

CBP SOFTWARE TOOLBOX, VERSION 2.0 INSTALLATION GUIDE

Cementitious Barriers Partnership

September 2013

CBP-TR-2013-004-2, Rev. 0

CBP SOFTWARE TOOLBOX, VERSION 2.0

INSTALLATION GUIDE

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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 1,000 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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TABLE OF CONTENTS

Acknowledgements	ii
Disclaimer	ii
Foreword	iii
Executive Summary	iv
List of Figures	vi
List of Tables	vi
List of Acronyms and Abbreviations	vii
1 Introduction.....	1
2 What Do You Need to Get Started?	3
2.1 System Requirements.....	3
2.2 What is Included in the CBP Software Toolbox?	3
2.3 How to Register for the CBP Software Toolbox.....	4
2.3.1 Obtaining the NetBIOS name for a host computer	4
2.4 How to Download the CBP Software Toolbox Software?.....	5
3 Installing the CBP Software Toolbox.....	6
3.1 Create a Project Space.....	6
3.2 Installing the GoldSim Player (Required).....	7
3.3 Installing the STADIUM® Runtime Executable	9
3.3.1 What if the STADIUM® executable is NOT named “stadium_goldsim_v2012b.exe”?	9
3.4 Installing Windows Dynamic-link Libraries (Required by STADIUM®).....	10
3.5 Installing LeachXS™/ORCHESTRA	11
3.6 JavaRE or the Java Runtime Environment (Required for LeachXS™/ORCHESTRA)	13
3.7 GNUPlot (Optional).....	14
4 Setting System Options after Installation	15
4.1 Configuring Windows to View the GoldSim Dashboard (Suggested).....	15
4.2 Setting Program Preferences (Program Shortcuts).....	15
5 Preparing a New Simulation Workspace	18
6 Technical Support	21
7 Glossary of Terms	22
8 Index.....	24
9 References.....	25

LIST OF FIGURES

Figure 2-1. Getting the Computer's NetBIOS name using getNetBIOScomputerNameA.exe	5
Figure 3-1. The CBPsoftwareToolbox_v2.0 Installers Folder	7
Figure 3-2. The GoldSim Player Installation Wizard	8
Figure 3-3. The GoldSim Player (GTG 2010a)	8
Figure 3-4. The STADIUM Folder in the Toolbox Codes folder	9
Figure 3-5. Revised STADIUMexecutableName.txt file	10
Figure 3-6. The LeachXS Lite Setup Wizard	11
Figure 3-7. The LeachXS™/ORCHESTRA Login Screen	12
Figure 3-8. The LeachXS™/ORCHESTRA Program including Advanced Modeling Capabilities	13
Figure 4-1. The Windows 7 Display Control Panel	15
Figure 4-2. Example of Editing the Toolbox Shortcut for MyTextEditor	17
Figure 5-1. The CBP Software Toolbox and GoldSim Run Controller	20

LIST OF ACRONYMS AND ABBREVIATIONS

CBP	Cementitious Barriers Partnership
CPU	central processing unit
CRESP	Consortium for Risk Evaluation with Stakeholder Participation
D&D	Decontamination and Decommissioning
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
URL	uniform resource locator

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1 INTRODUCTION

The Cementitious Barriers Partnership (CBP) has developed the CBP Software Toolbox, an integrated suite of software tools, to predict the structural, hydraulic, and chemical performance of cement barriers used in nuclear applications over extended time frames. The Toolbox 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 including: (i) sulfate ingress and attack, (ii) carbonation, (iii) oxidation, (iv) chloride attack, and (v) constituent leaching.

The new release of the CBP Software Toolbox is intended to replace the existing CBP Toolbox Version 1.0. If the user would like to further investigate models developed for version 1.0, please contact the CBP Team (Section 6) for assistance.

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

- LeachXS™/ORCHESTRA developed by the Energy Research Centre of the Netherlands (ECN) (Meeussen 2003, ECN 2012) and
- STADIUM® developed by SIMCO Technologies, Inc. (SIMCO 2008, Samson & Marchand 2007).

The GoldSim Monte Carlo simulation program (GTG 2010b, GTG 2010c) was chosen as the code integration platform to allow LeachXS™/ORCHESTRA and STADIUM® to be run probabilistically for a set of important, pre-defined degradation scenarios (Brown & Flach 2009). A GoldSim “Player” version allows running but not editing GoldSim models (except for simulation time and Monte Carlo parameters) (GTG 2010a). A general Dynamic-link Library (DLL) interface was developed by the CBP that links GoldSim with the partner codes (Smith III et al. 2010).

For each realization, the DLL uses an instructions file that controls creating the 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 the GoldSim model for analysis. As part of the GoldSim interface enhancements in Version 2.0, viewing simulation results using built-in GoldSim plotting functions has been replaced with two- and three-dimensional graphical displays of simulation results created using the gnuplot software (Smith III et al. 2013).

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

- What do you need to get started?
- Installing the CBP Software Toolbox
- Setting System Options after installation
- Preparing a new simulation workspace for the Software Toolbox

2 WHAT DO YOU NEED TO GET STARTED?

The CBP Software Toolbox is an integrated system that allows state-of-the-art partner codes (currently, STADIUM® and LeachXS™/ORCHESTRA) to be evaluated within a probabilistic framework. This section describes the requirements of the system needed to run the CBP Software Toolbox, the components of the Toolbox, and how to register and download the Toolbox.

