Cementitious Barriers Partnership: Introduction to GoldSim Dashboard User Interface (GUI) and CBP Software Communication Bridge, Version 2.0

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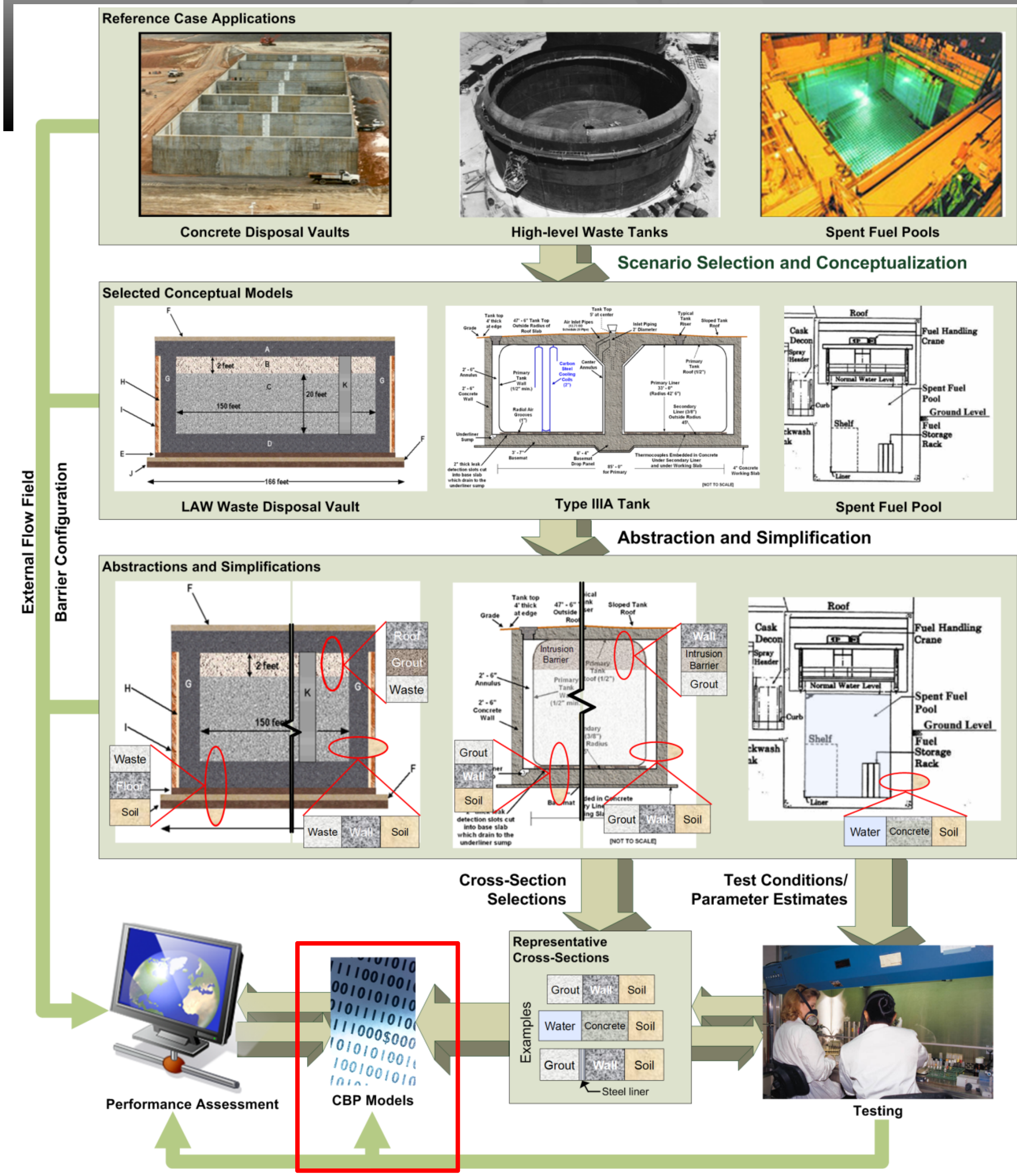
Richland, Washington
26-27 August 2014

