !50cm w/1cm spacing
0       25      d       poly    1.      0.01    25      !25cm w/1cm spacing
```

Table 6-8.   yMesh.dat file for example one-dimensional, three-layer mesh

```
!iFlag  key:
!       0=constant thickness
!       1=constant elevation
!       2=variable thickness
!       3=variable elevation
!dir    key:
!       p=positive
!       n=negative
!       c=center
!       d=disabled
!scheme key:
!       geom=geometric growth factor
!       poly=polynominal transformation
!       prev=previous polynomial transformation
!
!iFlag  ny      dir     scheme  skew    scale   dy|y|nPts
!       xi      yi
0                                       1       0       !bottom
0       1       d       poly    1       1       0.5     !top
```

Table 6-9.   mtypMesh.dat file for example one-dimensional, three-layer mesh

```
!mtyp key:
!  1=soil
!  2=concrete
!  3=saltwaste
!
!iFlag key:
! 0=zone indices from x and y mesh input
! 1=element indices
! 2=(x,y) trapezoidal zone with vertical sides
!
!iFlag  im|xm   ip|xp   jm|ymm  jp|ypm  mZone
!                       ymp     ypp
0       1       1       1       99      1       !soil
0       2       2       1       99      2       !concrete
0       3       3       1       99      3       !salt waste
```

Clicking on the **Make mesh** button on the line labeled "**2. Build mesh**" on the Mesh Generation Dashboard (Figure 6-5) runs the Mesh2d executable file contained in a subfolder within the **Codes** folder (Figure 5-2). The Mesh2d executable reads the input files edited in the previous "**Define Mesh**" Step and creates the computational grid that will be used in the simulation. The functions in the box labeled "**3. View mesh**" can be used to view the computational grid either in a text file or graphically. Currently, the Gnuplot plotting software is provided as the graphic programs for plotting the mesh. The Tecplot viewer is disabled in the

current version of the CBP Software ToolBox pending resolution of licensing issues. The mesh information is also written as a VTK graphics file suitable for viewing in VisIt (https://wci.llnl.gov/codes/visit/) and ParaView (http://www.paraview.org/), which are available to the user at no cost. The text output uses the default text editor to view the mesh file formatted for Tecplot viewing.

6.4.2 Running a STADIUM® Simulation from the CBP Software ToolBox

A STADIUM® simulation is controlled using the STADIUM® run controls dashboard shown in Figure 6-6. This Dashboard is opened from the simulation controls dashboard (Figure 6-4) by selecting the "**2. Run Controls**" button (in the STADIUM block), or from the mesh generation dashboard (Figure 6-5) by selecting the "**STADIUM Controls**" button, or generally by selecting the **Go** button on the GoldSim Run Controller (Figure 6-1) and then selecting "**STADIUM_DashBoard**" from the resulting list.
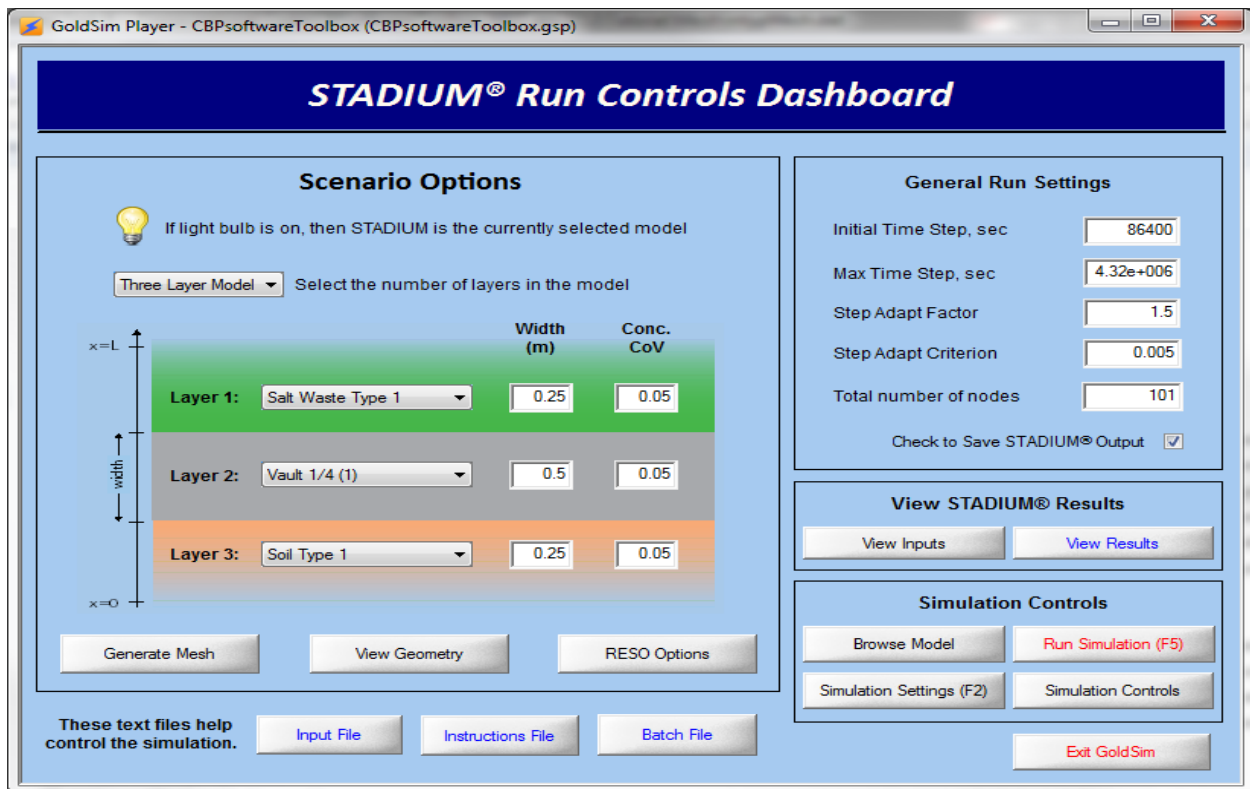
Figure 6-6.   STADIUM® Run Controls Dashboard

The STADIUM® run controls dashboard allows the user to enter basic data used for a STADIUM® simulation. Using the group of inputs labeled "**Scenario Options**" on the left hand side of the dashboard, the user first selects whether a two- or three-layer system is modeled. The materials present in each layer are selected from a list of available materials and the layer thicknesses in meters are entered. In the final input box for each layer, the user specifies the coefficient of variation (CoV) applied to the initial compositions for use in probabilistic calculations. *For probabilistic calculations, it is assumed in the ToolBox that the nominal compositions provided in the materials property spreadsheets are the mean values of normal distributions with*

the standard deviations specified by the concentration CoV entries. Truncated normal distributions have been used in the ToolBox becasue the chance that a negative sample concentration is generated increases as the standard deviation increases relative to the mean (for a normal distribution).

The group of "**General Run Settings**" contains four input boxes that allow the user to enter time step control parameters for the simulation and a box where the number of nodes in the mesh can be modified. A check box is located below these entries where the user selects whether or not to save the output from STADIUM® calculations. When the save option is checked, the integration software will create files in the **Runs** folder (Figure 5-7) saving output from each realization during a stochastic simulation.

Below the **Scenario Option** entries, control buttons are provided that allow the user to generate the computational mesh (Section 6.4.1), view the scenario geometry and related information (none of which can be altered by the user), and enter the STADIUM® RESO options. Clicking the **RESO Options** button opens the Dashboard shown in Figure 6-7 that allows the user to enter or select seven additional parameters that control STADIUM® solution methods. The STADIUM® manual (SIMCO 2008) should be consulted for an explanation of these additional features, and *it is highly recommended that only expert STADIUM® users change these values from their default values*.

The user can return to the Run Controls Dashboard (Figure 6-6) by either selecting the **STADIUM Options** button or the **Go** button on the GoldSim Run Controller and then "**STADIUM_DashBoard**" from the list.
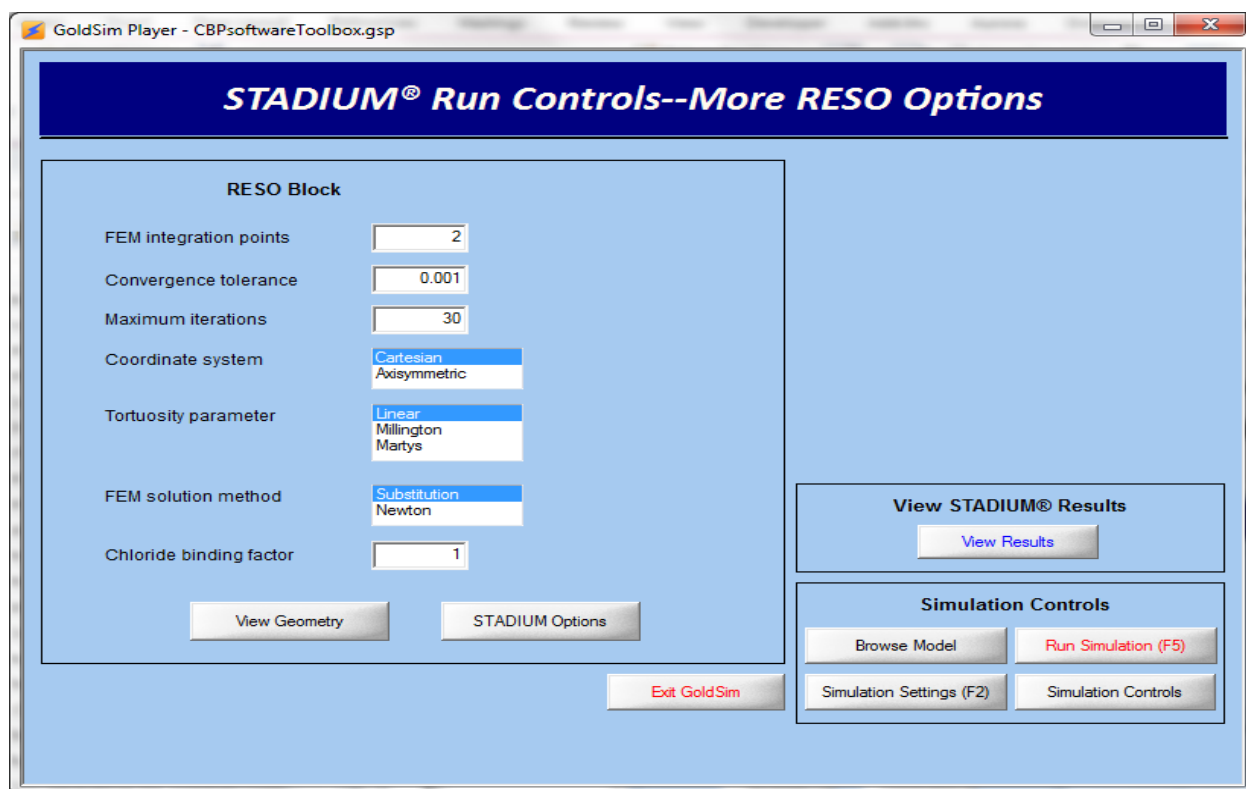

Figure 6-7. STADIUM® RESO solution control dashboard

Below the **Scenario Options** block on the Run Control Dashboard (Figure 6-6) are three control buttons that allow the user direct access to three text files that help control the STADIUM® simulation:

- **Input File** – Opens the input template file (e.g., `stad09d-cbp-task7-3layer.inp` in Figure 5-8 for a 3-layer model) used by the DLL interface to run the simulation.

- **Instructions File** – Opens the DLL instructions file (e.g., `DLL_STADIUM_3Layers.dat` for a 3-layer model as shown in Figure 5-3).

- **Batch File** – Opens the Windows batch file (e.g., `noscreen3.bat` for a 3-layer model as shown in Figure 5-8) that controls running of the STADIUM® executable.

It is recommended that only expert users change the information in these files.

6.4.3 Viewing STADIUM® Inputs and Results

Below the **General Run Settings** portion of the Run Control Dashboard (Figure 6-6) in the **View STADIUM® Results** block are two control buttons that allow the user to view inputs to and results from STADIUM® simulations. Selecting the **View Inputs** button opens the `STADIUM_Summary.xls` spreadsheet that summarizes the STADIUM® input used for each realization in separate worksheets as indicated in Figure 6-8. This workbook is useful for later analysis and is particularly valuable for stochastic runs where the input values are randomly assigned. Blank worksheets must already exist for each realization in the workbook.

Figure 6-8.   A Portion of the STADIUM_Summary.xls Workbook

Selecting the **View Results** button opens the Dashboard (Figure 6-9) that allows the user to view graphs of STADIUM® results for selected minerals or chemicals. These graphs are generated using built-in GoldSim plotting functions. The results available for plotting are those transferred back to GoldSim from the STADIUM® output files through the DLL interface.
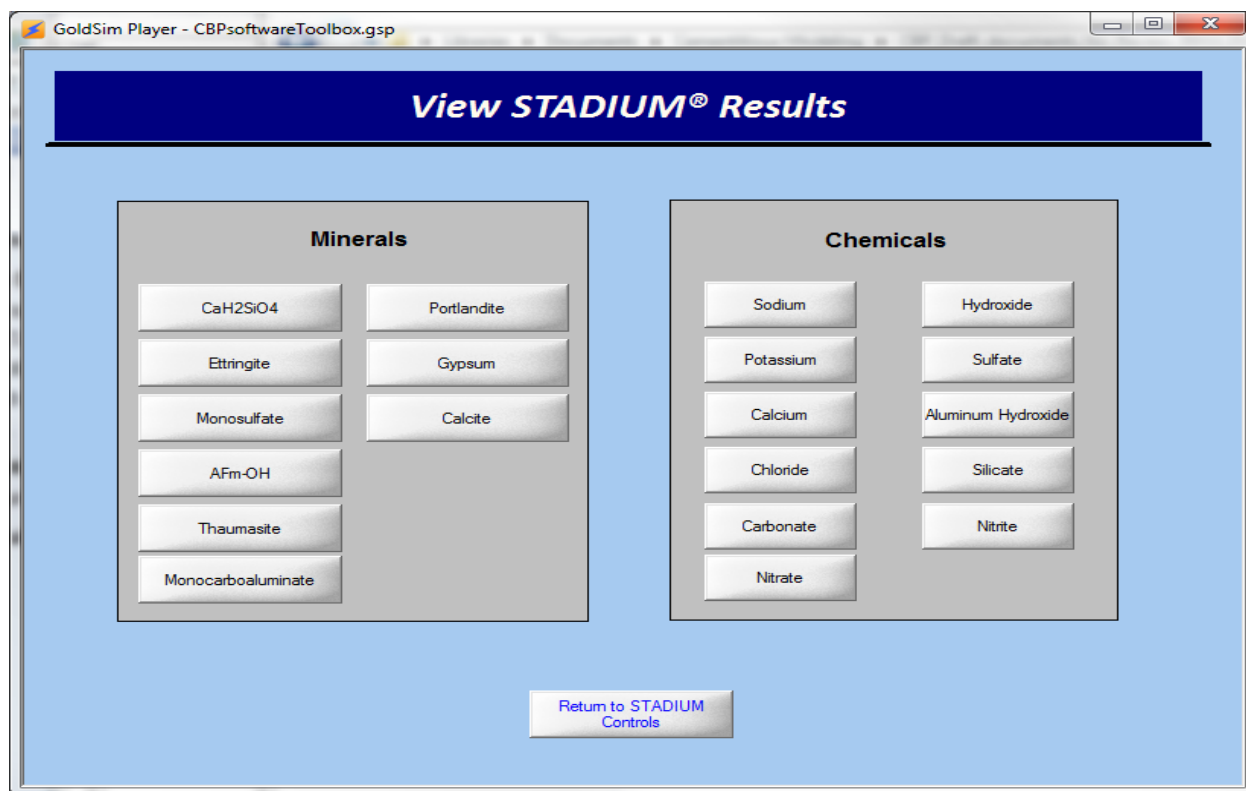
Figure 6-9.   Dashboard for selecting a plot of STADIUM® results

GoldSim plotting capabilities are primarily designed to produce time history graphs. Plots of special distributions, which will be of significant interest for evaluating the performance of cementitious materials, can also be created but may not be appropriate for all analyses. An example of such a special plot is shown in Figure 6-10 where the concentration of chlorine (Cl) at each computational node is plotted. In this example, the plot is for 100 years simulation of a two-layer system where the interface between layers is located at node 50. The Dashboard controls (Figure 6-9) can be used to generate quick plots of the results; other graphs can be generated by working with the computational results outside of the interface.

Figure 6-10. Example GoldSim results display plot for chloride concentration

6.5 General Dashboard Controls including Run Simulation

There are a set of common Dashboard control buttons (as shown on Figure 6-6, Figure 6-7, Figure 6-13 and Figure 6-16). These controls are:
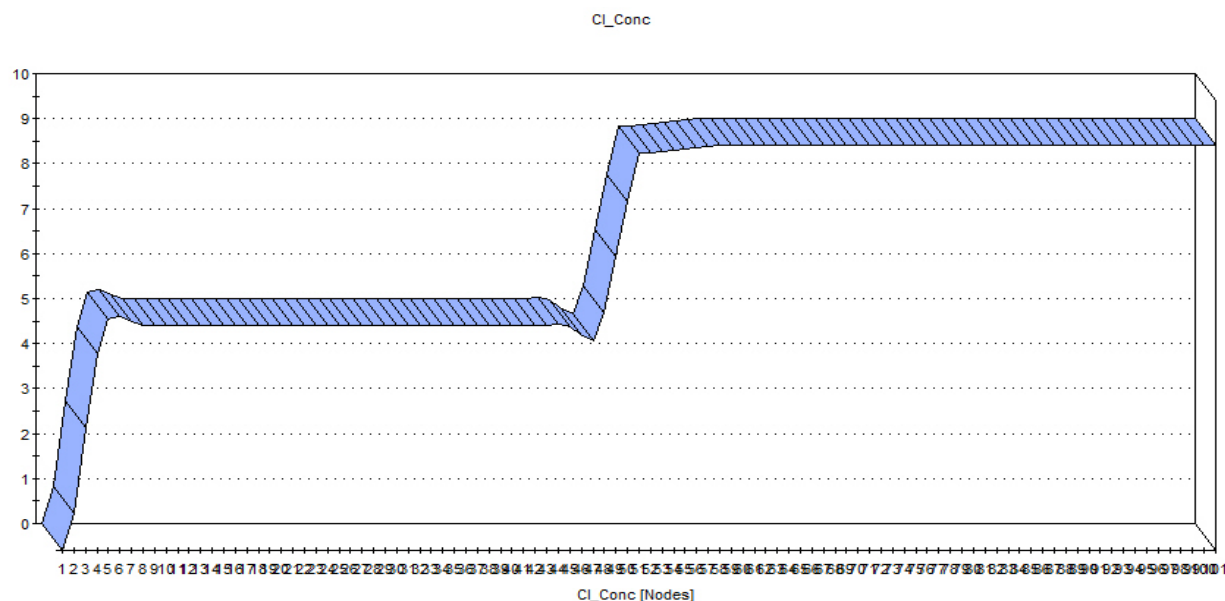
- **Browse Model** – Selecting this button opens the GoldSim model browser (Figure 6-1). The various elements used to define the CBP Software ToolBox can be examined. The components of the ToolBox are described in detail by Smith, et al. (2010b).