2.1 System Requirements

A system running the CBP Software Toolbox Version 2.0 must meet the following requirements:

- Desktop personal computer or laptop running Windows XP, Vista, or Windows 7
- Administrative Privileges on the system during the installation process
- Installation of Microsoft Visual C++ Redistributable (MSVCR100.DLL and VCOMP100) is required to run STADIUM® as described in Section 3.4
- CPU 1.6 GHz or higher (multicore processor such as Intel Core i7-2600 with 4GB at 3.40GHz is recommended)
- For XP machines, 512 MB of RAM required (1 GB or more recommended). For Vista and Windows 7 machines, 1 GB of RAM required (2 GB or more recommended)
- 16-bit color depth (32-bit recommended)
- Internet connection for software download (broadband connection preferred)
- Microsoft Internet Explorer 11 or higher
- GoldSim or GoldSim Player version 10.5.4.
- Because GoldSim is linked to Microsoft Excel in the Toolbox, Microsoft Windows Excel 2010 or later is required to be fully functional
- Disk Space required: 200 MB of free space in the target download directory and 40 MB of free space in Common Files folder. During the installation a minimum of 250 MB is required. Up to 1 GB of disk space or more may be required for repeated simulation of new models.
- Mouse, touchpad, or other pointing device

2.2 What is Included in the CBP Software Toolbox?

The CBP Software Toolbox Version 2.0 consists of:

- A GoldSim model (in this instance assumed to have been saved in a GoldSim Player file, CBPsoftwareToolbox_V2.0.gsp) that includes a series of Dashboards and external interface elements that control partner code evaluation (GTG 2010b). *GoldSim or GoldSim Player version 10.5.4 is required to run the model. Work is underway by the CBP Team to develop a Toolbox compliant with the latest version of GoldSim.*

- A CBP custom Dynamic-link Library (DLL) that is called from the GoldSim external interface element to link to the selected CBP partner code (Smith III et al. 2010).
- CBP partner codes including
 - 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 (ECN 2012). Geochemical speciation and chemical reaction/transport modeling capabilities are integrated into LeachXS using ORCHESTRA (Meeussen 2003).
 - 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 (Samson & Marchand 2007). 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 complete description of the program is provided by Flach & Smith III (2012).
- A text editor to modify the model files, including the finite element mesh creation files, needed to run a STADIUM® simulation.
- Gnuplot to view the finite element mesh created to run a STADIUM® simulation and a compiled gnuplot program to display simulation results (Smith III et al. 2013).

Installers for the CBP Software Toolbox Version 2.0 are included in the self-extracting archive that is downloaded as described in the Section 2.3.

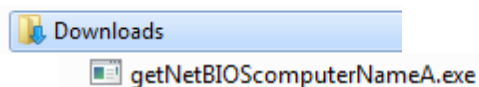
2.3 How to Register for the CBP Software Toolbox

The user should have received an e-mail from the CBP that provides a [hyperlink](#) to the CBP Software Toolbox Version 2.0 registration page. The user is asked to provide contact information including (required information):

- Name
- E-mail address
- Phone
- Computer NetBIOS name (Section 2.3.1)
- Organization
- Department
- Address
- City, State, Zip / Postal Code

2.3.1 Obtaining the NetBIOS name for a host computer

The CBP Software Toolbox registration page provides a [hyperlink](#) to either **Run** or download a small, executable program that retrieves the computer's NetBIOS name. Selecting the [hyperlink](#) allows the user to either **Run** or save an executable file named "getNetBIOScomputerNameA.exe" to the desired target location. For example, here it is assumed that the user saved the "getNetBIOScomputerNameA.exe" to the user's **Downloads** folder:



After the file named “getNetBIOScomputerNameA.exe” is either **Run** or downloaded and then executed (e.g., by double-clicking the program icon in the Windows Explorer window), the computer’s NetBIOS name is displayed as shown in Figure 2-1. The NetBIOS name (e.g., “CEE-KGB”) is entered in the appropriate field on the registration page.

Instructions for obtaining the computer’s NetBIOS name are provided on the CBP Software Toolbox registration page.

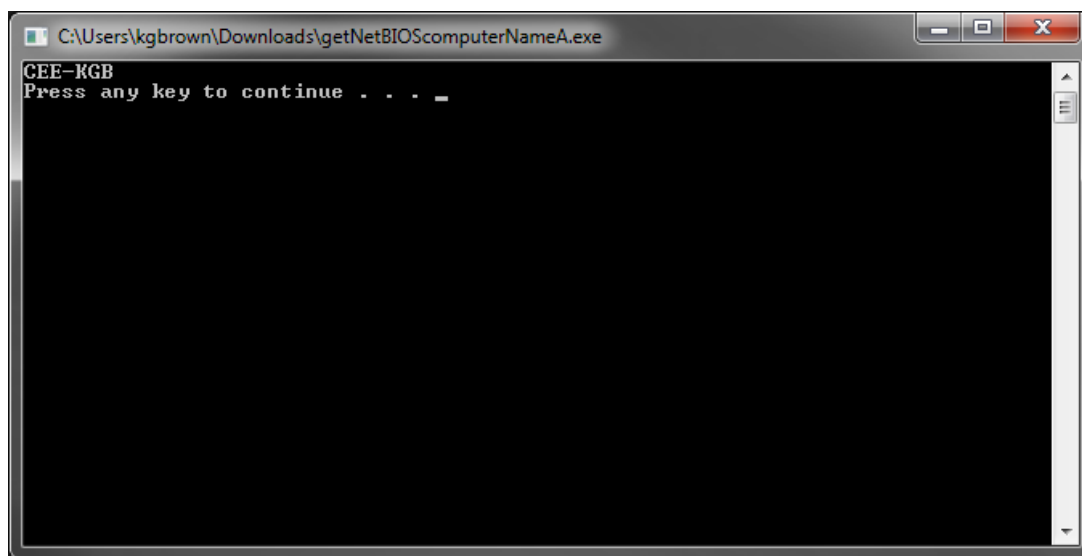
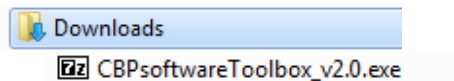


Figure 2-1. Getting the Computer’s NetBIOS name using getNetBIOScomputerNameA.exe

2.4 How to Download the CBP Software Toolbox Software?

Upon receipt of the required registration information, the CBP point of contact will provide a response containing a [hyperlink](#) that allows the user to download a self-extracting archive entitled “CBPsoftwareToolbox_v2.0.exe” containing the CBP Software Toolbox and supporting information.