CBP
Cementitious Barriers Partnership

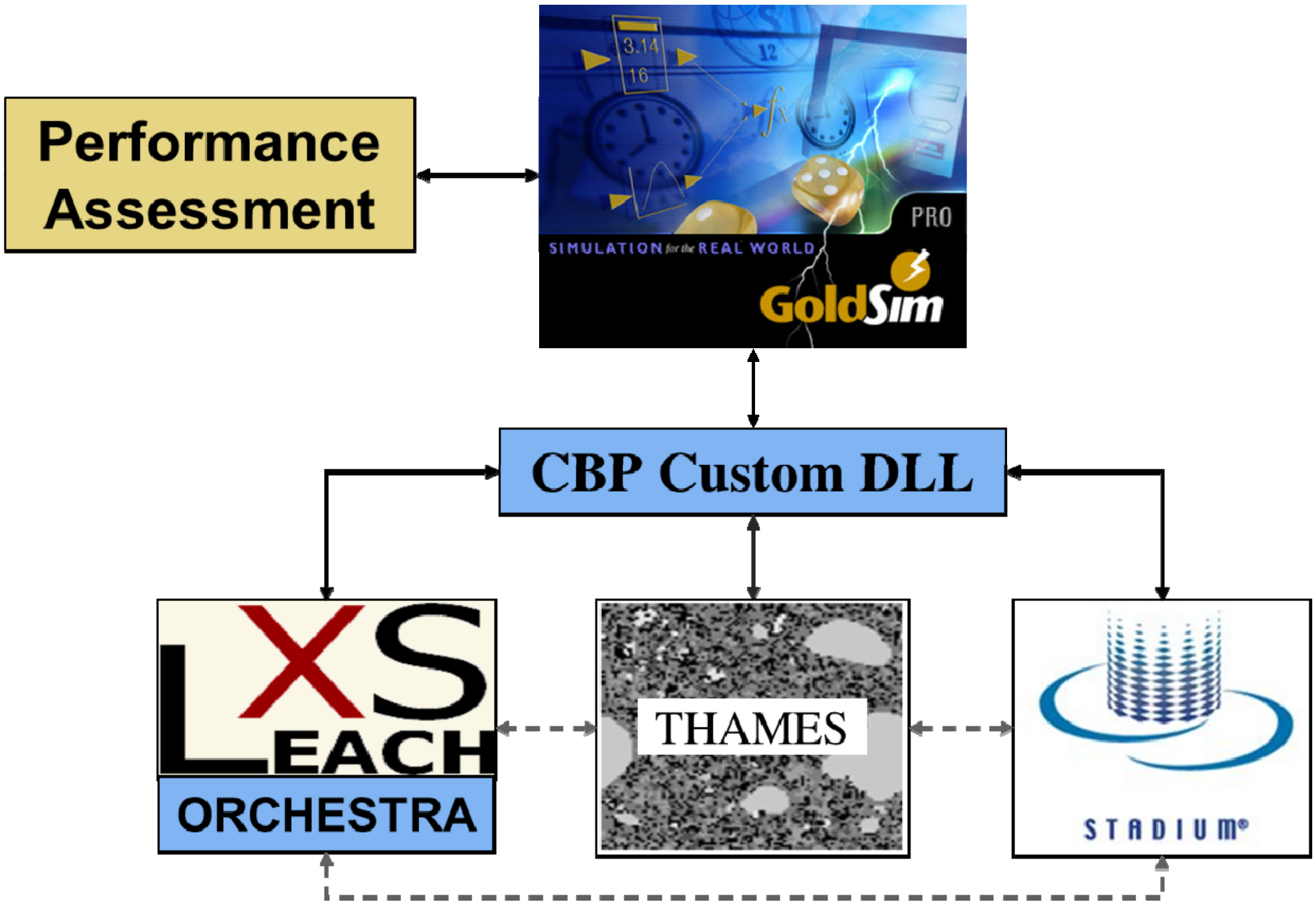
Workshop Summary

- CBP Software ToolBox, Version 2.0
  - Focus on sulfate attack (Low-Activity Waste), carbonation (HLW tanks), and percolation with radial diffusion (Tank Closure)
  - GoldSim model → Probabilistic wrapper for partner codes
  - Custom Dynamic-link library (DLL) developed (SRNL/VU) used to link to current partner codes
- Current Partner Codes
  - STADIUM® by SIMCO Technologies, Inc.
  - LeachXS™/ORCHESTRA by ECN/VU/DHI/NRG
  - THAMES (NIST) pending
- Uncertainty analysis using built-in GoldSim functionality
- Future Plans for Software ToolBox, Version 3.0



Linking Prototype Cases to Performance Models through System Abstraction and Validated by Laboratory and Field Testing