- **Simulation Settings (F2)** – Selecting this button opens the **Simulation Settings...** interface shown in Figure 6-19 that allows the user to control temporal and probabilistic settings for the model. *For the GoldSim Player version, the Windows function key* **F2** *is disabled.*

- **Run Simulation (F5)** – Selecting this button runs the simulation, equivalent to selecting **Run** on the **GoldSim Run Controller** (Figure 5-1). *For the GoldSim Player version, the function key* **F5** *is disabled*.

- **Simulation Controls** – Selecting this button returns to the Runs Control Dashboard (Figure 6-4).

6.6 Running a LeachXS™/ORCHESTRA Simulation

As the first step to run a LeachXS™/ORCHESTRA (LXO) simulation, the user should select one of the two LXO scenarios (**Sulfate Attack** or **Carbonation**) from the Combo Box on the Run Controls Dashboard (Figure 6-11); this Dashboard can be opened by clicking on the **Go** button on the **GoldSim Run Controller** and then selecting "**Main_DashBoard**" from the resulting list. When a scenario has been selected in the Combo Box, only its controls are active (and others are grayed and inactive). In general, the color green corresponds to LXO operations and information.
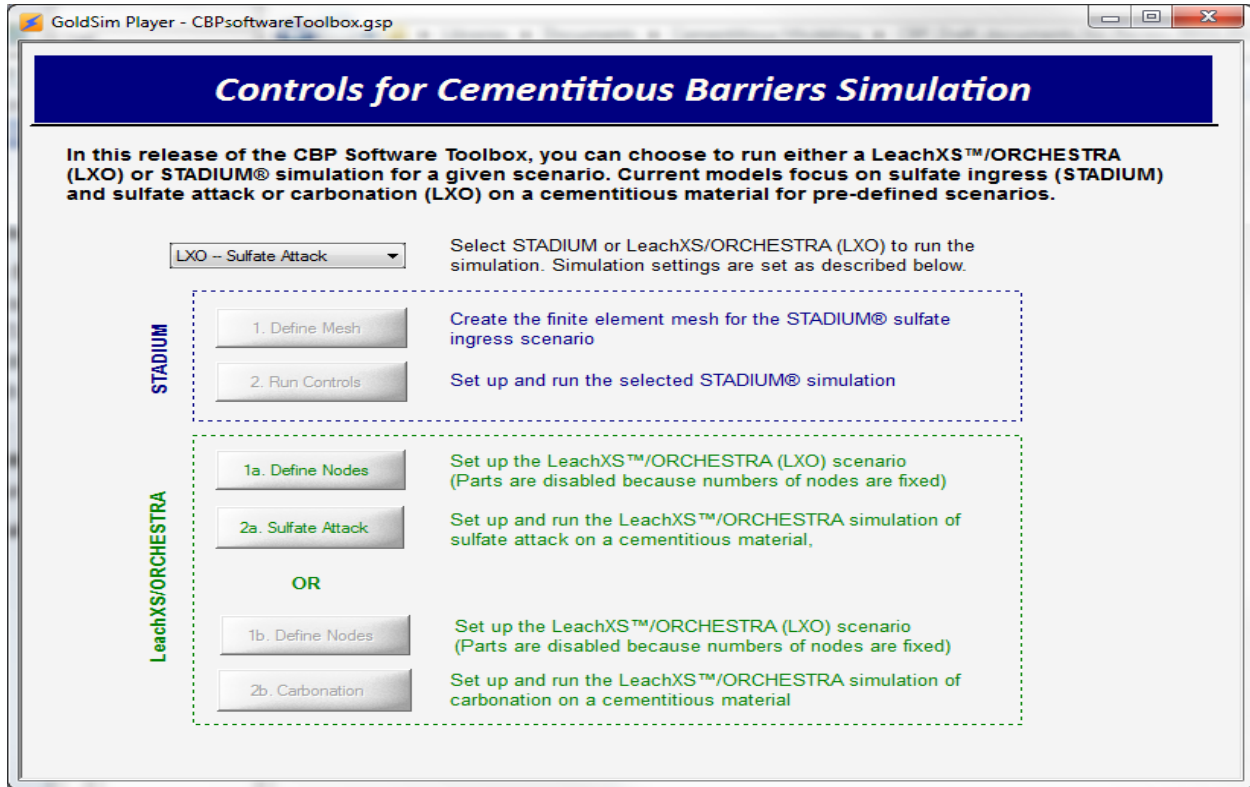
Figure 6-11. Runs Control Dashboard when LeachXS™/ORCHESTRA Sulfate Attack Selected

6.6.1 Simulating Sulfate Attack in LeachXS™/ORCHESTRA

When the "**LXO -- Sulfate Attack**" option is selected from the Combo Box on the **Runs Control Dashboard**, two active control buttons appear in the LeachXS™/ORCHESTRA (LXO) block as shown in Figure 6-11. The top control button, "**1a. Define Nodes**", in the LXO block opens the Dashboard illustrated in Figure 6-12. However, this Dashboard is currently only provided for information purposes because only a one-layer, one-dimensional model (with a boundary condition representing sulfate in an external salt waste layer) is supported based on the work performed by Sarkar (2010). Furthermore, the number of nodes (of constant dimensions) for the sulfate attack model is fixed (at 100) based on previous research.

Other versions of the sulfate attack models including two- and three-layer models with non-uniform node dimensioning have been investigated and will be included in subsequent versions.

Four text control buttons are provided at the bottom of the LXO Node that allow the user direct access to text files that help control the LXO simulation. These controls will be described below. *It is recommended that only experienced users change the information in these files*.

Figure 6-12. The LeachXS™/ORCHESTRA Dashboard for Defining Nodes

The user can return to the Runs Control Dashboard (Figure 6-11) by selecting the **Simulation Controls** button.

The control button entitled "**2a. Sulfate Attack**" in the LXO block opens the **LXO Controls Dashboard** illustrated in Figure 6-13. The LXO Runs Control Dashboard is similar to the STADIUM® Run Controls Dashboard (Figure 6-6). Using the group of inputs labeled "**Scenario and General Options**" on the left hand side of the dashboard, the user selects the concrete representing the vault layer. Currently, only the one-layer, one-dimensional system is modeled.

The layer thickness in meters can also be entered as well as the coefficient of variation (CoV) applied to the initial compositions for use in probabilistic calculations. For probabilistic calculations, it is assumed that the nominal compositions provided in the materials property spreadsheets are mean values of normal distributions with the standard deviations specified by the concentration CoV entries.

The check box entitled "**Treat data uncertainty for concrete compositions**" toggles on/off the treatment of data uncertainty (i.e., data sparseness) for the compositions related to the concrete compositions in the manner according to Sarkar (2010).
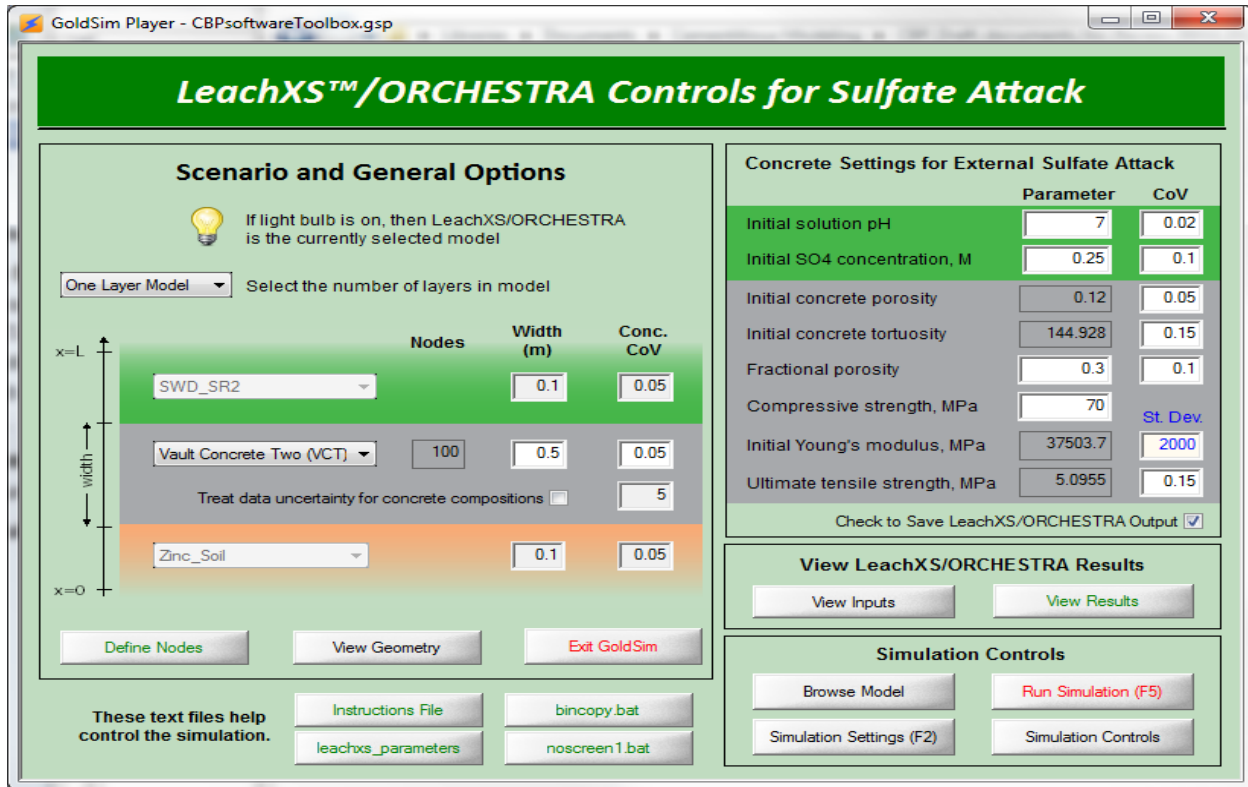
Figure 6-13. LeachXS™/ORCHESTRA Run Controls Dashboard for the Sulfate Attack Scenario

The LXO block labeled "**Concrete Settings for External Sulfate Attack**" contains a set of controls that allow the user to enter parameters related to the external sulfate boundary condition (the pH and SO_4 concentration representing the salt waste in contact with the concrete layer) and the concrete layer. For the concrete, the porosity and tortuosity are taken from a spreadsheet corresponding to the concrete selected. The fractional porosity relates to the sulfate attack model used by Sarkar (2010). *The compressive strength is used to estimate the Young's modulus and tensile strength; these parameters are not entered but are displayed for information purposes*. Values representing the variances in these parameters can also be entered by the user that describes the distributions used for probabilistic analysis as defined by Sarkar (2010).

Below these controls resides a check box where the user selects whether or not to save the output from the LXO calculations. When the **Save** option is checked, the integration software will create files in the **Runs** folder (Figure 5-7) saving output from each realization during a stochastic simulation.

Below the **Scenario and General Options** block on the Run Control Dashboard (Figure 6-13) are a set of control buttons that allow the user direct access to text files that help control the LXO simulation:

- **Instructions File** – Opens the DLL instructions file (e.g., `DLL_LXO_3Layers.dat` for a 3-layer model as shown in Figure 5-3).

- **Input File** – Opens the input template file (i.e., `leachxs_parameters.txt` as shown in Figure 6-14) used by the DLL interface to run the simulation.

- **Copy Batch File** – Opens the Windows batch file (e.g., `bincopy.bat` in Figure 5-4) that copies the files necessary for LXO to run properly.

- **Run Batch File** – Opens the Windows batch file (e.g., `noscreen1.bat` for a 1-layer model as shown in Figure 5-4) that controls execution of LXO.

It is recommended that only experienced users change the information in these files.
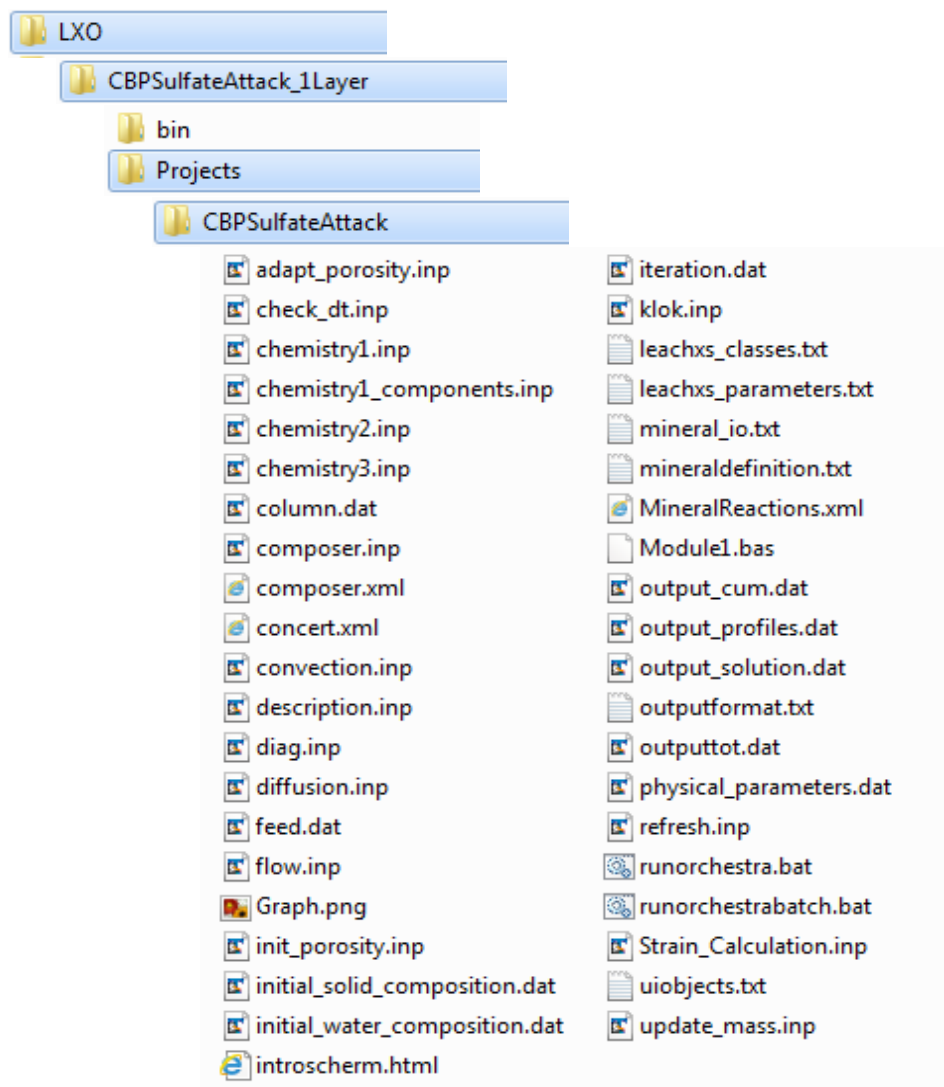

Figure 6-14. Example LeachXS™/ORCHESTRA Model Files (for 1-Layer Sulfate Attack)

6.6.2   Simulating Cement Carbonation in LeachXS™/ORCHESTRA

As the first step to run a LeachXS™/ORCHESTRA (LXO) simulation, the user should select one of the two LXO scenarios (**Sulfate Attack** or **Carbonation**) from the Combo Box on the Run Controls Dashboard (Figure 6-11); this Dashboard can be opened by clicking on the **Go** button on the **GoldSim Run Controller** and then selecting "**Main_DashBoard**" from the resulting list. When a scenario has been selected in the Combo Box, only its controls are active (and others are grayed and inactive).

When the "**LXO -- Carbonation**" option is selected from the Combo Box on the **Runs Control Dashboard** (Figure 6-4), a single active control button appears in the LeachXS™/ORCHESTRA (LXO) block as shown in Figure 6-15. The Runs Control Dashboard can be opened by clicking on the **Go** button on the **GoldSim Run Controller** and then selecting "**Main_DashBoard**" from the resulting list. Unlike the LXO Sulfate Attack model, the top control button, "**1b. Define Nodes**", in the LXO block is inactive because the number of nodes and other information are fixed for this initial version of the carbonation model.

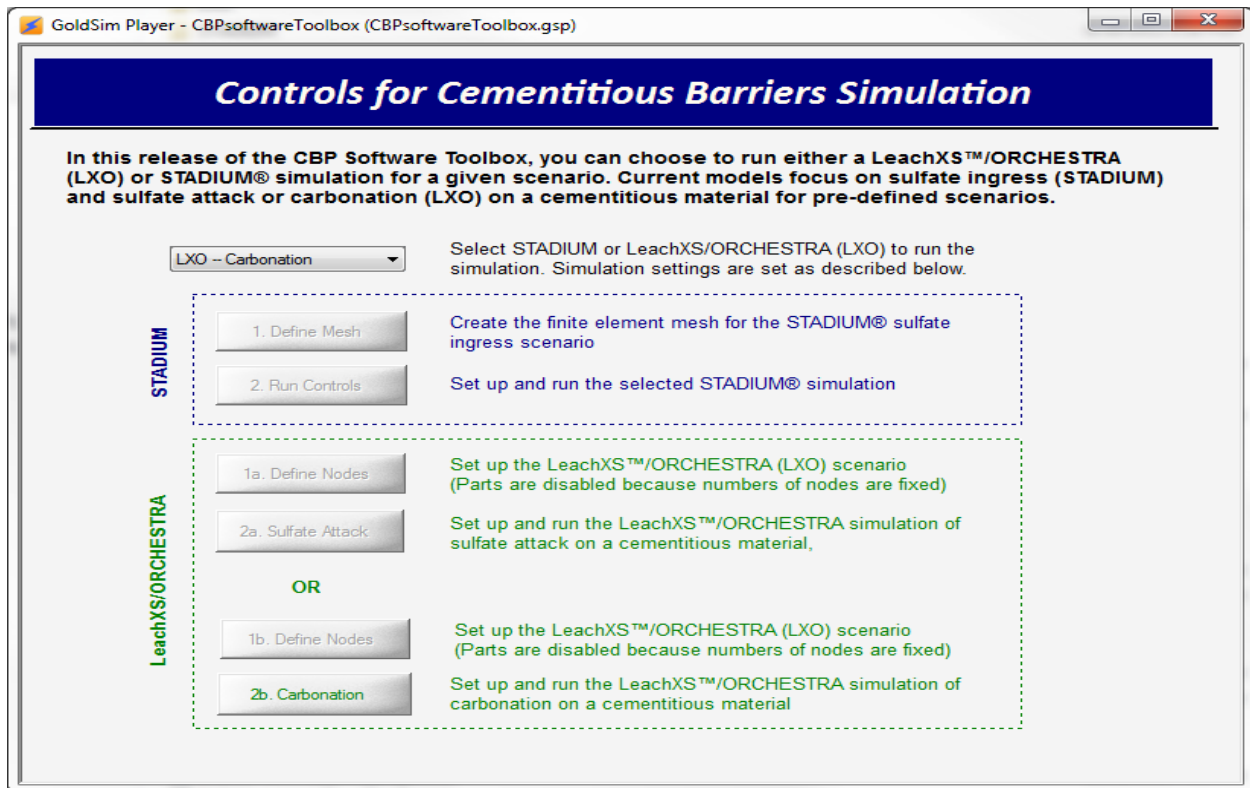**Figure 6-15. Runs Control Dashboard when LeachXS™/ORCHESTRA Carbonation Selected**

The active control button, entitled "**2b. Carbonation**" in the LXO block, opens the **LXO Controls Dashboard** illustrated in Figure 6-16, which is still under development. This LXO Runs Control Dashboard is similar to the STADIUM® Run Controls Dashboard (Figure 6-6). Using the group of inputs labeled "**Scenario and**

General Options" on the left hand side of the dashboard, the user selects the concrete representing the vault layer. Currently, only the one-layer, one-dimensional system is modeled.