A logical place to download the Toolbox self-extracting archive would be in the **Downloads** folder as shown in this example:



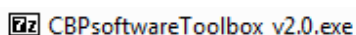
3 INSTALLING THE CBP SOFTWARE TOOLBOX

The software needed to install CBP Toolbox Version 2.0 is contained in the “CBPsoftwareToolbox_v2.0.exe” self-extracting archive downloaded as described in Section 2.4; it is assumed for the sake of this example that the user downloaded the Toolbox archive into the **Downloads** folder.

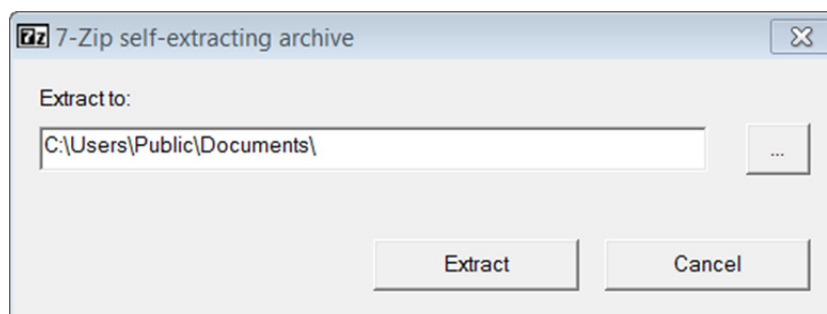
The new release of the CBP Software Toolbox (Version 2.0) is intended to replace the existing CBP Toolbox Version 1.0. Thus the new Toolbox software should be installed in a new directory separate from the Toolbox Version 1.0 software. If the user would like to further investigate models developed for version 1.0, please contact the CBP Team (Section 6) for assistance.

3.1 Create a Project Space

The “CBPsoftwareToolbox_v2.0.exe” self-extracting archive shown below should be launched from Windows Explorer. The 7-Zip program used to create the archive is not required to be on the user’s system for extraction.



The folders/files in the above archive should be extracted to a location of the user’s choice, for example:



The software installers for the required and optional software are provided in the folder ...\\CBPsoftwareToolbox_v2.0\\Installers (Figure 3-1). The software components are contained in the following folders:

- **GNUPlot** – plotting software (optional, for plotting STADIUM® computational mesh).
- **GoldSim** – GoldSim Player (required). The fully functional, commercial version of GoldSim Pro can be obtained from <http://www.goldsim.com/Home/>. GoldSim RT is required to run the CBP Toolbox.
- **JavaRE** – Java Runtime Environment (required for LeachXS™/ORCHESTRA, but often previously installed). The 32- and 64-bit versions of the Java Runtime Environment are provided. See www.java.com for more information.
- **LeachXS-ORCHESTRA** – LeachXS™/ORCHESTRA (required for LeachXS™/ORCHESTRA simulations). Two installation files are provided: 1) LeachXS™/ORCHESTRA

(LeachXS_2_0_XX.zip) and 2) the CBP case files (CBP Cases 19-Mar-2014.zip). Both files need to be unzipped and installed.

- **STADIUM** – This folder is currently empty except for the installer required for the Open MP DLLs described in Section 3.4. An evaluation copy of the STADIUM® runtime executable, locked to the user's designated computer, is provided by SIMCO Technologies, Inc. upon request.

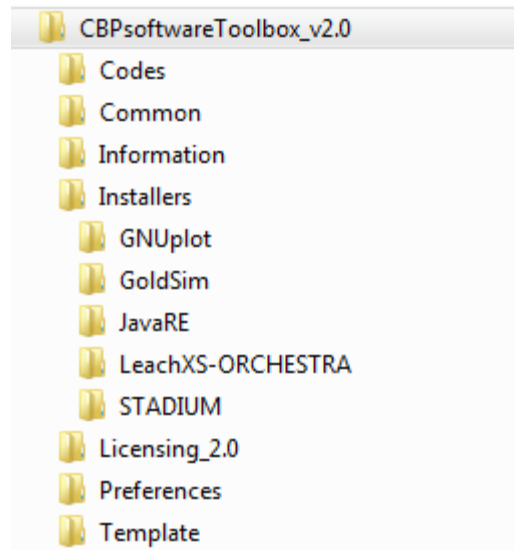
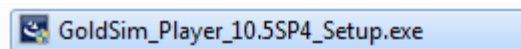


Figure 3-1. The CBPsoftwareToolbox_v2.0 Installers Folder

3.2 Installing the GoldSim Player (Required)

The GoldSim Player (GTG 2010a) installer is located in the
...\CBPsoftwareToolbox_v2.0\Installers\GoldSim folder:



When the installer is launched, the GoldSim Player 10.5 Wizard is launched (after checking system requirements) as shown in (GTG 2010a).



Figure 3-2. The GoldSim Player Installation Wizard

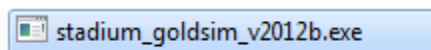
The instructions in the Wizard should be followed to install the GoldSim Player needed to run the CBP Software Toolbox. Upon installation, the GoldSim Player can be tested by launching the application from the Windows Start menu. If the installation was successful, the GoldSim Player will begin as shown in Figure 3-3.



Figure 3-3. The GoldSim Player (GTG 2010a)

3.3 Installing the STADIUM® Runtime Executable

An evaluation copy of the STADIUM® runtime executable, locked to the user's designated computer (e.g., Section 2.3.1 and Figure 2-1), will be provided by SIMCO Technologies, Inc. upon request:



The CBP Software Toolbox may be shipped with the evaluation version of STADIUM® included in the appropriate folder. If a valid version of the STADIUM® runtime executable is not included in the ...\\Codes\\STADIUM folder, the user should

1. Request an evaluation version of the STADIUM® runtime executable from SIMCO Technologies, Inc. using the contact information listed on the <http://cementbarriers.org> site. SIMCO Technologies, Inc. will provide a way to download an evaluation version of the STADIUM® executable file.
2. Place the valid STADIUM® runtime executable provided by SIMCO Technologies, Inc. in the ...\\Codes\\STADIUM folder (Figure 3-4).