General Integrated Model Concept



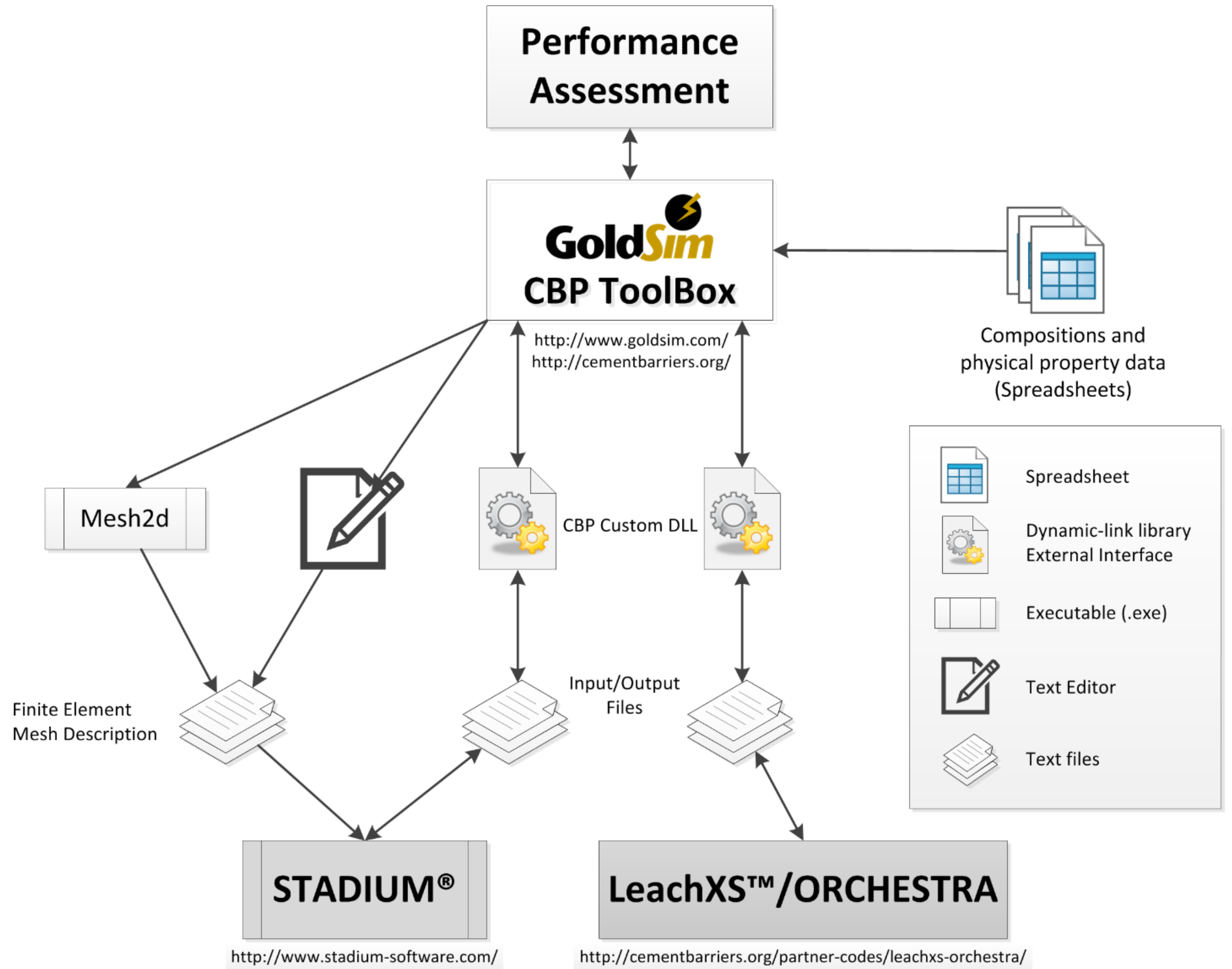
General Design Principles

- Model development is proceeding in phases
  - Weakest appropriate coupling amongst models
- Parallel improvement of partner codes and coupling where appropriate
  - Influence, but stay within, CBP partners' code development path
  - Accept reasonable existing duplication of functionality (e.g., bulk chemistry) but require consistency
- Data and I/O considerations
  - Common repository (spreadsheet/database) for common data
  - Common data formats, so an output can be an input
  - Common graphics format (SRNL custom graphics)
  - Consistent solutions