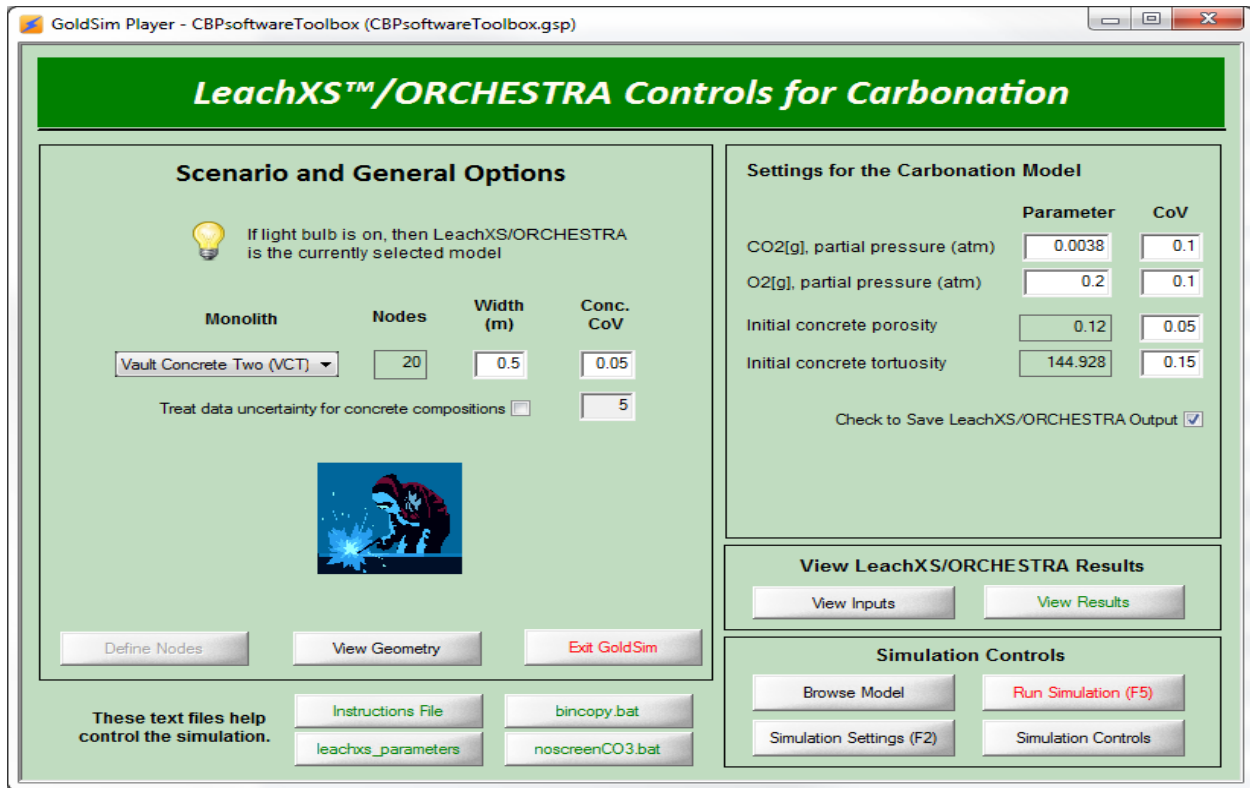

Figure 6-16. LeachXS™/ORCHESTRA Run Controls Dashboard for the Carbonation Scenario

The layer thickness in meters can also be entered as well as the coefficient of variation (CoV) applied to the initial compositions for use in probabilistic calculations. For probabilistic calculations, it is assumed that the nominal compositions provided in the materials property spreadsheets are mean values of normal distributions with the standard deviations specified by the concentration CoV entries.

The check box entitled "**Treat data uncertainty for concrete compositions**" toggles on/off the treatment of data uncertainty (i.e., data sparseness) for the compositions related to the concrete compositions in the manner according to Sarkar (2010).

Four text control buttons are provided at the bottom of the LXO Node that allow the user direct access to text files that help control the LXO simulation. These controls were described in Section 6.6.1 for the LXO Sulfate Attack model. *It is recommended that only expert users change the information in these files*.

The LXO block labeled "**Settings for the Carbonation Model**" contains a set of controls that allow the user to enter parameters related to carbonation of the concrete layer. For the concrete, the porosity and tortuosity are taken from a spreadsheet corresponding to the concrete selected. The partial pressures of CO_2 and O_2 (e.g., that

may change as a function of soil depth for buried structures), can be entered by the user. Values representing the variances in these parameters can also be entered by the user that describes the distributions used for probabilistic analysis.

Below these controls resides a check box where the user selects whether or not to save the output from the LXO calculations. When the **Save** option is checked, the integration software will create files in the **Runs** folder (Figure 5-7) saving output from each realization during a stochastic simulation.

6.6.3 Viewing LeachXS™/ORCHESTRA Inputs and Results

The Run Controls Dashboards for Sulfate Attack (Figure 6-13) and Carbonation (Figure 6-15) contains a **View LeachXS™/ORCHESTRA Results** block that contains two control buttons that allow the user to view inputs to and results from LXO simulations. Selecting the **View Inputs** button opens either the `LXO_Summary.xls` or `LXO_Summary_CO3_by_rows.xls` spreadsheet for the Sulfate Attack or Carbonation model, respectively, that summarizes the LXO input used for each realization in separate worksheets (for Sulfate Attack) or in separate rows (for Carbonation). The Sulfate Attack summary is similar to that for STADIUM® (Figure 6-8); however, the Carbonation Summary displays the information differently (realization by row instead of by worksheet) as illustrated in Figure 6-17. These workbooks are useful for later analysis and may be particularly valuable for stochastic runs where the input values are randomly assigned. Blank worksheets must already exist for each realization in the `LXO_Summary.xls` workbook (for Sulfate Attack). Additional worksheets can be added to the summary workbook as described in Microsoft Excel Help.

Figure 6-17. A Portion of the LXO_Summary_CO3_by_row.xls Workbook

Selecting the **View Results** button opens the Dashboard (Figure 6-18) that allows the user to view graphs of LeachXS™/ORCHESTRA results for selected minerals or chemicals. These graphs are generated using built-in GoldSim plotting functions. The results available for plotting are those transferred back to GoldSim from the LeachXS™/ORCHESTRA output files through the DLL interface.
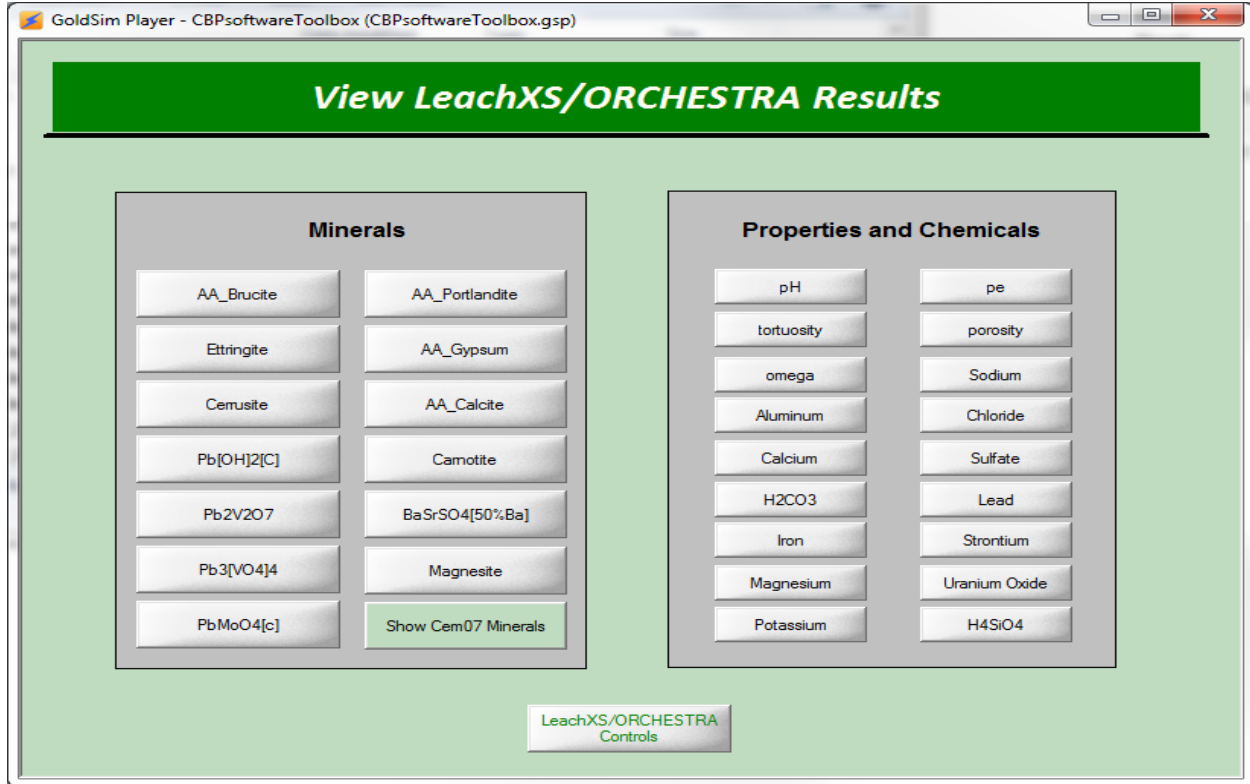
Figure 6-18. Dashboard for selecting a plot of LeachXS™/ORCHESTRA results

GoldSim plotting capabilities are primarily designed to produce time history graphs. Plots of special distributions, which will be of significant interest for evaluating the performance of cementitious materials, can also be created but may not be appropriate for all analyses. An example of such a special plot was shown in Figure 6-10 where the concentration of chlorine (Cl) at each computational node is plotted. The Dashboard controls (Figure 6-18) can be used to generate quick plots of the results; other graphs can be generated by working with the computational results outside of the interface.

6.7 Defining Simulation Settings

There is a control button entitled **Simulation Settings (F2)** located on multiple Dashboard elements in the ToolBox (e.g., Figure 6-6, Figure 6-7, Figure 6-13 and Figure 6-16).Selecting this button opens the **Simulation Settings...** interface shown in Figure 6-19 that allows the user to control temporal and probabilistic settings for the model. *For the GoldSim Player, the Windows function key F2 is disabled.*
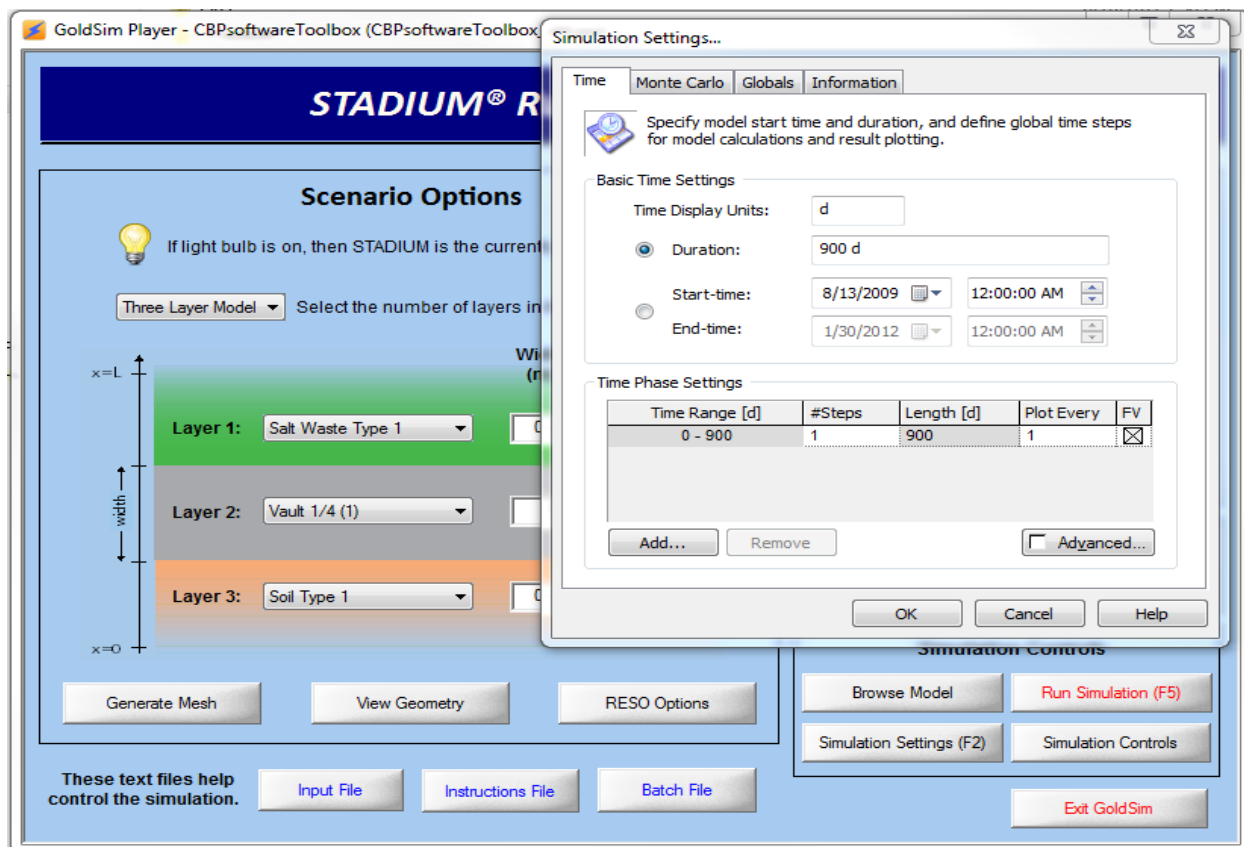
Figure 6-19. GoldSim Simulation Settings window for time control

The first tab (**Time**) on this window is used to control the total simulation time and the time steps used in the model. The simulation duration is passed to STADIUM® as the simulation time by the DLL; however, the STADIUM® time step control is specified separately as discussed in Section 6.4.2. A single GoldSim time step should be specified so that the DLL will only run the codes linked to GoldSim one time (to completion). The final results from the partner code are then transferred to GoldSim by the DLL.

The second tab on the **Simulation Settings...** window (**Monte Carlo**) is used to specify whether a deterministic or Monte Carlo simulation is to be made. For Monte Carlo simulations, this window is also used to set the number of realizations made, which results are saved in memory, and stochastic sampling parameters. An example of the Monte Carlo simulation settings panel is shown in Figure 6-20.
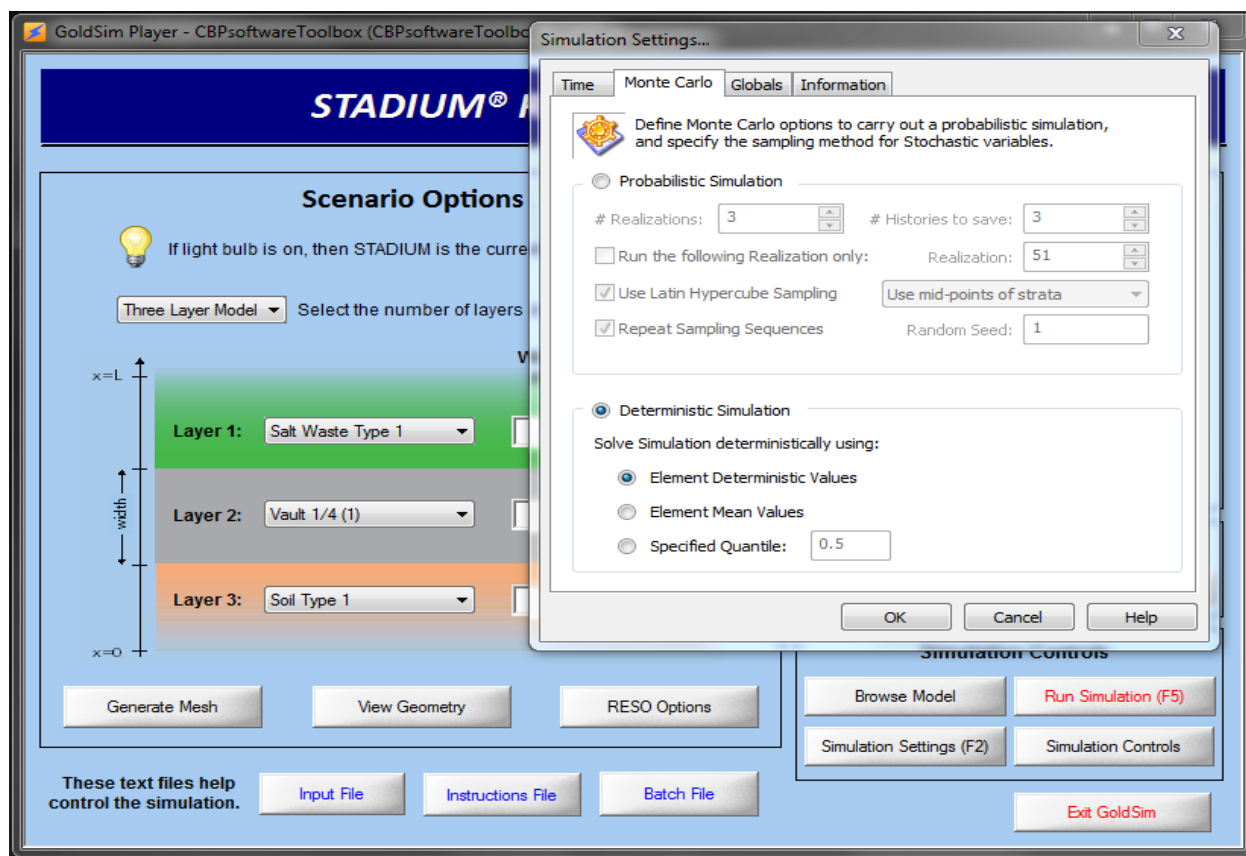
Figure 6-20. GoldSim simulation settings window for Monte Carlo control

6.8 Help

Help is provided for selected general topics concerning the CBP Software ToolBox. The Help facilities are accessed from the Top-Level or Root container (Figure 6-1); a **Quick Start Guide** container has also been provided (explained below) that is accessible from this container. The Top-Level container is generally accessed in the GoldSim Player version by selecting **Go** from the **GoldSim Run Controller** and then "**Go to Model Root…**" from the resulting list. (The **Browse Model** control button on the Run Controls Dashboards will also take the user to the Top Level or Root Container as described in Section 6.5.)