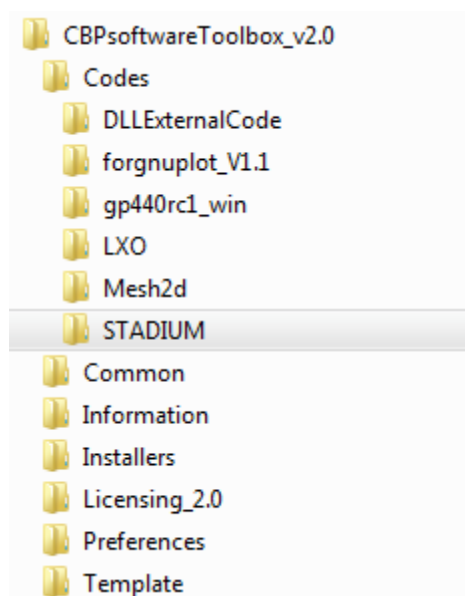
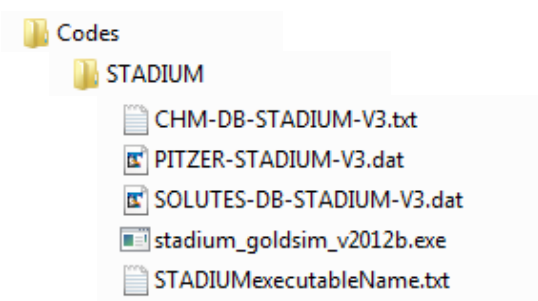


Figure 3-4. The STADIUM Folder in the Toolbox Codes folder

3.3.1 What if the STADIUM® executable is NOT named "stadium_goldsim_v2012b.exe"?

It is assumed that the evaluation version of the STADIUM® executable provided by SIMCO Technologies, Inc. to the user will be named "stadium_goldsim_v2012b.exe". This file is placed in the appropriate directory as described above (Section 3.3). To run a simulation, a Windows batch file is created by GoldSim

using the name of the STADIUM® executable file contained in the `STADIUMexecutableName.txt` file residing in the `...\Codes\STADIUM\` directory:



If the STADIUM® executable is not named “`stadium_goldsim_v2012b.exe`”, the name in the `STADIUMexecutableName.txt` file must be changed to the new file name for the STADIUM executable will be successfully opened at runtime. For example, assuming that the new STADIUM® executable file is named “`stadium_goldsim_v2012b.exe`”, then the contents of the `STADIUMexecutableName.txt` file should be that shown in Figure 3-5. Any text editor can be used.

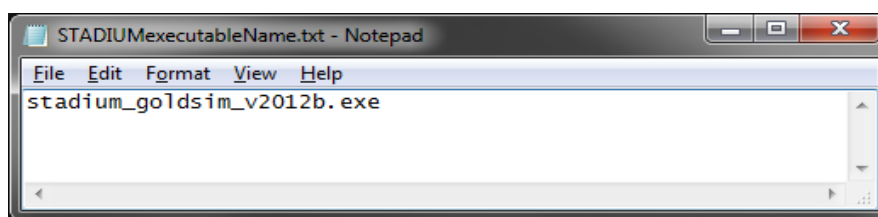


Figure 3-5. Revised `STADIUMexecutableName.txt` file

3.4 Installing Windows Dynamic-link Libraries (Required by STADIUM®)

STADIUM® requires the Windows Dynamic-link Libraries (DLLs) `MSVCR100.DLL` and `VCOMP100.dll`. If these DLLs are not already present on your system, download and install the Microsoft Visual C++ Redistributable Package from:

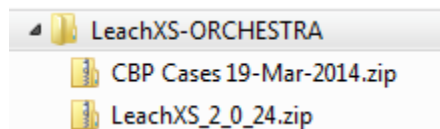
<http://www.microsoft.com/download/en/details.aspx?id=5555>.

This package manages the Open MP multi-processor capabilities within STADIUM®.

Alternatively, the “`vcredist_x86.exe`” installer, available from the above [hyperlink](#), is provided in the `...\CBPsoftwareToolbox_v2.0\Installers\STADIUM` folder.

3.5 Installing LeachXS™/ORCHESTRA

The LeachXS™/ORCHESTRA program is installed using the installers found in the ...\\CBPsoftwareToolbox_v2.0\\Installers\\LeachXS-ORCHESTRA folder:



Launching the installer will start the LeachXS Setup Wizard as shown in Figure 3-6.