Phased CBP ToolBox Development

- Phase I: Use existing CBP partner codes "as is"
  - No coupling between LeachXS/ORCHESTRA (LXO) and STADIUM
  - Use CBP Custom Dynamic-link library (DLL)
  - Focus on sulfate attack, carbonation, and cracking
- Phase II: Coupling through functions
  - Modest coupling where appropriate
  - Add THAMES partner code (virtual microprobe)
  - Enhanced I/O may be needed for partner codes to support integration path
  - May use "system call" DLLs using instructions file (run time)

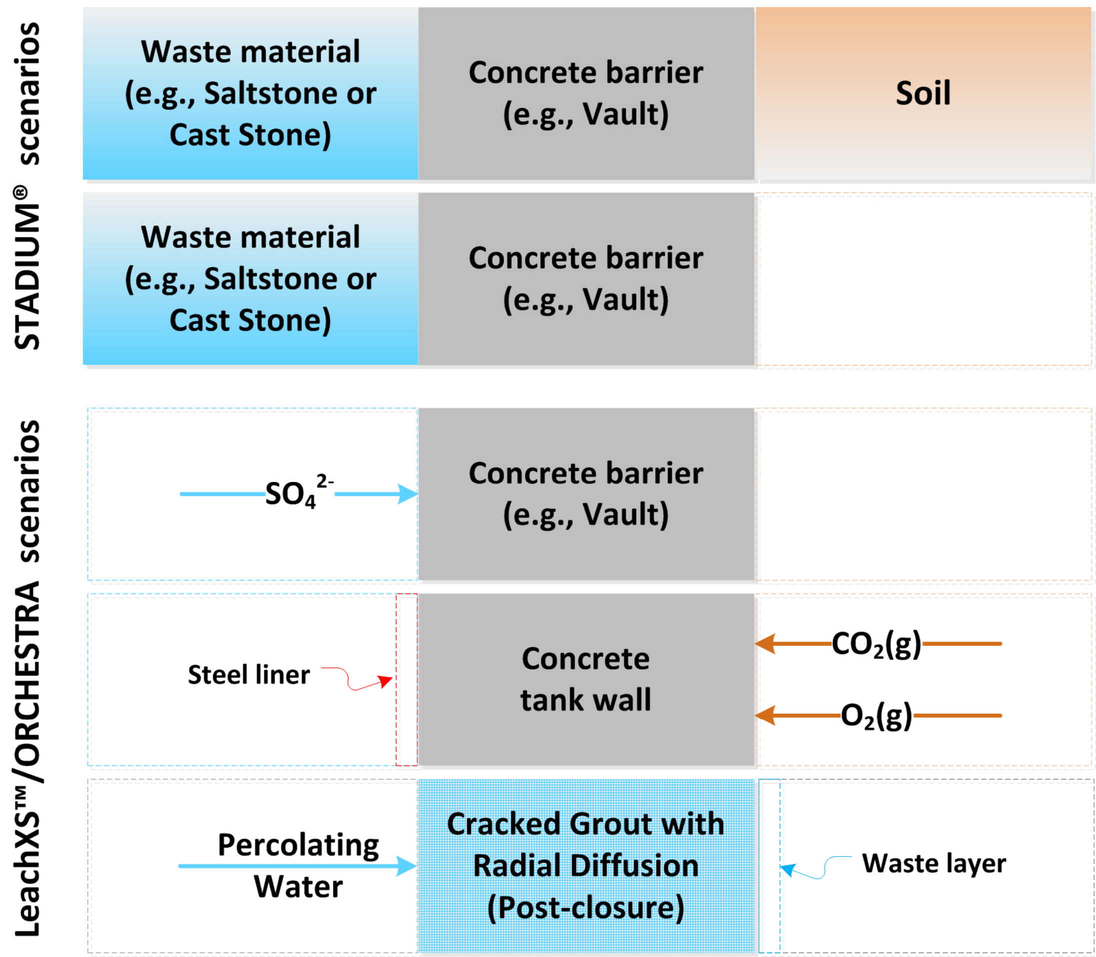
CBP Software ToolBox—Phase I



CBP ToolBox Development—Process

1. Conceptualize problem scenario and determine appropriate model and coupling, if needed
   - Need to consider availability of needed data
2. Develop scenario in appropriate partner code(s)
   - No coupling between LXO and STADIUM (Phase I)
   - STADIUM → SIMCO Technologies, Inc.
   - LeachXS/ORCHESTRA (LXO) → LeachXS
3. Set up necessary model file(s) to run simulation
   - Instructions file → Model file
   - DLL_STADIUM_#Layers.dat → stad09d-cbp-task7-#layers.inp
   - DLL_LXO_#Layers.dat → leachxs_parameters.txt
4. Run simulation