The Help container is on the upper left-hand side of the Top-Level or Root container (Figure 6-1). The Help container is opened by selecting the ⊞ control on the upper left-hand corner of the **Help** icon. The contents of the **Help** container are displayed in Figure 6-21. Each of the subcontainers shown contains material that provides a limited amount of information on the following subjects:

- **CBP_Description** provides a brief description of the CBP project and goals related to the ToolBox.
- **Terminology** provides a listing of relevant terms (ASTM 2008).

- **DOE_Applications** provides illustrations of a number of applications relevant to DOE.

- **DLL_Description** provides a brief description of the Generic Dynamic-link Library developed by the CBP.

- **Partner_Codes** provides brief descriptions of the LeachXS™/ORCHESTRA and STADIUM® partner codes.

- **Nuclear_Facility_Applications** provides illustrations of a number of applications relevant to nuclear facilities.
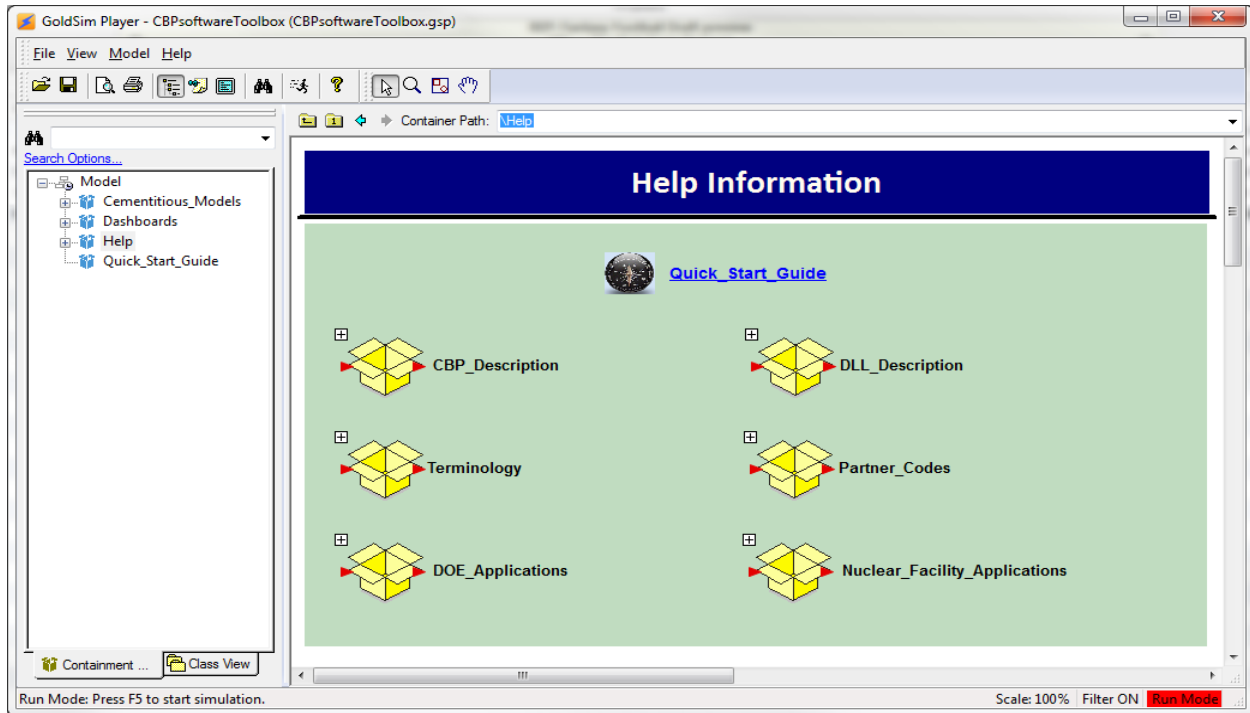

Figure 6-21. Contents of the CBP Software ToolBox Help container

7 TUTORIALS

The design and general operation of the CBP GoldSim Dashboard (GTG 2010a, GTG 2010d) interface to LeachXS™/ORCHESTRA and STADIUM® are presented in the CBP technical reports:

- *CBP Software Summaries for LeachXS™/ORCHESTRA, STADIUM®, THAMES, and GoldSim*, CBP-TR-2009-003 (Brown & Flach 2009a)

- *CBP Phase I Code Integration*, CBP-TR-2011-009-1 (Smith III et al. 2010b)

- *CBP Code Integration GoldSim DLL Interface*, CBP-TR-2010-009-2 (Smith III et al. 2010a)

An example model simulation was provided by Smith, et al. (2010a). Complementary tutorials on specific operations are presented here for the LeachXS™/ORCHESTRA and STADIUM® partner codes. The exercises were developed during user workshops conducted at the National Institute of Standards and Technology (Washington, DC), the Savannah River Site (Aiken, SC), and the Hanford Site (Richland, WA) between April and June 2012.

As described in the CBP Software ToolBox Installation Guide (Brown et al. 2012), the initial installation of the Toolbox includes the **Template** folder (Figure 5-3) that is used as a template for creating new simulations, such as those in the present tutorial exercises. The **Template** folder can be copied as many times as desired to create additional workspaces. The tutorial exercises which follow assume that a copy of the **Template** folder was created and renamed **Tutorials** (Figure 7-1), which will initially have the contents shown in Figure 5-3.
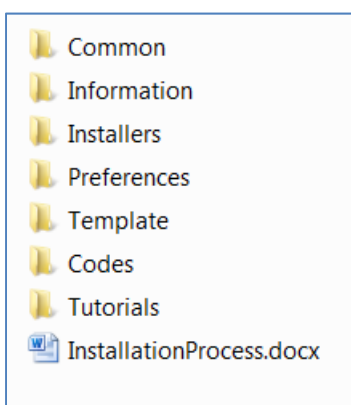

Figure 7-1.   Tutorials folder created by copying the Template folder

7.1 STADIUM® Tutorials

Two STADIUM® tutorials are provided: one deterministic based on default settings and one probabilistic to demonstrate how to modify settings before running a simulation.

7.1.1 STADIUM® Tutorial #1 – Deterministic simulation with default settings

The CBP GoldSim Dashboard interface to STADIUM® comes pre-configured to make a single deterministic simulation of external sulfate ingress / attack on a three-layer, one-dimensional, saltwaste-concrete-soil system. This tutorial is focused on using the Dashboard controls and **GoldSim Run Controller** to open and launch a typical STADIUM® simulation and ensure that STADIUM® is operable on the host computer.

The first step is to launch the GoldSim Player file named "`CBPsoftwareToolbox.gsp`" (Figure 5-3) that opens the Top-Level or Root container shown in Figure 6-1.

Double clicking on the START button shown in Figure 6-1 opens the Simulation Controls Dashboard shown in Figure 6-4, where the user can define the scenario and access simulation controls for the selected partner codes. In general, the color blue corresponds to STADIUM® information.

Next the STADIUM® "**2. Run Controls**" button is selected that takes the user directly to the pre-configured scenario, bypassing the "**Define Mesh**" control for this tutorial. The CBP STADIUM® Runs Control Dashboard (Figure 6-6) and **GoldSim Run Controller** will appear.

The pre-configured scenario is run by either clicking on the "**Run Simulation (F5)**" button on the CBP Runs Control Dashboard or clicking "**Run**" on the **GoldSim Run Controller**. *For the GoldSim Player version, the function key* **F5** *is disabled and will not start the simulation.* When running, a series of command-line windows will appear, with the top-level window running STADIUM®, as shown in Figure 7-2.
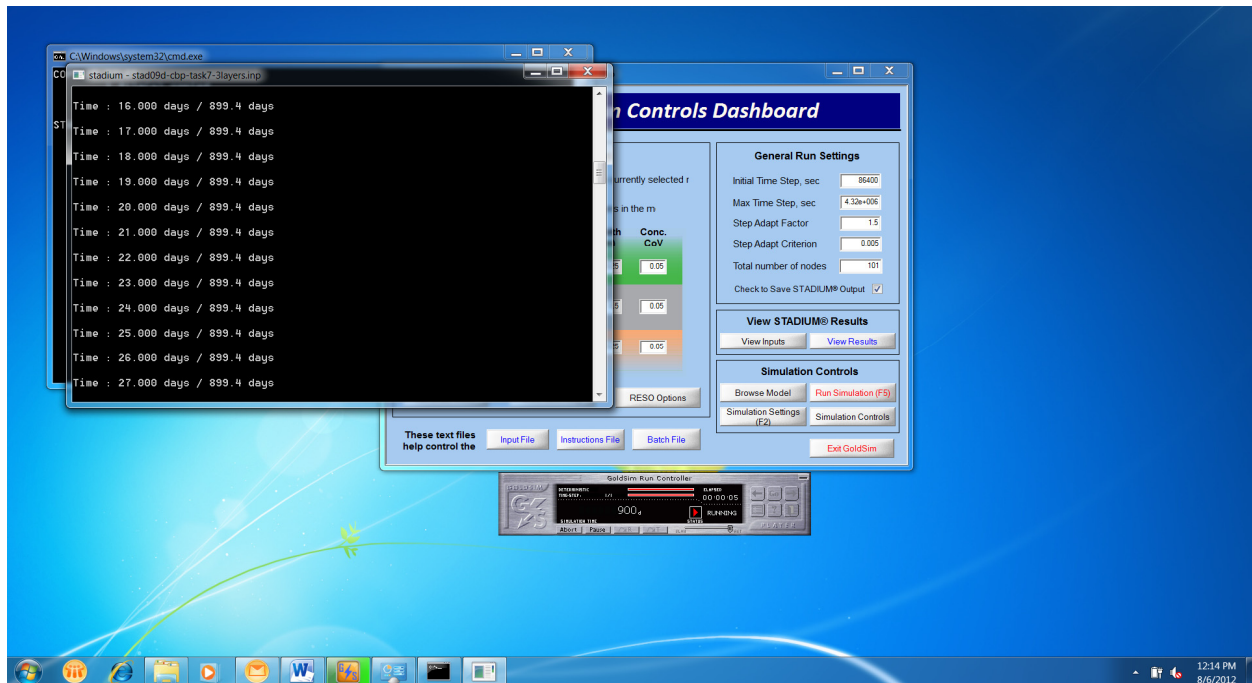
Figure 7-2.   STADIUM® transient simulation in process

The pre-configured scenario is set to run for only a short simulation period, 900 days, and should complete in a few minutes time depending on computer capabilities. GoldSim signals completion of the run as illustrated in Figure 7-3; click "OK" to proceed.
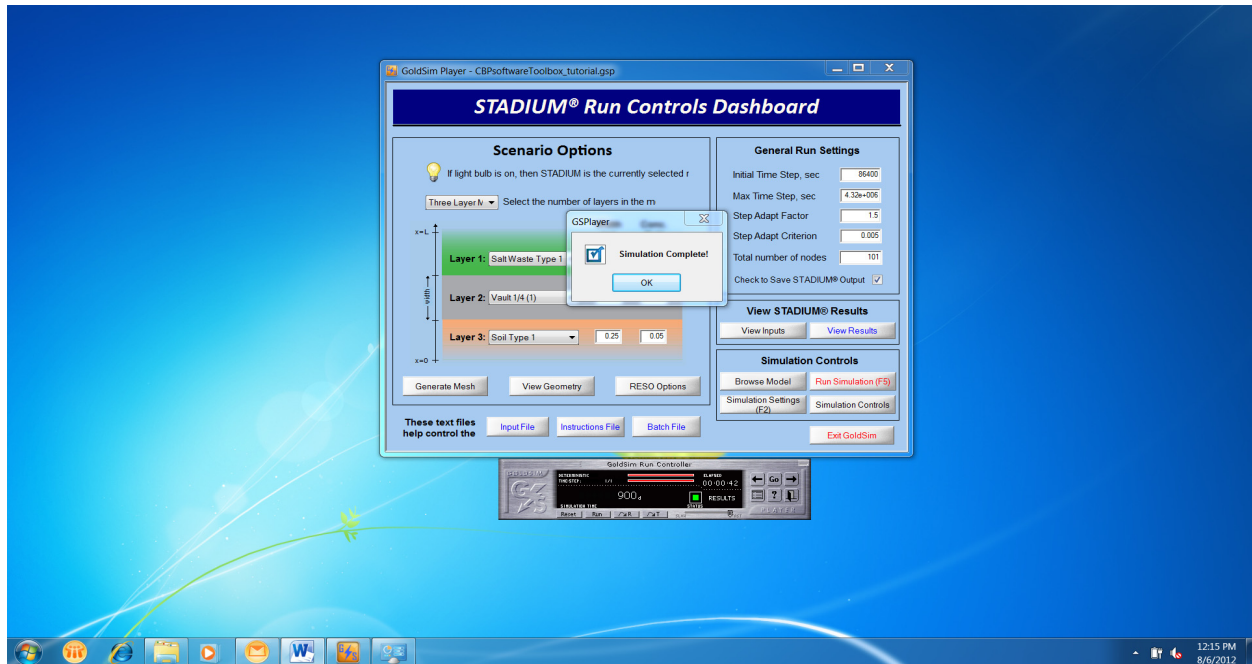
Figure 7-3.   STADIUM® transient simulation at completion

Simulation results can be viewed by pressing the "**View Results**" button (as described in Section 6.4.3). Note that these results are plotted as a function of node number instead of the spatial coordinate (Figure 7-4). The complete set of STADIUM® input and output files for the simulation can be found in the **Runs** folder (Figure 5-7). Deterministic simulation files are placed in a folder named "**realization_0**" (Figure 7-5).
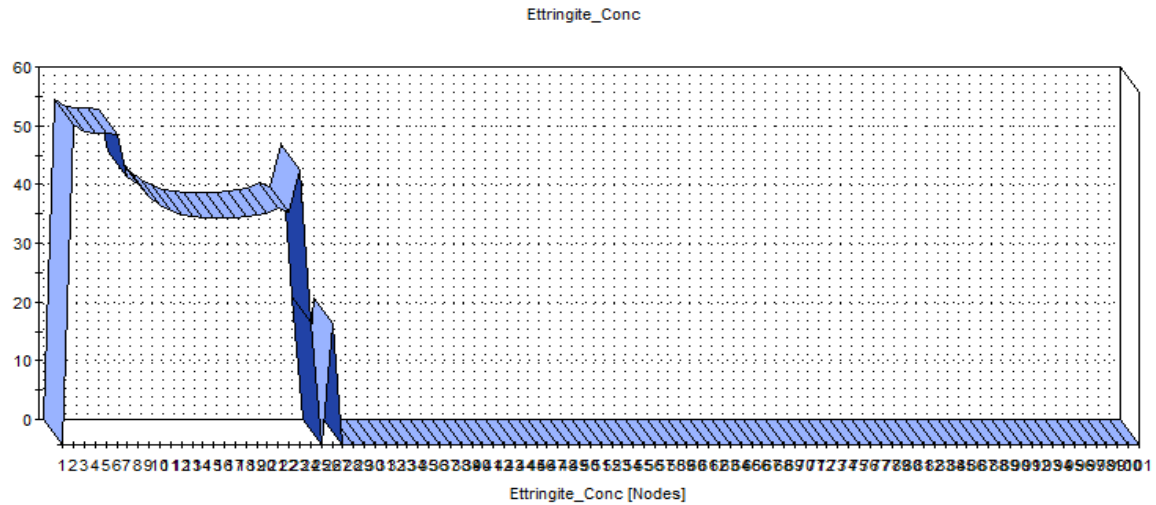
(a)
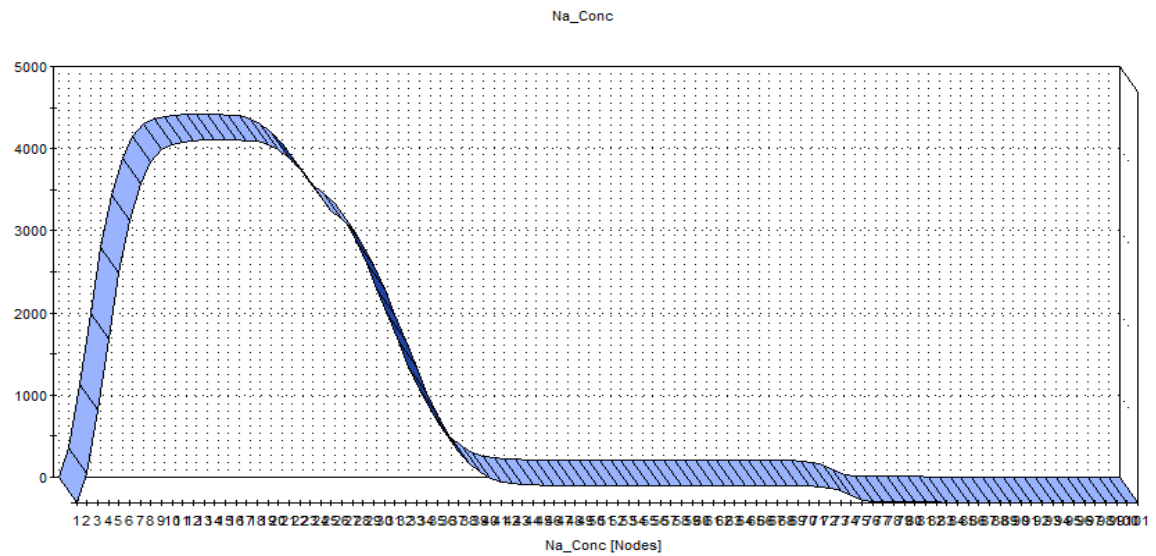
(b)

Figure 7-4.   Example STADIUM® results as a function of node number: (a) ettringite, (b) sodium
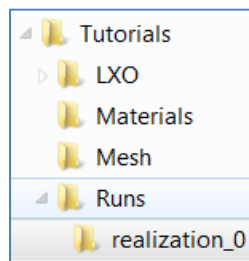
Figure 7-5.   Runs folder containing deterministic simulation results in the "realization_0" folder

7.1.2 STADIUM® Tutorial #2 – Monte Carlo simulation with modified settings

This tutorial modifies the pre-configured STADIUM® scenario using the following steps:

1. Omit the soil layer and switch to a two-layer saltwaste-concrete system
2. Increase the salt waste thickness to 0.5 meters
3. Decrease the total number of computational elements (grid cells) from 100 to 50, 25 in each material, for a total of 51 nodes (i.e., grid vertices).