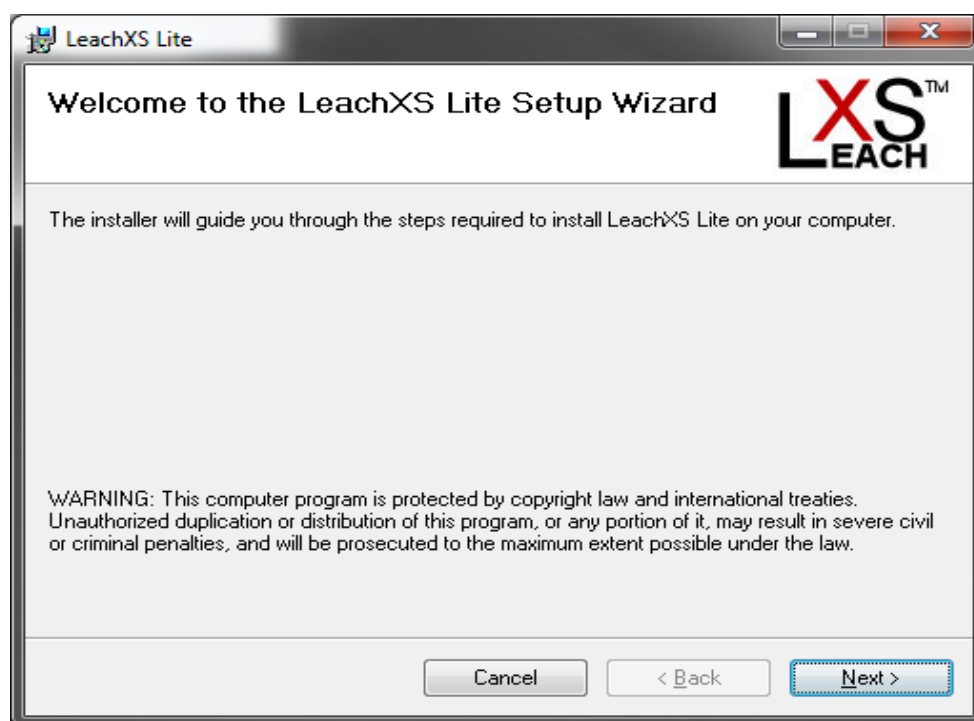


Figure 3-6. The LeachXS Lite Setup Wizard

The directions provided by the setup wizard (Figure 3-6) should be followed to install the LeachXS™/ORCHESTRA program (ECN 2012). The LeachXS Lite™ Shortcut placed on the desktop or available from the Windows Start menu can be used to open LeachXS™/ORCHESTRA.

The second installation file should also be unzipped and used to install the CBP case files.

A valid user name and license key will be provided to the registrant by ECN via e-mail based on the NetBIOS name entered during the registration process (Figure 2-1). This information is entered into the LeachXS Lite™

login screen as shown in Figure 3-7. When installed appropriately (including a valid license key), the LeachXS™/ORCHESTRA program with selected Advanced Modeling capabilities will start up as shown in Figure 3-8.

The LeachXS™/ORCHESTRA (LXO) program was used to develop the one-dimensional, one-layer LXO models for sulfate attack, carbonation, and percolation with radial diffusion that are currently used in the CBP Software Toolbox (Brown et al. 2013). These models will 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 the LXO advanced modeling capabilities.



Figure 3-7. The LeachXS™/ORCHESTRA Login Screen



Figure 3-8. The LeachXS™/ORCHESTRA Program including **Advanced Modeling** Capabilities

3.6 JavaRE or the Java Runtime Environment (Required for LeachXS™/ORCHESTRA)

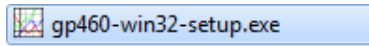
The Java Runtime Environment (JavaRE) is required for LeachXS™/ORCHESTRA to run. Typically JavaRE is installed on computers. If JavaRE is not installed, the user can either: 1) load JavaRE from one of the installers in the ...\\CBPsoftwareToolbox_v2.0\\Installers\\JavaRE folder:

jre-7u65-windows-i586.exe
jre-7u65-windows-x64.exe

or 2) use the Java download site at <http://www.java.com/en/> to both check to see if JavaRE already resides on the computer and to download the most recent version of JavaRE. The instructions in the Java installer wizard should be followed to correctly install the program.

3.7 GNUPlot (Optional)

GNUPlot must be installed to view the finite element mesh created for STADIUM®. GNUPlot can be installed from the file in the ...\\CBPsoftwareToolbox_v2.0\\Installers\\GNUPlot folder:



The instructions in the wizard should be followed *using all default parameters* to install the program.

4 SETTING SYSTEM OPTIONS AFTER INSTALLATION

After installing the necessary software components (Section 3), various Windows and program elements must be set properly for best Toolbox performance. These settings are described in this section.

4.1 Configuring Windows to View the GoldSim Dashboard (Suggested)

The CBP GoldSim Dashboard element used for the CBP Software Toolbox was designed for 100% font scaling. The Windows Display Control Panel Setting (e.g., for Windows 7 in Figure 4-1) should be set to “Smaller - 100%” (i.e., not the Default setting) for best viewing of the Dashboards in the CBP Software Toolbox Version 2.0, as opposed to display magnification. There are similar Control Panel Settings available for Windows Vista and XP.

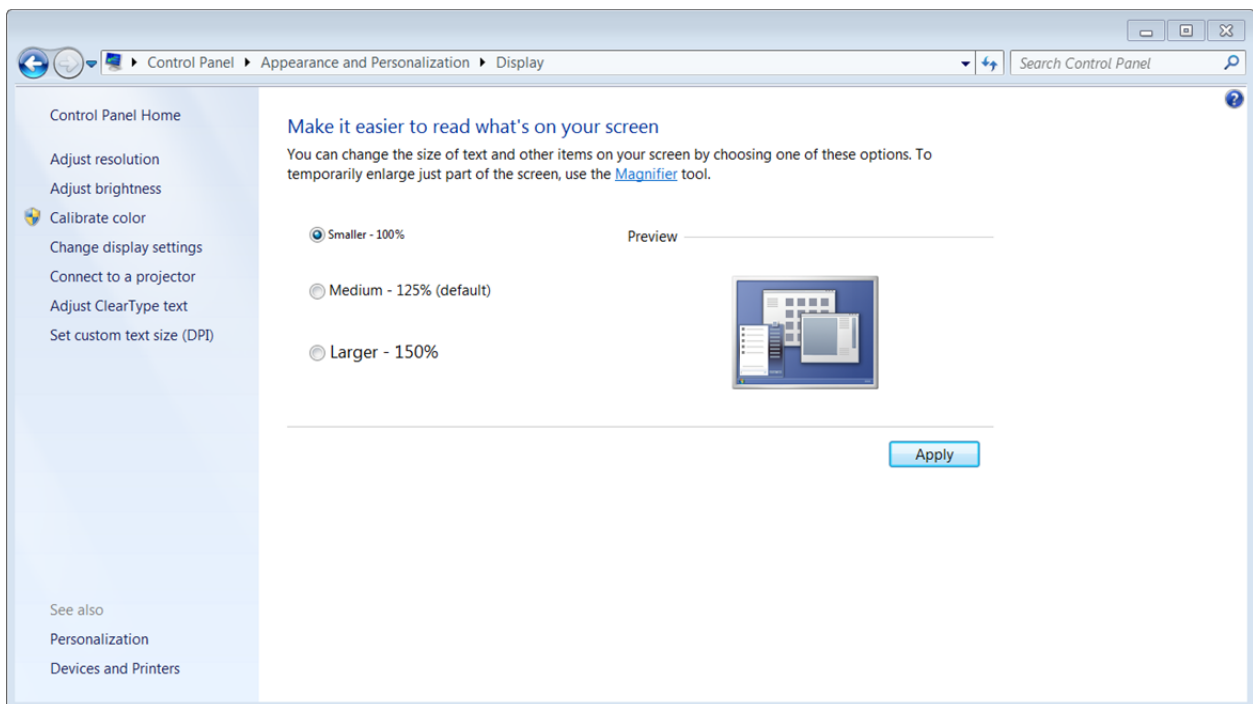
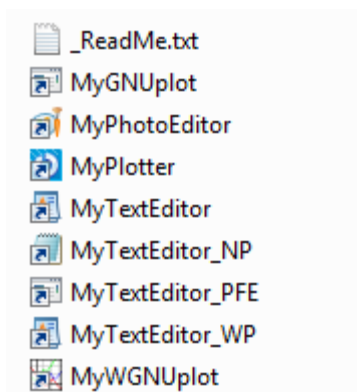


Figure 4-1. The Windows 7 Display Control Panel

4.2 Setting Program Preferences (Program Shortcuts)

Program Shortcuts are needed to prepare data for simulations and view input files and results; these Shortcuts are found in the ... \CBPsoftwareToolbox_v2.0\Preferences folder:



These Shortcuts have the default settings indicated below and should be edited, as needed, for your computer system:

- MyTextEditor - Text file editor of user choice, e.g., “C:\WINDOWS\NOTEPAD.EXE”
(see example shortcuts MyTextEditor_*)
- MyPhotoEditor - Image file editor or viewer of user choice, e.g.,
“%SystemRoot%\system32\mspaint.exe”
- MyGNUplot - GNUplot command-line executable, e.g.,
“C:\Program Files\gnuplot\bin\gnuplot.exe”
- MyWGNUplot - GNUplot GUI executable, e.g.,
“C:\Program Files\gnuplot\bin\wgnuplot.exe”

A simple way to edit a Shortcut is by selecting (right-clicking on the icon) and then editing the information on the **Shortcut** tab of the **Properties** pop-up menu item as shown in Figure 4-2.

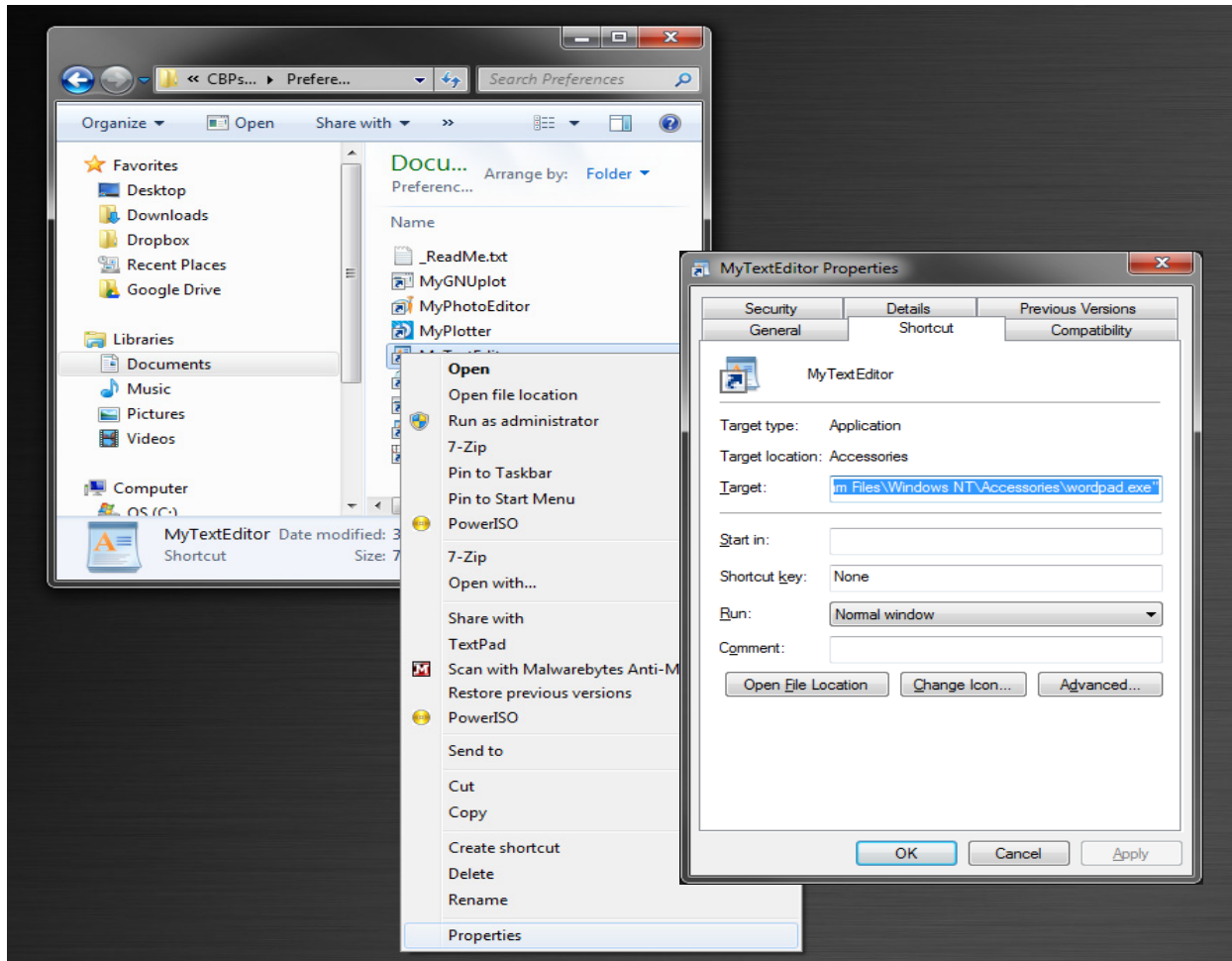
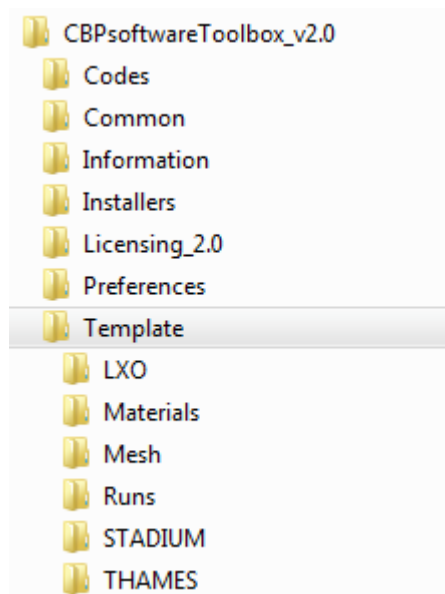