4. Run three probabilistic (Monte Carlo) simulations

While not comprehensive, this exercise illustrates how to make some of the more likely changes that would be needed to customize the pre-configured scenario. Because the CBP GoldSim Dashboard couples existing stand-alone codes, some changes can be effected directly through Dashboard controls while others are performed through manual edits to input files.

The first step above is an example of changing the simulation using the Dashboards. The scenario is changed from three-layers to two-layers using the pull-down menu in the STADIUM® Run Controls dashboard (Figure 6-6); this change also requires changing the input file to the mesh generation program.

The mesh specifications are accessed from either the Run Controls Dashboard (Figure 6-6) by selecting the "**Generate Mesh**" button or from the Simulation Controls Dashboard (Figure 6-4) by clicking on the "**1. Define Mesh**" button. Either button takes the user to the Mesh Generation Dashboard (Figure 6-5). A user manual for the Mesh2d finite element mesh generation program is available (Flach & Smith III 2012); this document is provided with the CBP Software ToolBox in the **…\Information\Mesh2d** folder.

The "**Open xMesh**" button opens the x-coordinate grid specification input file, named "`xMesh.dat`". Figure 7-6 shows the edits needed for this tutorial, including commenting out the last data line representing the soil layer. The other edits correspond to Steps 2 and 3 (above). The new computational mesh is created by selecting the "**Make Mesh**" button. Selecting the "**Run batch file**" and then "**View batch plot**" buttons will display an image of the grid (Figure 7-7).

```
!iFlag key:
!     0=constant interval
!     1=constant position
!dir key:
!     p=positive
!     n=negative
!     c=center
!     d=disabled
!scheme key:
!     geom=geometric growth factor
!     poly=polynominal transformation
!     prev=previous polynomial transformation
!
!iFlag     nx     dir    scheme        skew  scale dx|x
                                  1      0     !origin at x=0
0      25     c      poly 1.35 0.01  50    50 cm w/1cm spacing
0      25     n      poly 1.56 0.01  50    !50cm w/1cm spacing
!0     25     d      poly 1.   0.01  25    !25cm w/1cm spacing
```

Figure 7-6.   Edits made to the "xMesh.dat" file for STADIUM® Tutorial #2
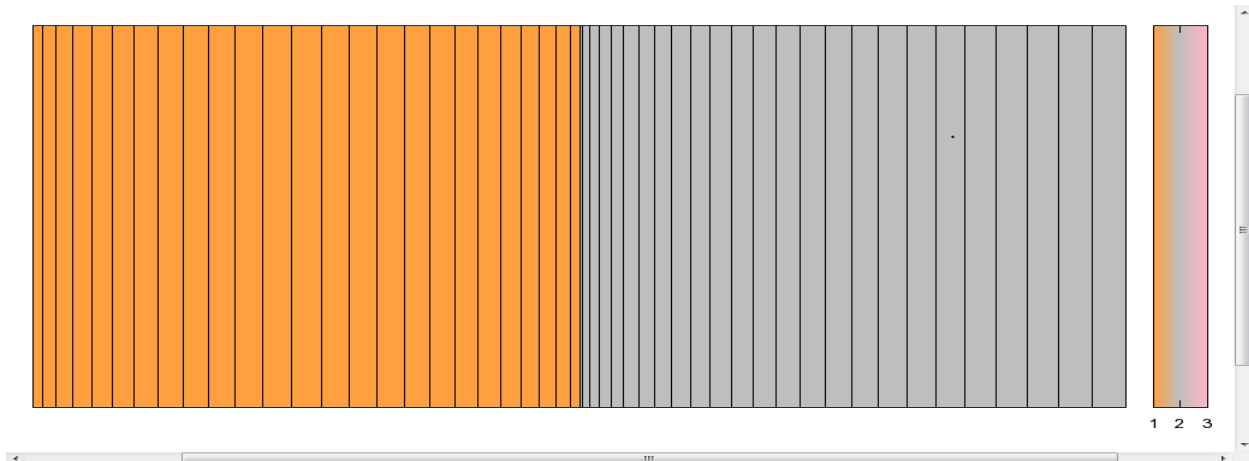
Figure 7-7.   New computational mesh for STADIUM® Tutorial #2

The next step is to open the STADIUM® Run Control Dashboard to make changes; this Dashboard is opened by either selecting the "**STADIUM Controls**" button on the Generate Mesh Dashboard or by selecting Go from the GoldSim Run Controller and then "**STADIUM_DashBoard**" from the resulting list. Figure 7-8 highlights the remaining edits to be made to the Run Controls Dashboard.

Figure 7-8.   Changes to STADIUM® Run Controls Dashboard for Tutorial #2

STADIUM® is a stand-alone program run from the CBP Software ToolBox using a command-line invocation. The ToolBox Dashboards and a supporting library function in an external DLL modify the STADIUM® input files, run the code, and retrieve data from output files following specifications in a "DLL instructions" file. The file is accessed from the "**Instructions File**" button on the Run Controls dashboard. The format of the DLL instructions file is described in *CBP Code Integration GoldSi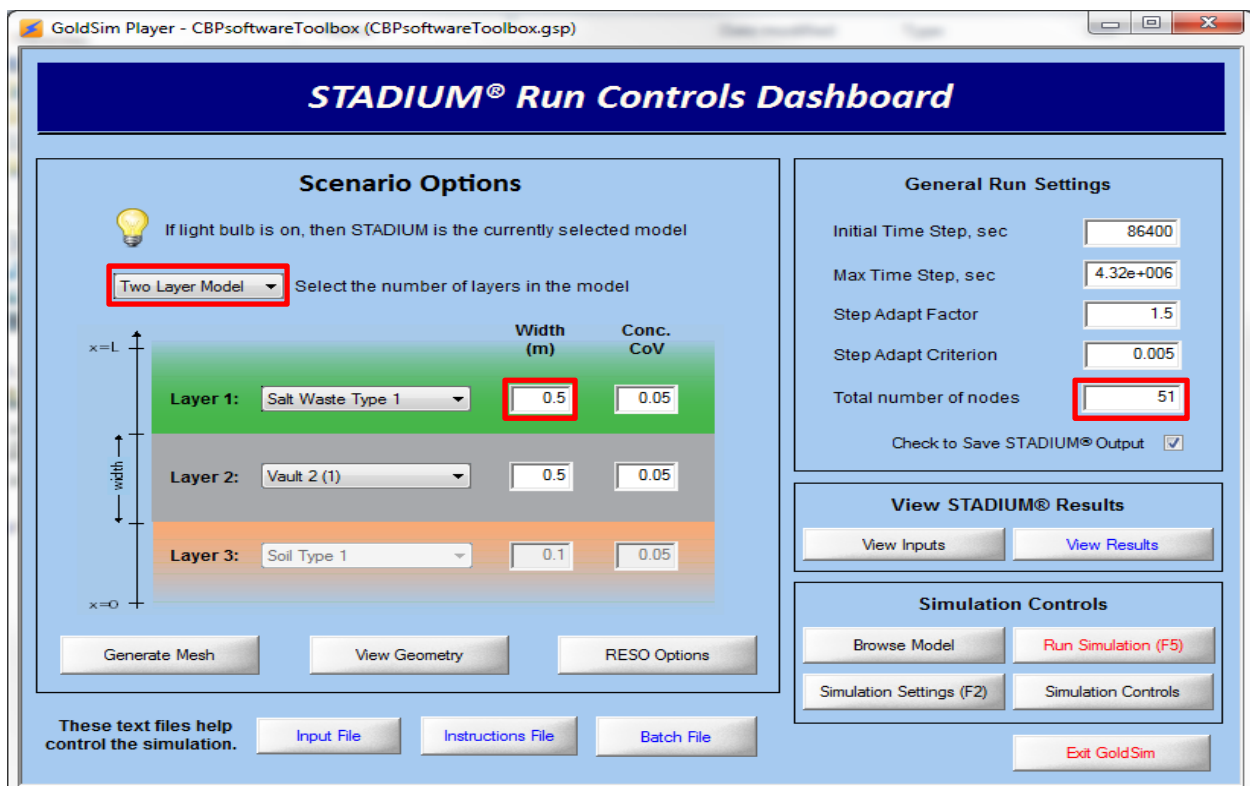m DLL Interface* (Smith III et al. 2010a); this document is provided with the CBP Software ToolBox in the **...\Information\CBP_DLL** folder. Because the grid size was reduced from 101 nodes to 51 nodes (Figure 7-8), the DLL library function must be told to only retrieve 51 values from the output STADIUM® output file. The corresponding edits are shown in Figure 7-9.

```
!-------------------------------------------------------------
GET   stad09d-cbp-task7-2layers.out.xls      space ignore
      1      value 2.0   1      -0.1  col   4              51    11
      3312   value 2.0   1      -0.1  col   18             51    9
```

Figure 7-9.   **Changes** made to the DLL instructions file for STADIUM® Tutorial #2

The final changes are to switch the GoldSim simulation mode from Deterministic to Probabilistic and to specify the number of simulations. Clicking on the "**Simulation Settings (F2)**" button on the Run Controls menu brings up the GoldSim dialog window shown in Figure 7-10, which highlights the required changes.
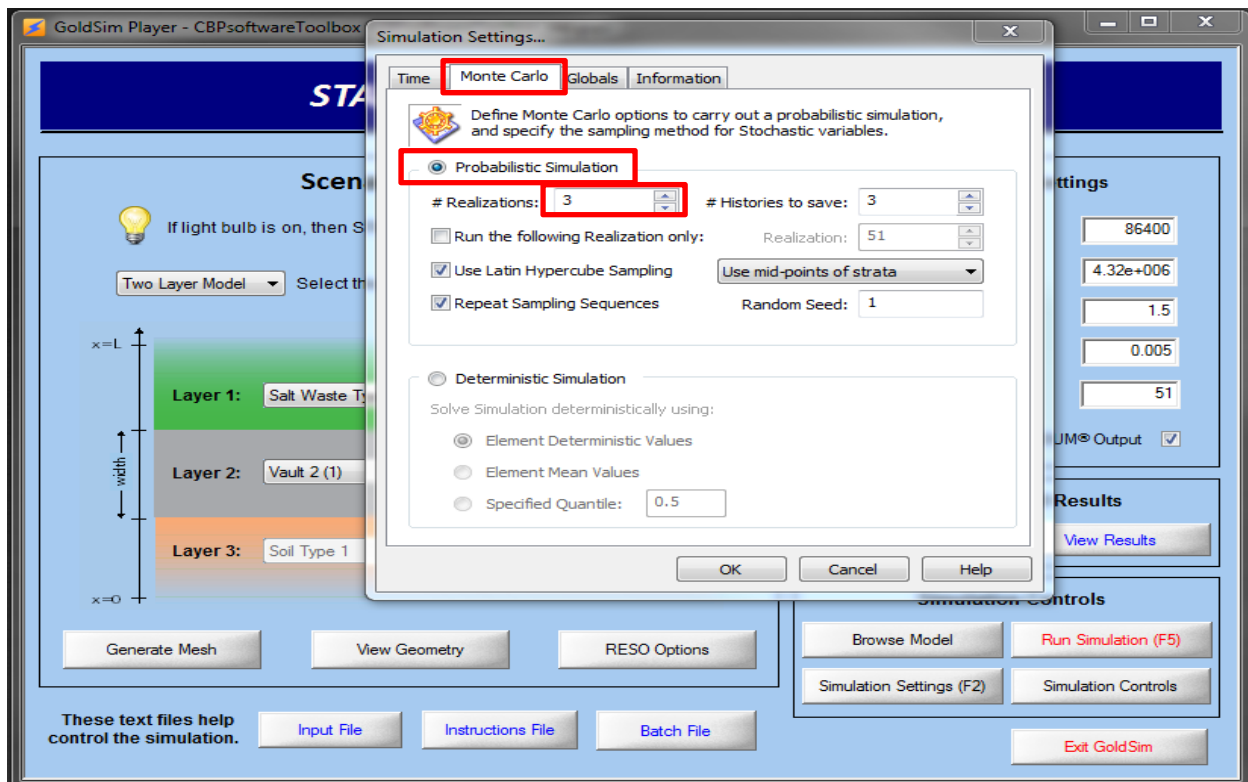

Figure 7-10. Changes to GoldSim Simulation Settings

As with Tutorial #1, STADIUM® simulations are launched either by selecting the "**Run Simulation (F5)**" button on the CBP Runs Dashboard or by selecting "**Run**" on the **GoldSim Run Controller**. *For the GoldSim Player version, the function key* **F5** *is disabled and will not start the simulation.* When running, a series of command-line windows will appear, with the top-level window running STADIUM®, as shown in Figure 7-2.

As before, the simulation time is short, 900 days, so that the three simulations will finish within a reasonable time frame. When all three STADIUM® simulations are complete, a GoldSim dialog window appears as shown in Figure 7-3. If the "**Check to Save STADIUM® Output**" box was checked on the Runs Control Dashboard (Figure 6-6) (current default), then the input and output file from each simulations is saved to the **...\Tutorials\Runs** subfolders "**realization_1**" through "**realization_ 3**" corresponding to the three realizations. If the "**Check to Save STADIUM® Output**" box is unchecked, the all input and output files are successively placed in the "**realization_0**" folder; only the input and output file from the last simulation are preserved.

7.2 LeachXS™/ORCHESTRA (LXO) Tutorials

A set of LeachXS™/ORCHESTRA tutorials are provided in this guide: one based on deterministic sulfate attack using default settings, one probabilistic sulfate attack simulation to demonstrate how to modify settings before running a simulation, and a deterministic cement carbonation simulation.

7.2.1 LXO Tutorial #1 – Deterministic Sulfate Attack simulation with default settings

The CBP GoldSim Dashboard interface comes pre-configured to make a single deterministic STADIUM® simulation of external sulfate ingress/attack on a three-layer system (Section 7.1.1). This tutorial is instead focused on using the Dashboard controls and **GoldSim Run Controller** to open and launch a typical LeachXS™/ORCHESTRA (LXO) sulfate attack simulation on a one-layer, one-dimensional, concrete vault (with a boundary condition representing salt waste) and to ensure that LXO is operable on the host computer.

The first step is to launch the GoldSim Player file named "CBPsoftwareToolbox.gsp" (Figure 5-3) that opens the Top-Level or Root container shown in Figure 6-1. Double clicking on the **START** button shown in Figure 6-1 opens the Simulation Controls Dashboard shown in Figure 6-4, where the user can define the scenario and access simulation controls for the selected partner codes. In general, the color green corresponds to LXO information.

The "**LXO -- Sulfate Attack**" option should be selected from the Combo Box on the **Runs Control Dashboard**; two active control buttons appear in the LXO block as shown in Figure 6-11.

Next the LXO "**2a. Sulfate Attack**" button is selected that takes the user directly to the pre-configured LXO scenario, bypassing the "**1a. Define Nodes**" control for this tutorial. The CBP LXO Runs Control Dashboard (Figure 6-13) and **GoldSim Run Controller** will appear.

The pre-configured scenario is run by either clicking on the "**Run Simulation (F5)**" button on the CBP Runs Control Dashboard or clicking "**Run**" on the **GoldSim Run Controller**. *For the GoldSim Player version, the function key* **F5** *is disabled and will not start the simulation.* When running, a series of command-line windows will appear as shown in Figure 7-11 and then LeachXS™/ORCHESTRA appears as shown in Figure 7-12.
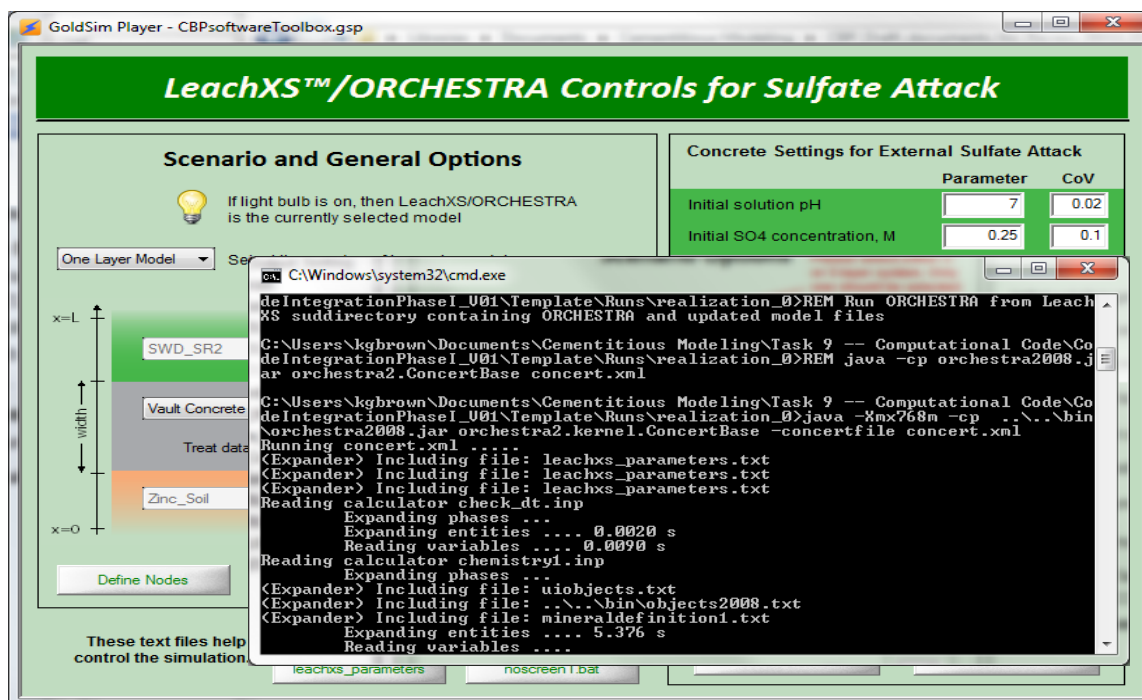
Figure 7-11. LeachXS™/ORCHESTRA transient simulation in process
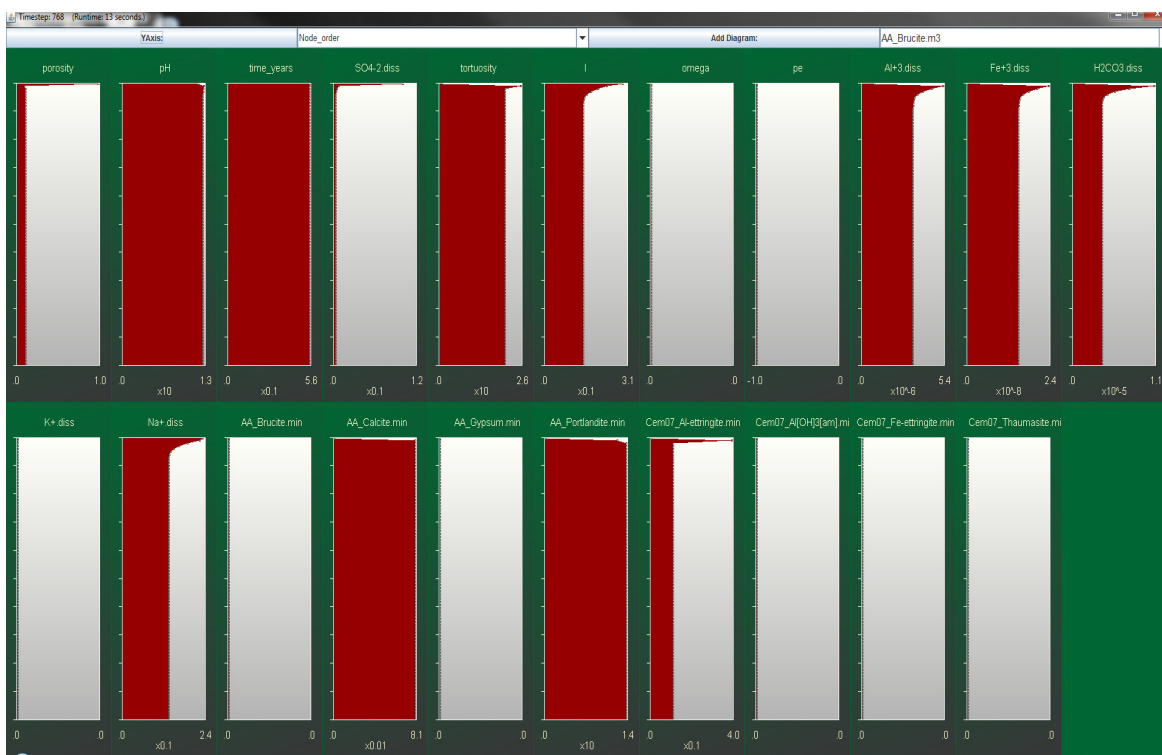

Figure 7-12. LeachXS™/ORCHESTRA running during a simulation

The pre-configured scenario is set to run for only a short simulation period, 900 days, and should complete in a few minutes time depending on computer capabilities. GoldSim signals completion of the run as illustrated in Figure 7-13; click "**OK**" to proceed.
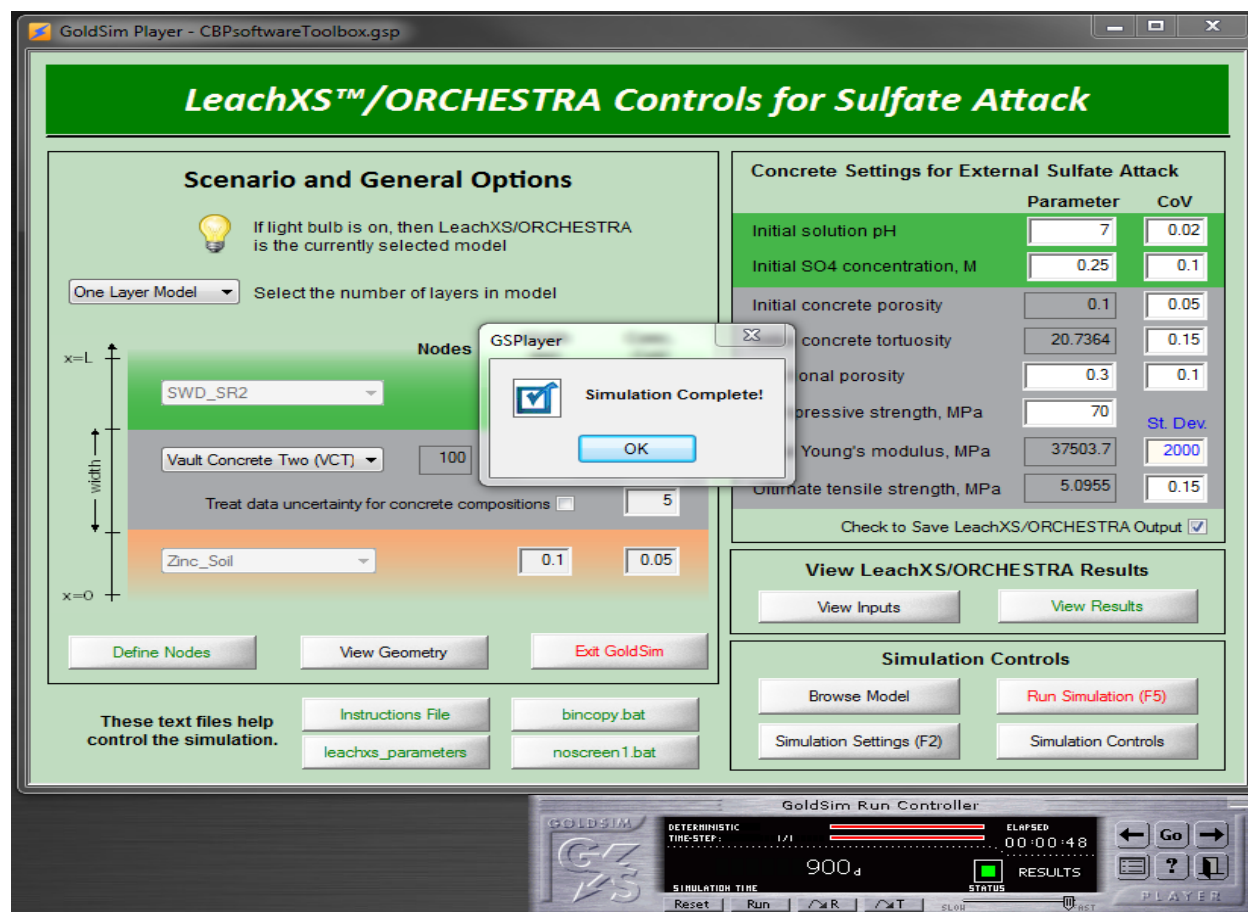
Figure 7-13. LeachXS™/ORCHESTRA transient simulation at completion

Simulation results can be viewed by pressing the "**View Results**" button (as described in Section 6.6.3). Note that these results are plotted as a function of node number instead of the spatial coordinate (Figure 7-14). The complete set of LXO input and output files for the simulation can be found in the **Runs** folder (Figure 5-7). Deterministic simulation files are placed in a folder named "**realization_0**" (Figure 7-5).

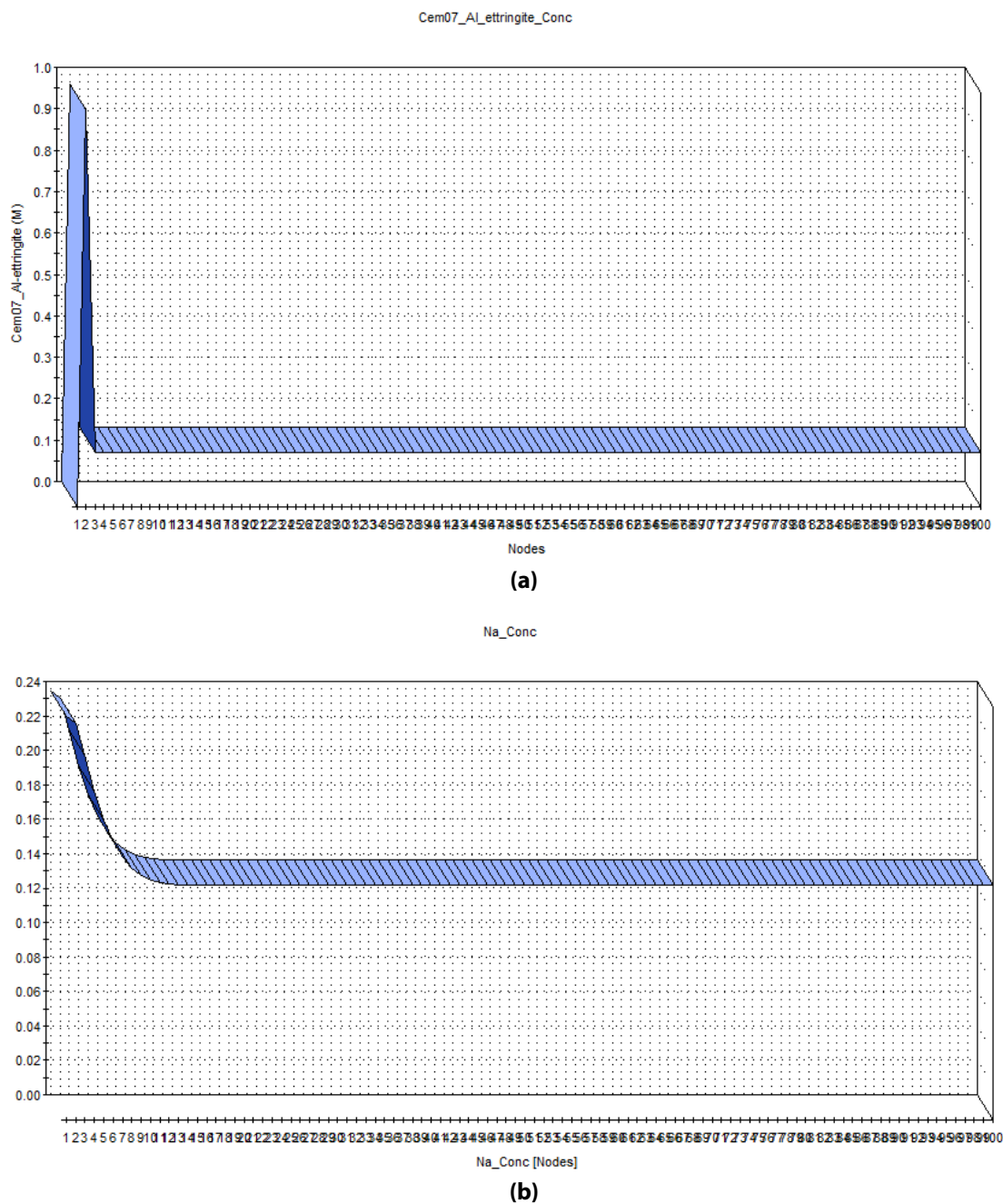**Figure 7-14. Example LeachXS™/ORCHESTRA results by node number: (a) ettringite, (b) sodium**

7.2.2   LXO Tutorial #2 – Monte Carlo sulfate attack simulation with modified settings

This tutorial modifies the pre-configured LeachXS™/ORCHESTRA (LXO) scenario using the following steps:

1. Change the concrete composition to Vault Concrete One (VCO)
2. Decrease the concrete vault thickness to 0.25 meters
3. Increase the initial sulfate (SO_4) concentration to 0.5M
4. Run three probabilistic (Monte Carlo) simulations

While not comprehensive, this exercise illustrates how to make some of the more likely changes that would be needed to customize the pre-configured LXO scenario. Because the CBP GoldSim Dashboard links to existing stand-alone codes, some changes can be made directly through Dashboard controls while others must be performed through manual edits to input files.

The changes for this tutorial are examples of changing the simulation using the Dashboards. The concrete composition is changed using the appropriate pull-down menu in the LXO Controls Dashboard (Figure 6-11). The other changes (#2 and #3) are made using the LXO Controls Dashboard as highlighted in Figure 7-15.

No changes made for this tutorial require changing any of the instructions or template text files as described in Section 6.6.1; all changes are made using Dashboard controls.

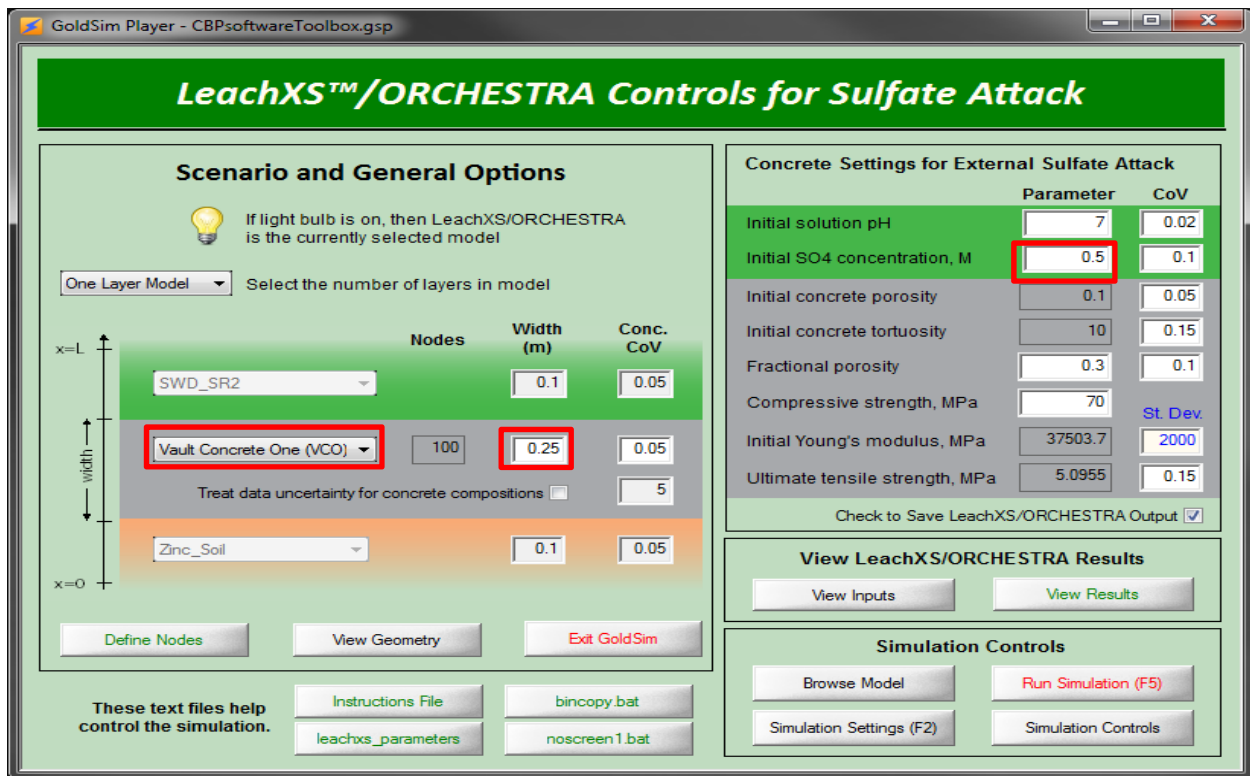**Figure 7-15. Changes to LeachXS™/ORCHESTRA Run Controls Dashboard for Tutorial #2**

The final changes are to switch the GoldSim simulation mode from Deterministic to Probabilistic and to specify the number of simulations. Clicking on the "**Simulation Settings (F2)**" button on the Run Controls menu brings up the GoldSim dialog window shown in Figure 7-16, which highlights the required changes.
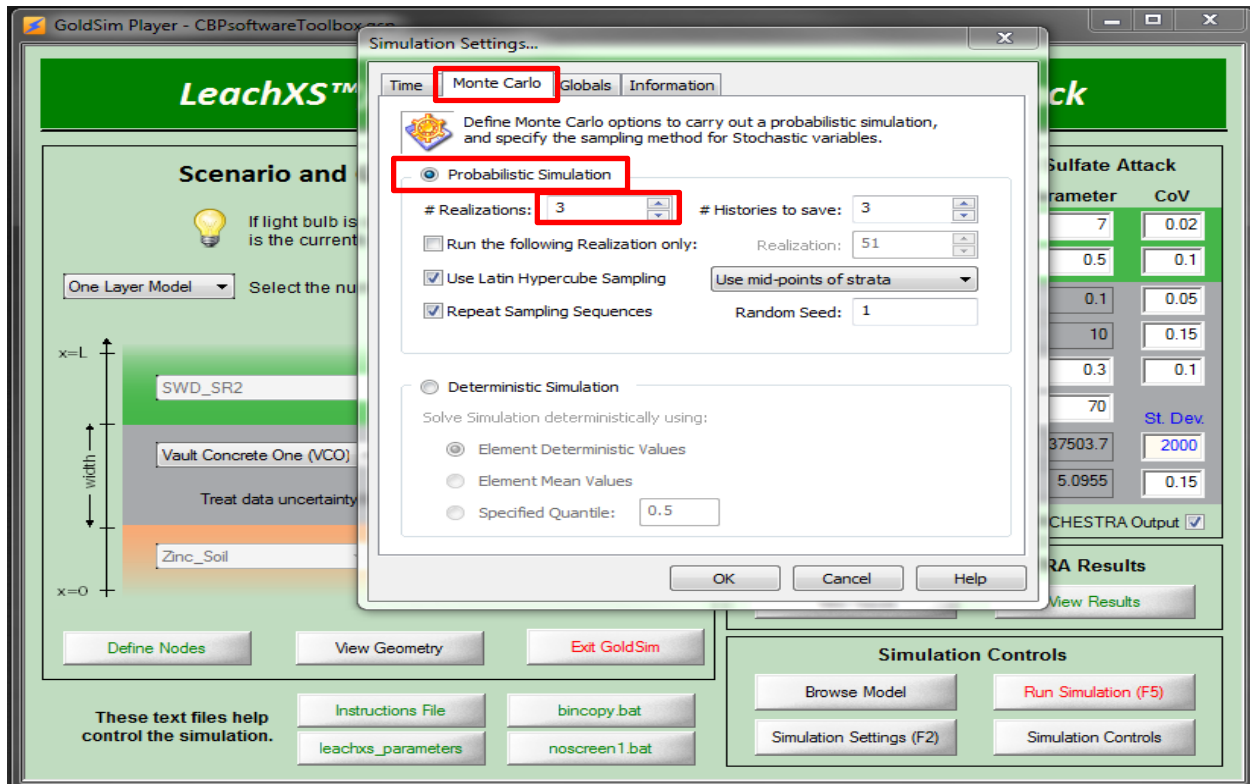
Figure 7-16. Changes to GoldSim Simulation Settings for LeachXS™/ORCHESTRA Tutorial #2

LXO simulations are launched either by selecting the "**Run Simulation (F5)**" button on the Runs Dashboard or by selecting "**Run**" on the **GoldSim Run Controller**. *For the GoldSim Player version, the function key **F5** is disabled and will not start the simulation.* When running, a series of command-line windows will appear as shown in Figure 7-11 and then LeachXS™/ORCHESTRA appears as shown in Figure 7-12.