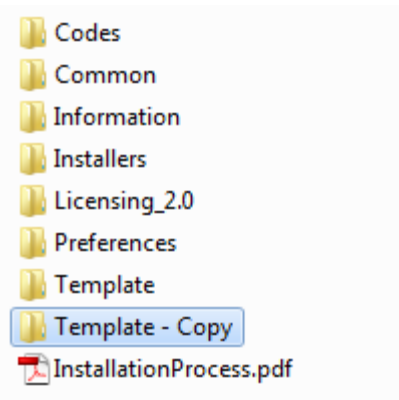
Figure 4-2. Example of Editing the Toolbox Shortcut for MyTextEditor

5 PREPARING A NEW SIMULATION WORKSPACE

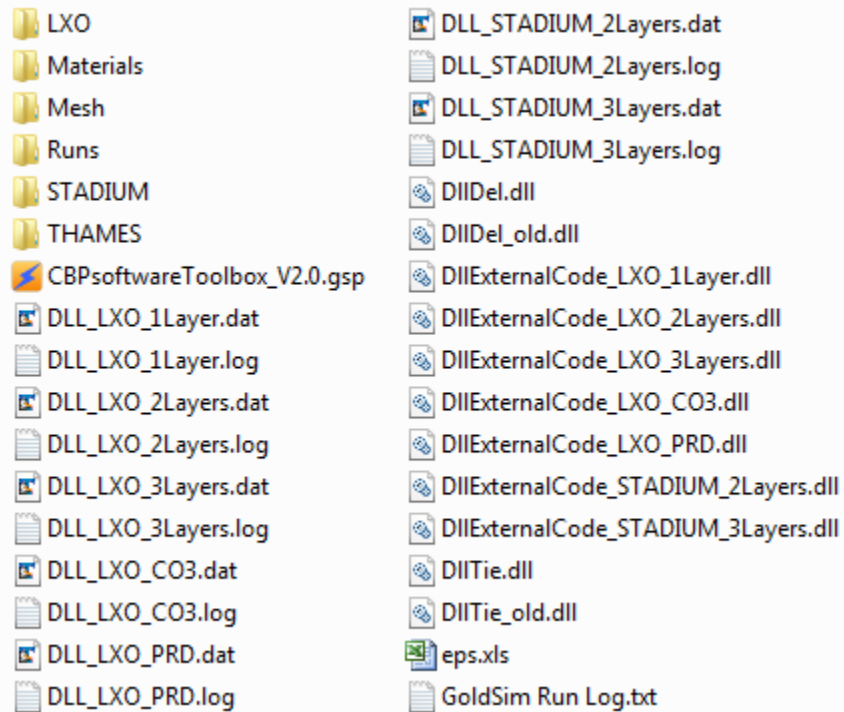
The basic information needed to run simulations using the CBP Software Toolbox is contained in the **Template** folder:



To prepare the simulation workspace, the **Template** folder should be copied:



The new folder should be renamed (e.g., “MyProject”) and the renamed folder should be opened to run a simulation as show below:



Please do not perform work in the Template folder.

To run a simulation, the GoldSim Player file CBPsoftwareToolbox_v2.0.gsp is launched. The CBP Software Toolbox is opened using the GoldSim Player as illustrated in Figure 5-1.