The simulation time is short, 900 days, so that the three simulations will finish within a reasonable time frame. When all three LXO simulations are complete, a GoldSim dialog window appears as shown in Figure 7-13. If the "**Check to Save STADIUM® Output**" box was checked on the Runs Control Dashboard (Figure 6-6) (current default), then the input and output file from each simulations is saved to the **...\Tutorials\Runs** subfolders "**realization_1**" through "**realization_ 3**" corresponding to the three realizations. If the "**Check to Save LeachXS/ORCHESTRA Output**" box is unchecked, the all input and output files are successively placed in the "**realization_0**" folder; only the input and output file from the last simulation are preserved.

Simulation results can be viewed by pressing the "**View Results**" button (as described in Section 6.6.3). Note that these results are plotted as a function of node number instead of the spatial coordinate (Figure 7-17). The complete set of LXO input and output files for the simulation can be found in the **Runs** folder (Figure 5-7). Deterministic simulation files are placed in a folder named "**realization_0**" (Figure 7-5).
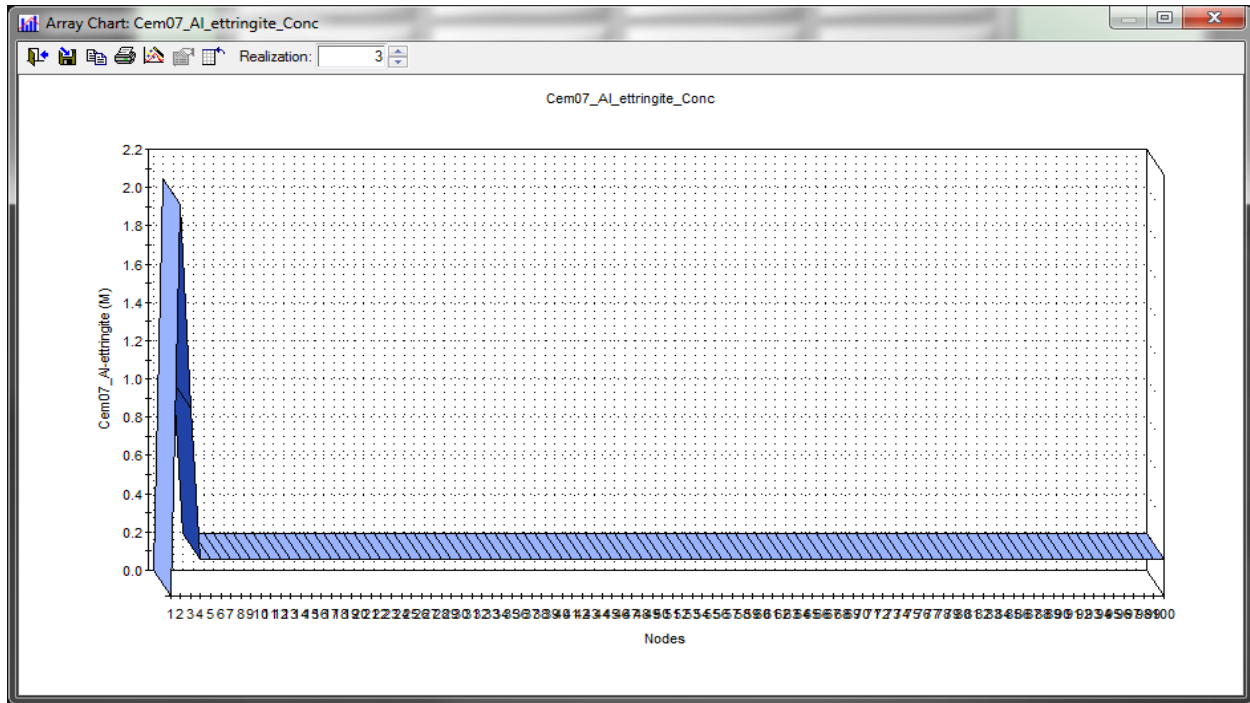
(a) **Ettringite**
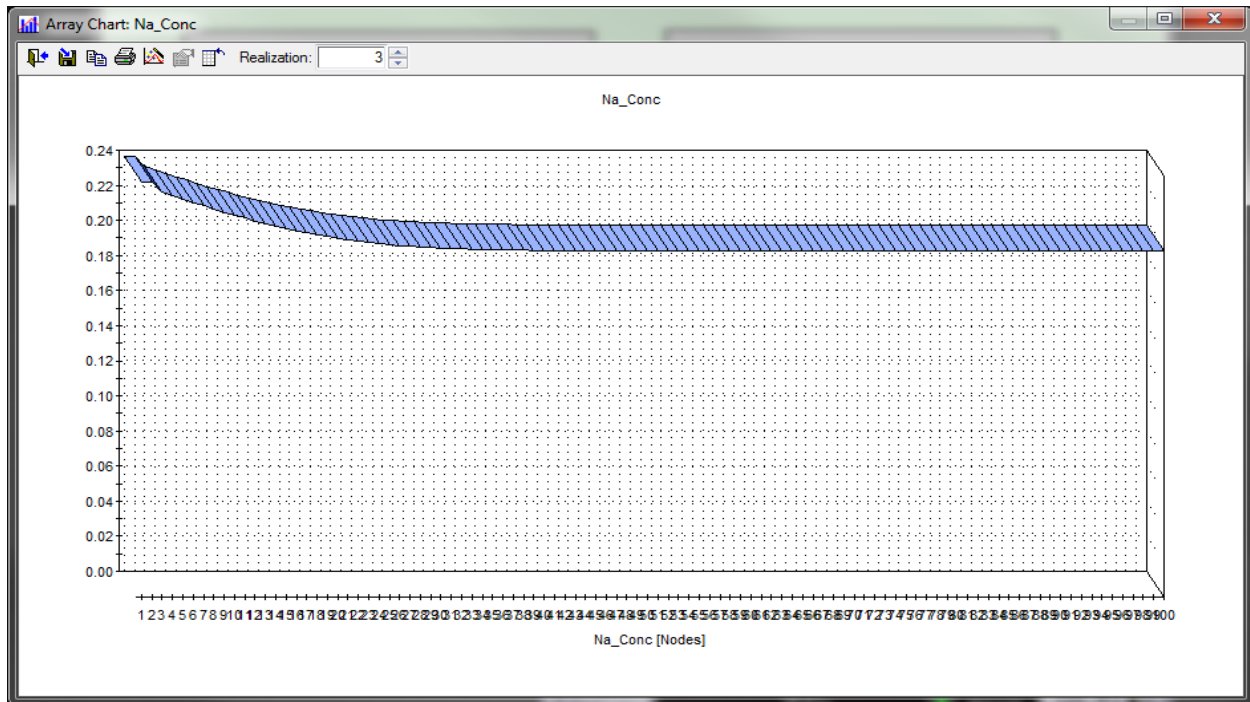
(b) **Sodium**

Figure 7-17. Example LeachXS™/ORCHESTRA probabilistic results by node for third realization

7.2.3   LXO Tutorial #3 – Deterministic carbonation simulation with modified settings

The CBP GoldSim Dashboard interface comes pre-configured to make a single deterministic STADIUM® simulation of external sulfate ingress/attack on a three-layer system (Section 7.1.1). This tutorial is instead focused on using the Dashboard controls and **GoldSim Run Controller** to launch a LeachXS™/ORCHESTRA (LXO) cement carbonation simulation on a one-layer, one-dimensional, concrete monolith and to ensure that LXO is operable on the host computer.

The first step is to launch the GoldSim Player file named "`CBPsoftwareToolbox.gsp`" (Figure 5-3) that opens the Top-Level or Root container (Figure 6-1). Double clicking on the **START** button shown in Figure 6-1 opens the Simulation Controls Dashboard (Figure 6-4), where the user can define the scenario and access simulation controls for the selected partner codes. In general, the color green corresponds to LXO information.

The "**LXO -- Carbonation**" option is selected from the Combo Box on the **Runs Control Dashboard**; a single, active control button appears in the LXO block as shown in Figure 6-15.

Next the LXO "**2b. Carbonation**" button is selected that takes the user directly to the LXO Carbonation scenario. The appropriate CBP LXO Run Controls Dashboard (Figure 6-16) and **GoldSim Run Controller** appears.

This tutorial modifies the pre-configured LeachXS™/ORCHESTRA Carbonation scenario using the following steps:

1. Change the concrete composition to Standard Vault Concrete (SVC)
2. Decrease the concrete vault thickness to 0.25 meters
3. Increase the $CO_2(g)$ partial pressure to 0.0050 atm

While not comprehensive, this exercise illustrates how to make some of the more likely changes that would be needed to customize the pre-configured LXO scenario. Because the CBP GoldSim Dashboard links to existing stand-alone codes, some changes can be made directly through Dashboard controls while others must be performed through manual edits to input files.

The changes for this tutorial are examples of changing the simulation using the Dashboards. The concrete composition is changed using the appropriate pull-down menu in the LXO Controls Dashboard (Figure 6-16). The other changes (#2 and #3) are made using the LXO Controls Dashboard as highlighted in Figure 7-18.

No changes made for this tutorial require changing any of the instructions or template text files as described in Section 6.6.1; all changes are made using Dashboard controls.
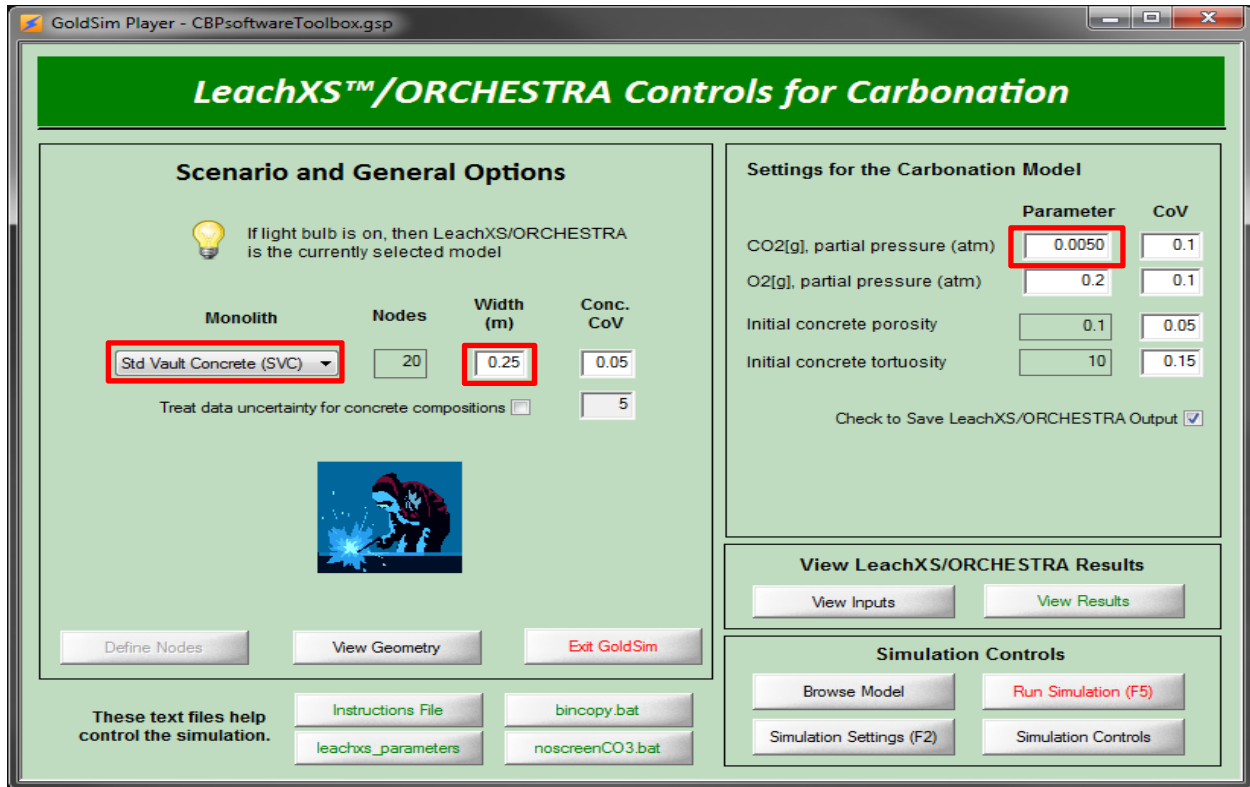
Figure 7-18. Changes to LeachXS™/ORCHESTRA Run Controls Dashboard for Tutorial #3

The LXO Carbonation scenario is run by either clicking on the "**Run Simulation (F5)**" button on the CBP Runs Control Dashboard or clicking "**Run**" on the **GoldSim Run Controller**. *For the GoldSim Player version, the function key* **F5** *is disabled and will not start the simulation.* When running, a series of command-line windows will appear as shown in Figure 7-19 and then LeachXS™/ORCHESTRA appears as shown in Figure 7-20.

Figure 7-19. LeachXS™/ORCHESTRA transient carbonation simulation in process

Figure 7-20. LeachXS™/ORCHESTRA running during a simulation

The LXO Carbonation scenario is set to run for only a short simulation period, 900 days, and should complete in a few minutes time depending on computer capabilities. GoldSim signals completion of the run as illustrated in Figure 7-21; click "**OK**" to proceed.
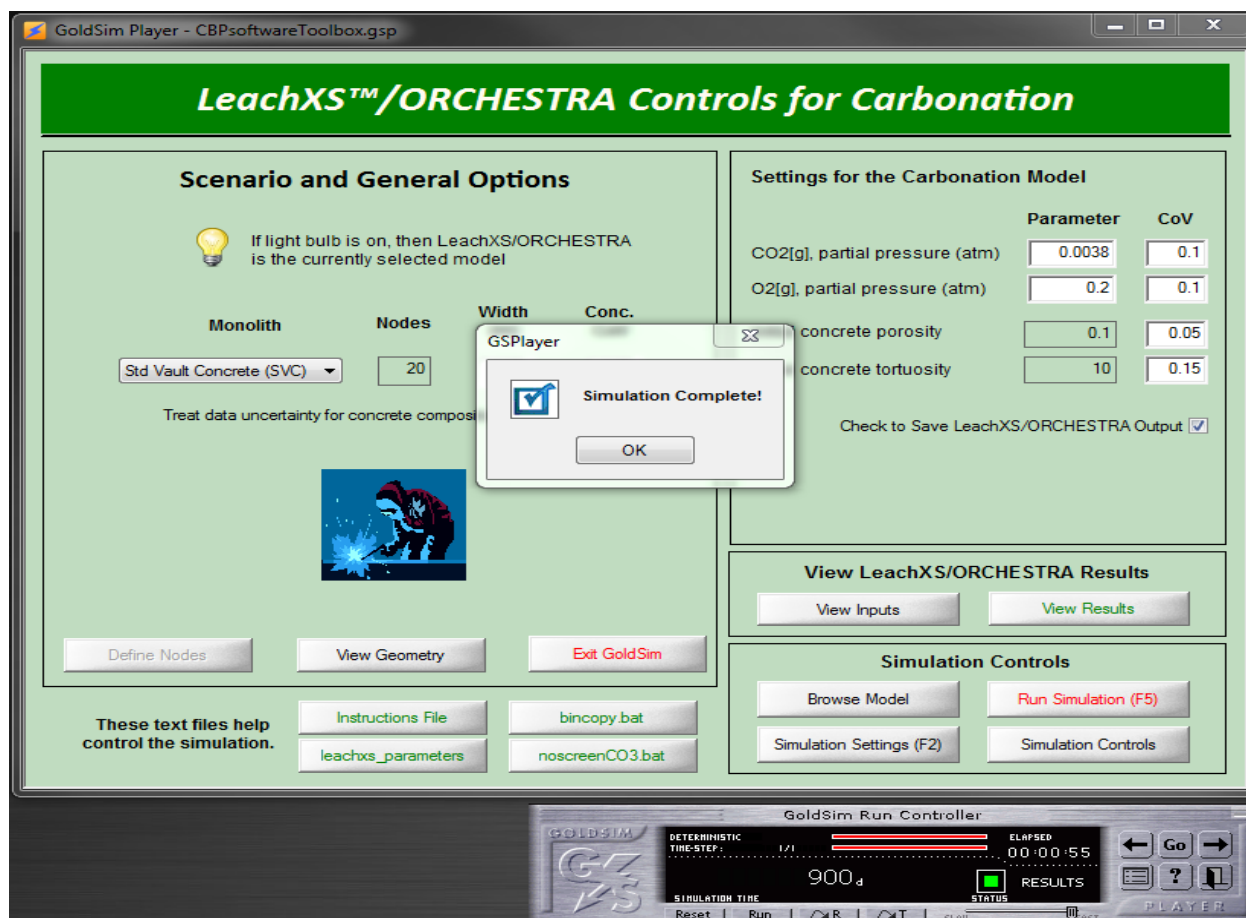

Figure 7-21. LeachXS™/ORCHESTRA transient simulation at completion

Simulation results can be viewed by pressing the "**View Results**" button (as described in Section 6.6.3). Note that these results are plotted as a function of node number instead of the spatial coordinate (Figure 7-22). The complete set of LXO input and output files for the simulation can be found in the **Runs** folder (Figure 5-7). Deterministic simulation files are placed in a folder named "**realization_0**" (Figure 7-5).
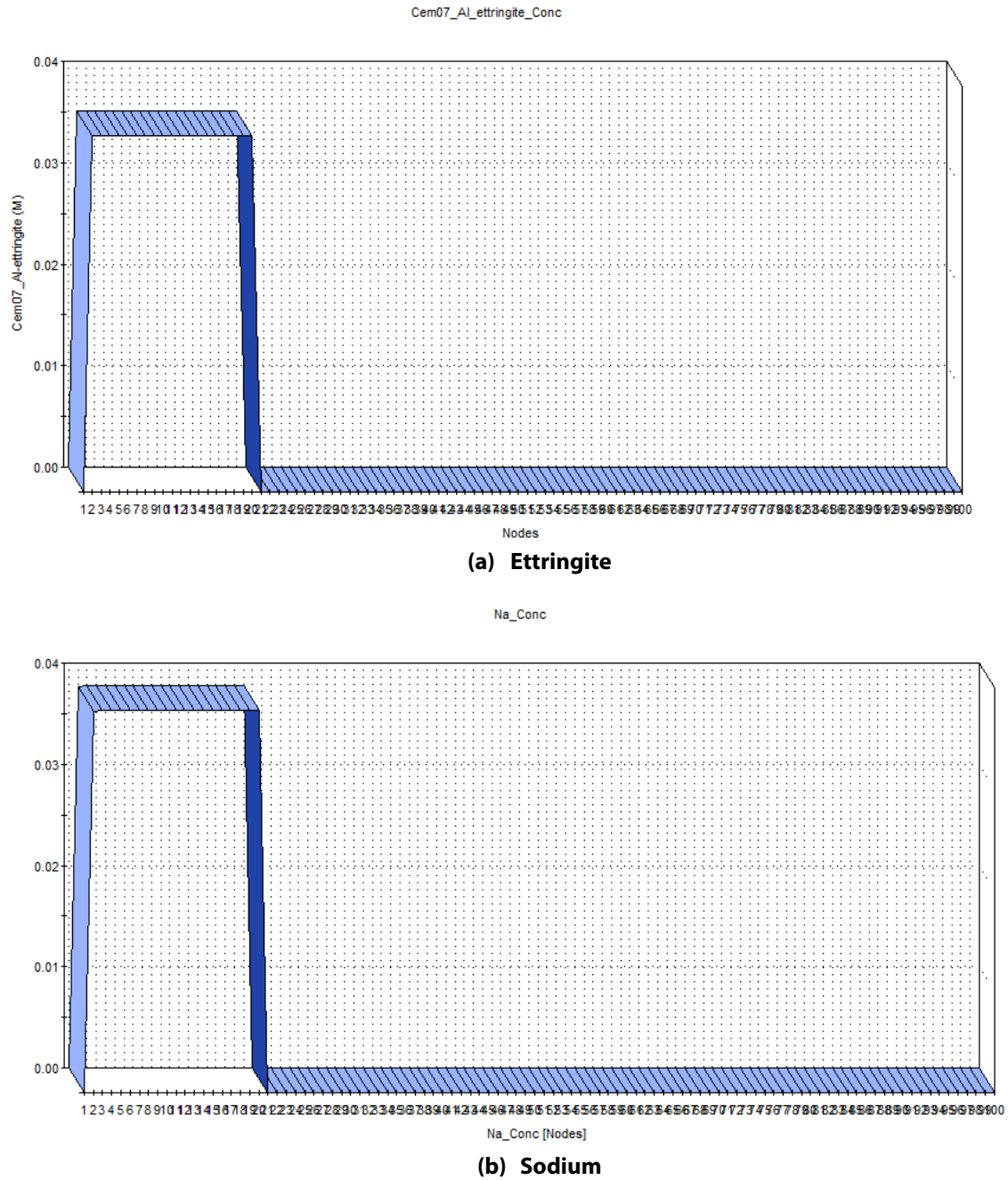
(a) Ettringite

(b) Sodium

Figure 7-22. Example LeachXS™/ORCHESTRA cement carbonation results by node number

8 KNOWN ISSUES WITH THE CBP SOFTWARE TOOLBOX

Issues have been identified with the CBP Software ToolBox that are being diagnosed. However, these issues do not prevent the user from successfully using the ToolBox.

8.1 Exception Thrown after Multiple Simulations without Exiting ToolBox

An exception may be intermittently thrown after completion of a simulation because one or more of the (exponent of the) floating-point results exceeds the maximum allowed size for that data type as illustrated in Figure 8-1. Typically this type of exception is thrown after a simulation has already been completed and a new simulation is being performed.
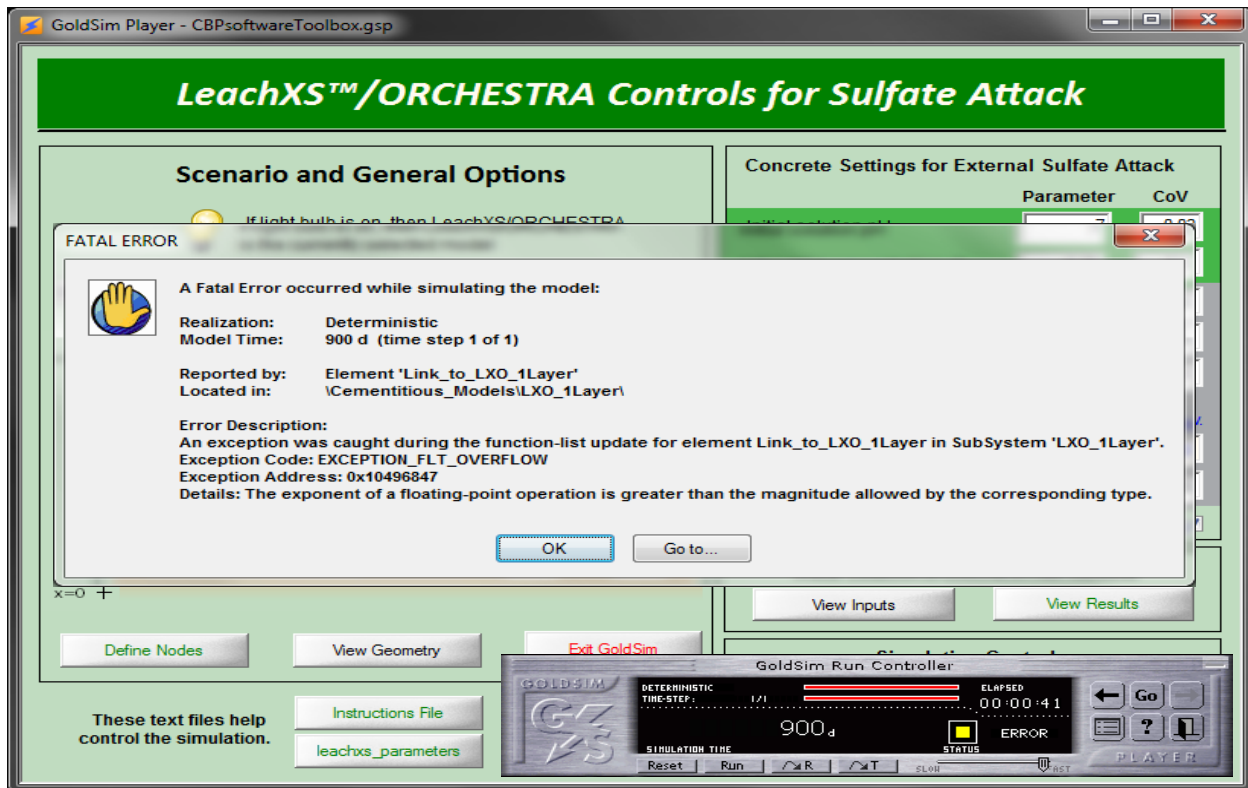

Figure 8-1.   Example of the exception thrown during ToolBox simulation

The intermittent nature of this issue can be demonstrated by observing results from simulations. The sodium concentration result in Figure 8-2(a) is obtained when one selects **OK** in the error window shown in Figure 8-1 and then views the sodium result. The **GoldSim Run Controller** was then used to **Reset** and then **Run** the same simulation again. The simulation ran to completion without error; the sodium results are displayed in Figure 8-2(b). *If a floating-point exception is thrown as illustrated in* Figure 8-1*, it is recommended that the simulation be* **Reset** *and* **Run** *again*. If the error persists, **Exit** the ToolBox and restart.
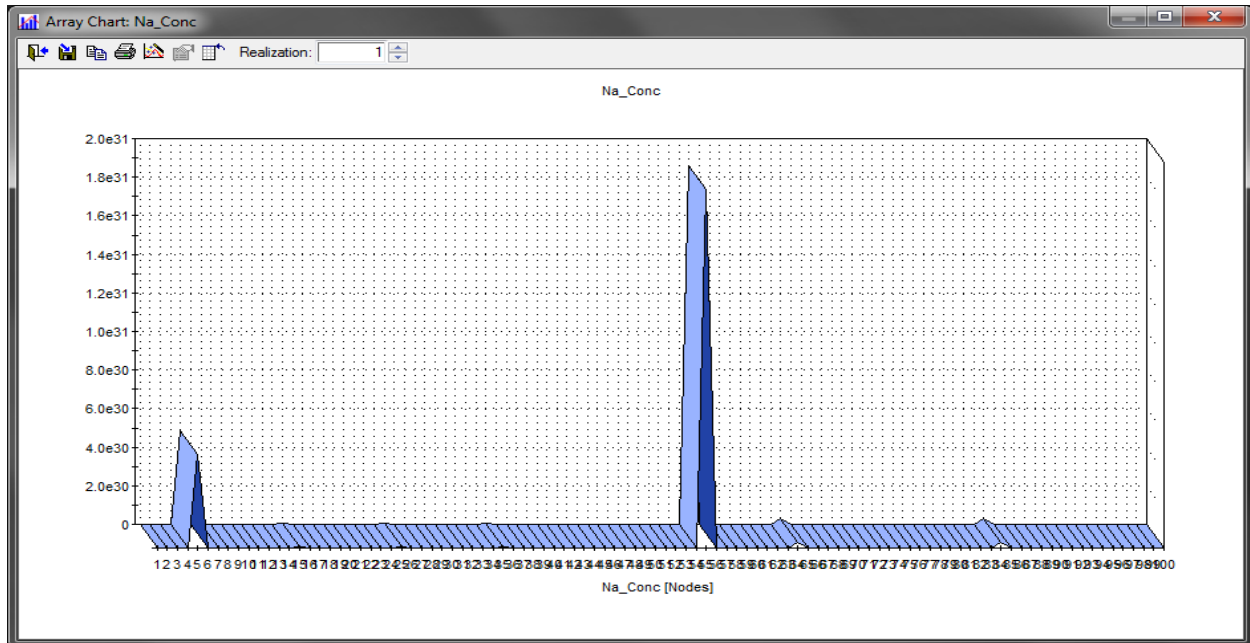
(a) Sodium result when floating-point exception thrown
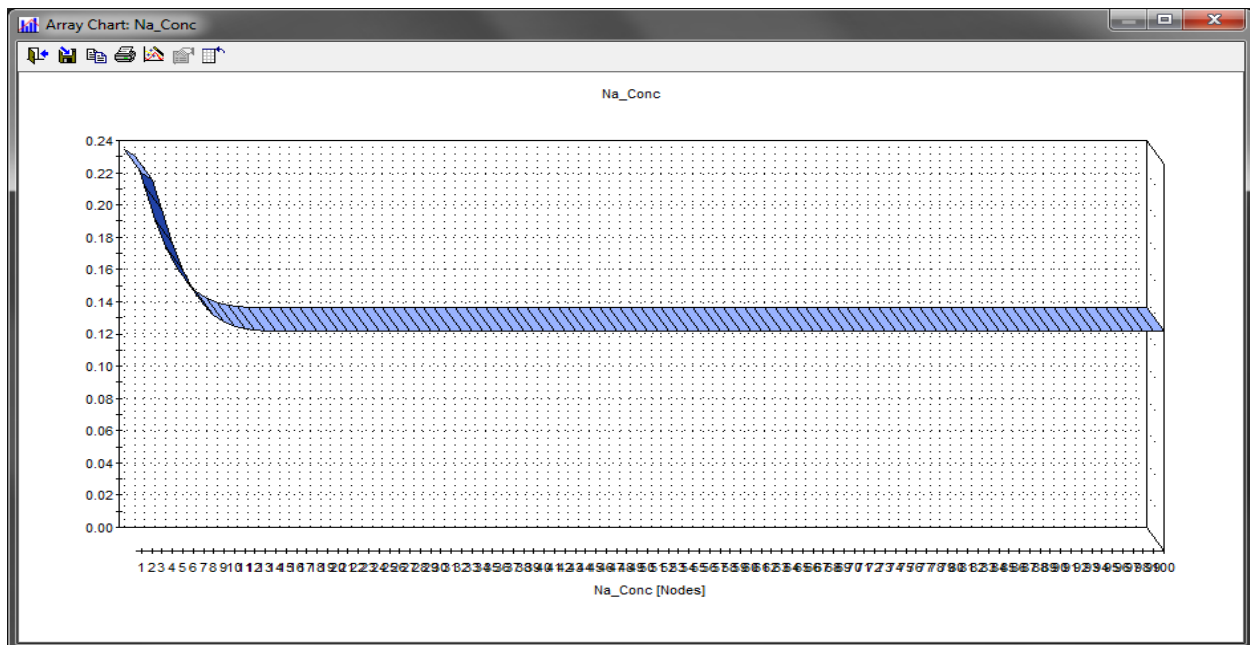
(b) Sodium result for successful simulation

Figure 8-2.   Example Sodium Results for Simulations using the CBP Software ToolBox

8.2   Erroneous Display of Results

During the training workshop held at NIST (Washington, DC), it was noticed that running a simulation intermittently resulted in results plots that resembled that in Figure 8-2(a) without the floating-point exception being thrown (Figure 8-1).

If results are displayed erroneously as illustrated in Figure 8-2(a)*, it is recommended that the simulation be* **Reset** *and* **Run** *again*. If the error persists, **Exit** the ToolBox and restart.

8.3   Running a Realization without a Corresponding Summary Worksheet

Microsoft Excel worksheets are provided that are used to summarize the input parameters used in the various realizations in a simulation. For the STADIUM® and LeachXS™/ORCHESTRA sulfate attack simulations, each worksheet corresponding to a realization is populated at run time. Blank worksheets should already exist for each realization in the pertinent workbooks. (The maximum number of worksheets in a workbook is limited by available memory where worksheets can be added as described in Microsoft Excel Help.)

If a realization is run corresponding to a non-existent worksheet, then GoldSim will add worksheets up to that corresponding to the realization; however, the headings typically associated with the input information will be missing as shown in Figure 8-3. In the example shown in this figure, the 51st realization has been run when only 50 worksheets have been added to the summary workbook. The input information is placed in a new worksheet entitled "**Sheet1**" without headings.
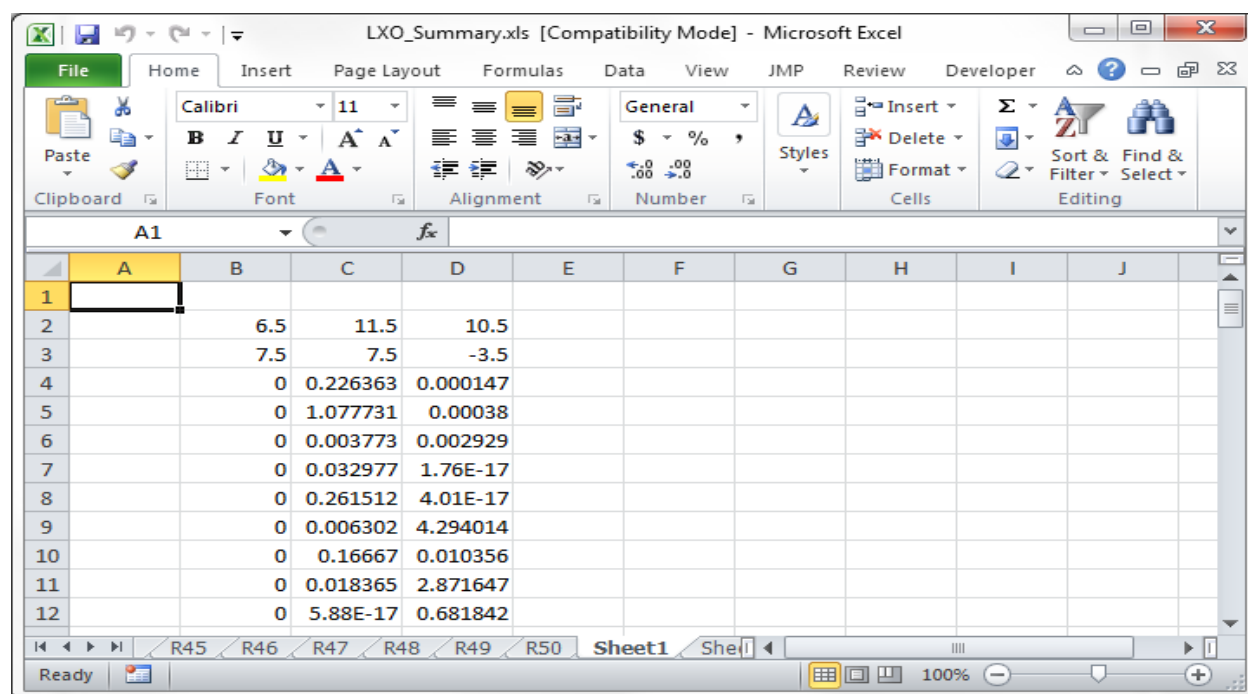

Figure 8-3.   Input Summary for Realization 51 when 50 Worksheets are Prepared

9 TECHNICAL SUPPORT

If you are experiencing problems with installing the CBP Software ToolBox or have any questions concerning its use, please contact either:

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Consortium for Risk Evaluation with Stakeholder Participation (CRESP) III
Nashville, TN 37235
E-mail: kevin.g.brown@vanderbilt.edu (Preferred method)
Phone: 615-343-0391

or

Gregory P. Flach, Ph.D.
Savannah River National Laboratory
773-42A, Savannah River Site, Aiken, SC 29808
E-mail: gregory.flach@srnl.doe.gov (Preferred method)
Phone: 803-725-5195

10 GLOSSARY OF TERMS

Browser

An alternative view of a GoldSim model, in which elements are displayed in a tree-like structure, and organized either hierarchically or by type.

Carbonation

Carbonation denotes various natural processes that result in the neutralization of concrete. The most significant such process is the reaction of atmospheric carbon dioxide with calcium hydroxide forming calcium carbonate that reduces the pH of the concrete and increases the potential for corrosion of steel reinforcement.

Container

Object within a GoldSim model that is analogous to a folder that is used to organize the model in a hierarchical manner.

Dashboard

Specialized user interface that can be built into a Player file. A dashboard looks like a "control panel", with buttons, sliders and display panels, and provides a mechanism by which inputs to a model can be modified within the Player.

Deterministic (probabilistic)[1]

Consistent with the principles of "determinism" that hold that specific causes completely and certainly determine the effects of all sorts. The term "probabilistic" is associated with an evaluation that explicitly accounts for likelihood in the analysis in an integrated fashion.

Dynamic-link Library (DLL)

A DLL is a library containing code and data that can be used by more than one program at run time, which helps promote code reuse and efficient memory usage.

Element

Object that represents a basic building block of a GoldSim model.

Graphics Pane

The primary portion of the GoldSim interface, where the graphical depiction of the model is shown.

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[1] Taken from the US NRC full-text glossary at http://www.nrc.gov/reading-rm/basic-ref/glossary/full-text.html.

Realization

A single model execution within a Monte Carlo simulation that represents one possible path the system could follow through time.

Run Controller

A dialog used to control the manner in which a GoldSim simulation is run from the Player.

Sulfate Attack

The deleterious chemical/physical reaction between sulfate in groundwater or soil and various solid components in cement that result in expansion and cracking of concrete.

Superfile

The top-tier input to Mesh2d is a superfile containing filenames and high-level option specifications.

ToolBox (also CBP Software ToolBox)

An integrated system that allows state-of-the-art partner codes (namely, STADIUM® and LeachXS™/ORCHESTRA) to be evaluated under a GoldSim probabilistic framework.

11 INDEX

12 REFERENCES

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