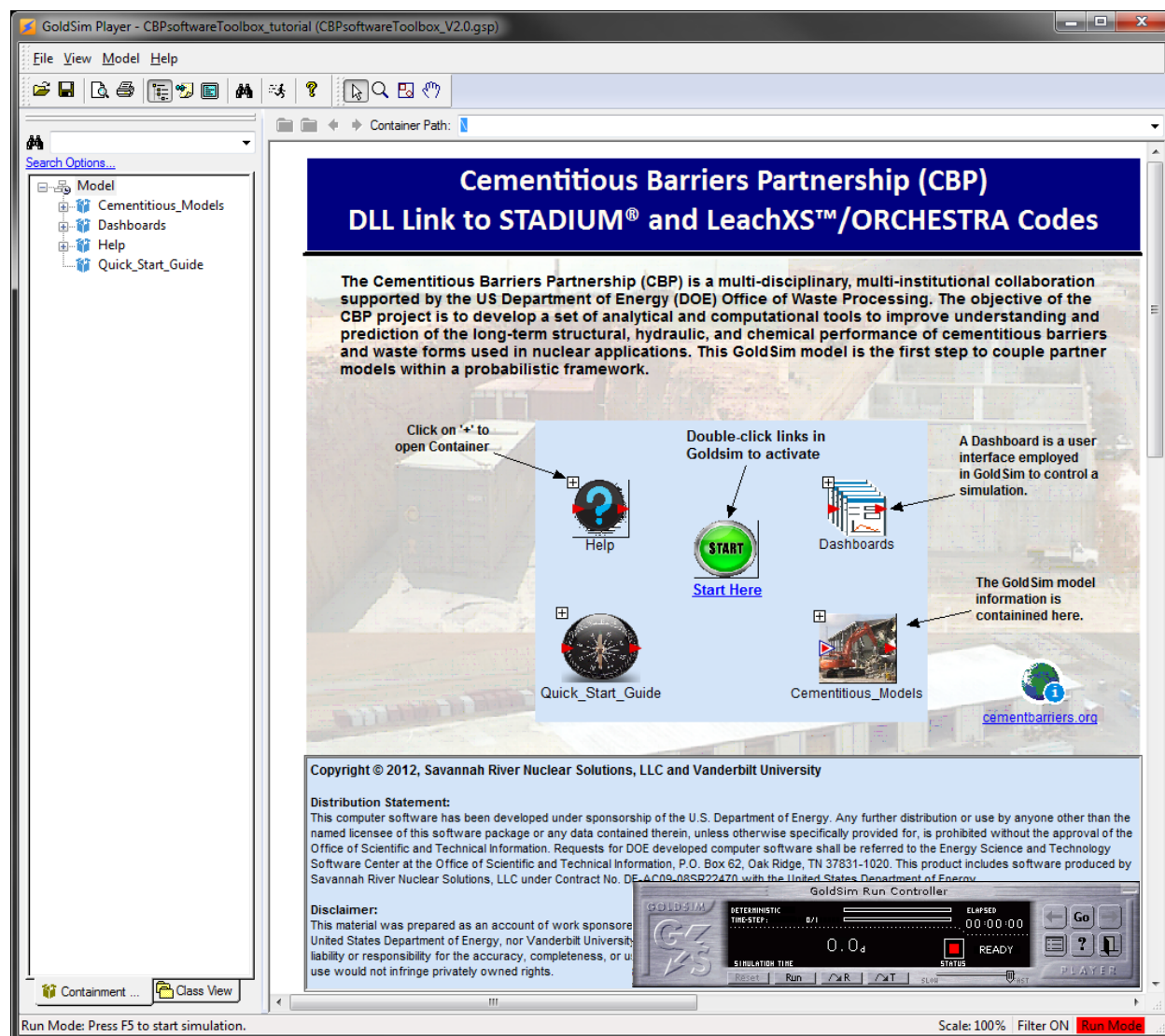


Figure 5-1. The CBP Software Toolbox and GoldSim Run Controller

6 TECHNICAL SUPPORT

If you are experiencing problems with installing the CBP Software Toolbox Version 2.0 or have any questions concerning its use, please contact either:

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7 GLOSSARY OF TERMS

Browser

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

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 is built into a GoldSim Player file. A dashboard resembles a "control panel", with buttons, sliders and display panels that provides a mechanism by which inputs to a model can be modified within the Player.

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

An object that represents the 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 to the user.

NetBIOS name

A name assigned to a Windows computer using the common 15-character NetBIOS format, which is the original networking protocol for DOS and Windows personal computers.

Player

A free version of GoldSim that allows running but not editing GoldSim models.

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.

Self-extracting archive

An executable program containing one or more compressed files that, when run, automatically decompresses the files.

Shortcut (Windows)

An icon that points to a program or data file; double-clicking a shortcut is the same as double-clicking the original file.

Toolbox

An integrated suite of software tools developed by the CBP, to predict the structural, hydraulic, and chemical performance of cement barriers used in nuclear applications over extended time frames.

8 INDEX

7-Zip, 6
Advanced Modeling, 12, 13
carbonation, 1, 12
CBP Software Toolbox, i, 1, 2, 3, 4, 5, 6, 8, 9, 12, 15, 18, 19, 20, 21
cementitious barriers, iii, 1
Cementitious Barriers Partnership, vi, 1
chloride attack, 1
Control Panel Settings, 15
Dashboard, 3
DLL, vi, 1, 3, 4, 10, 22
Dynamic-link Library, 1, 4, 22
executable file, 4, 9, 10
external application, 1
external interface element, 4
finite element mesh, 4, 14
font scaling, 15
Gnuplot, 4, 6, 14
GoldSim, vi, 1, 3, 4, 6, 7, 8, 9, 15, 19, 20, 22, 23
instructions file, 1
Java Runtime Environment, 6, 13
JavaRE, 6, 13, 14
leaching, 1
Leaching eXpert System, vi, 4
LeachXS Lite, 11, 12
LeachXS™/ORCHESTRA, vi, 1, 3, 4, 6, 11, 12, 13
Mesh2D, 4
Microsoft Excel, 3
NetBIOS name, 4, 5, 12, 22
ORCHESTRA, vi, 4
performance, iii, 1, 15, 23
Player, 1, 3, 6, 7, 8, 19, 22
point of contact, 5
realization, 1
registration, 4, 5, 12
self-extracting archive, 4, 5, 6
Shortcuts, 15, 16
simulation, iii, 1, 2, 3, 4, 9, 18, 19, 22, 23
STADIUM®, vi, 1, 3, 4, 6, 7, 9, 10, 14
sulfate attack, 1, 12
sulfate ingress, 1
THAMES, vi
Wizard, 7, 8, 11

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