CBP ToolBox—Conceptualize Problem



Multi-layered sulfate ingress or chloride attack case

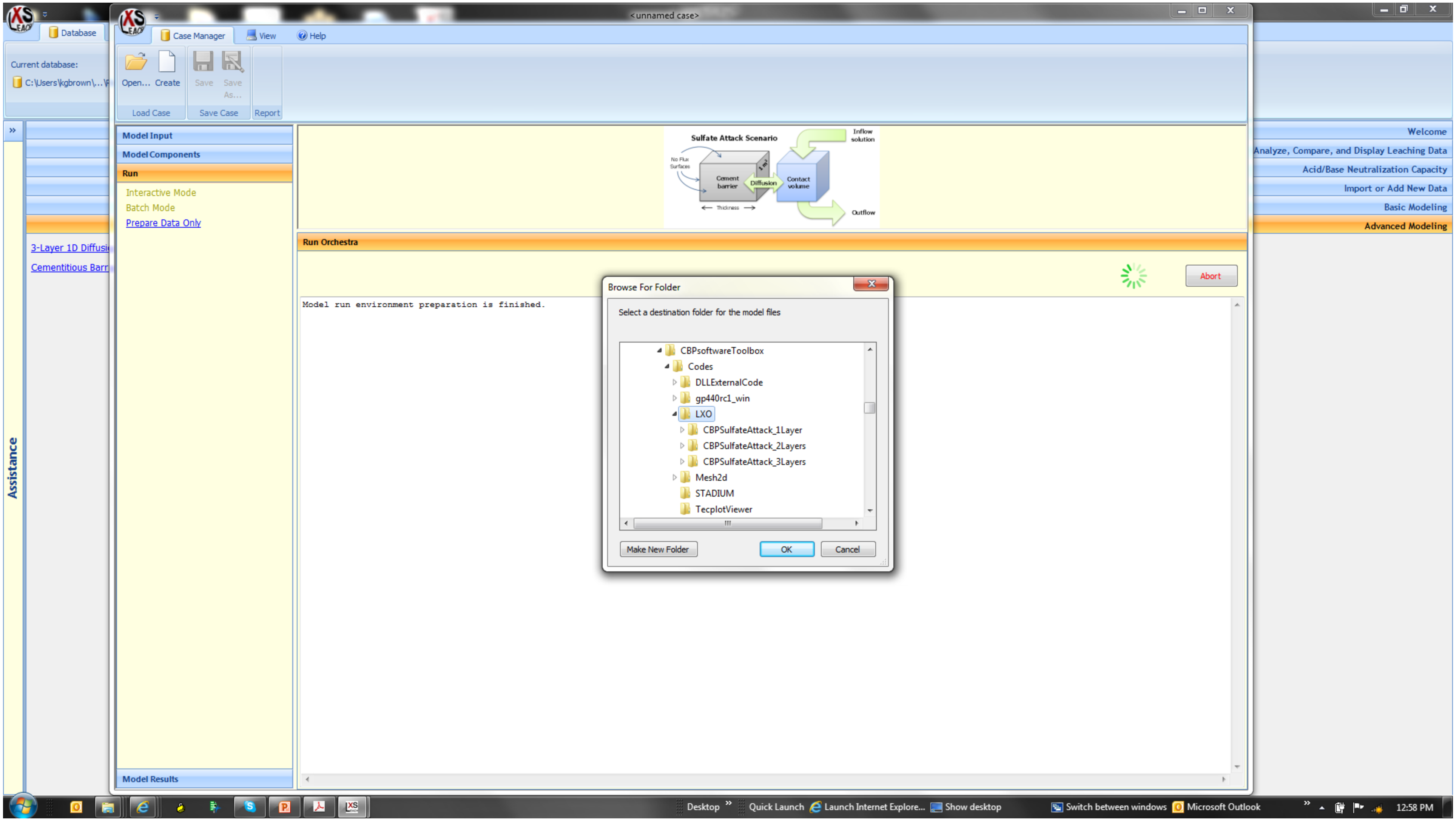
Simplified two-layer sulfate ingress or chloride attack case

Simplified one-layer sulfate attack case with boundary condition representing salt waste

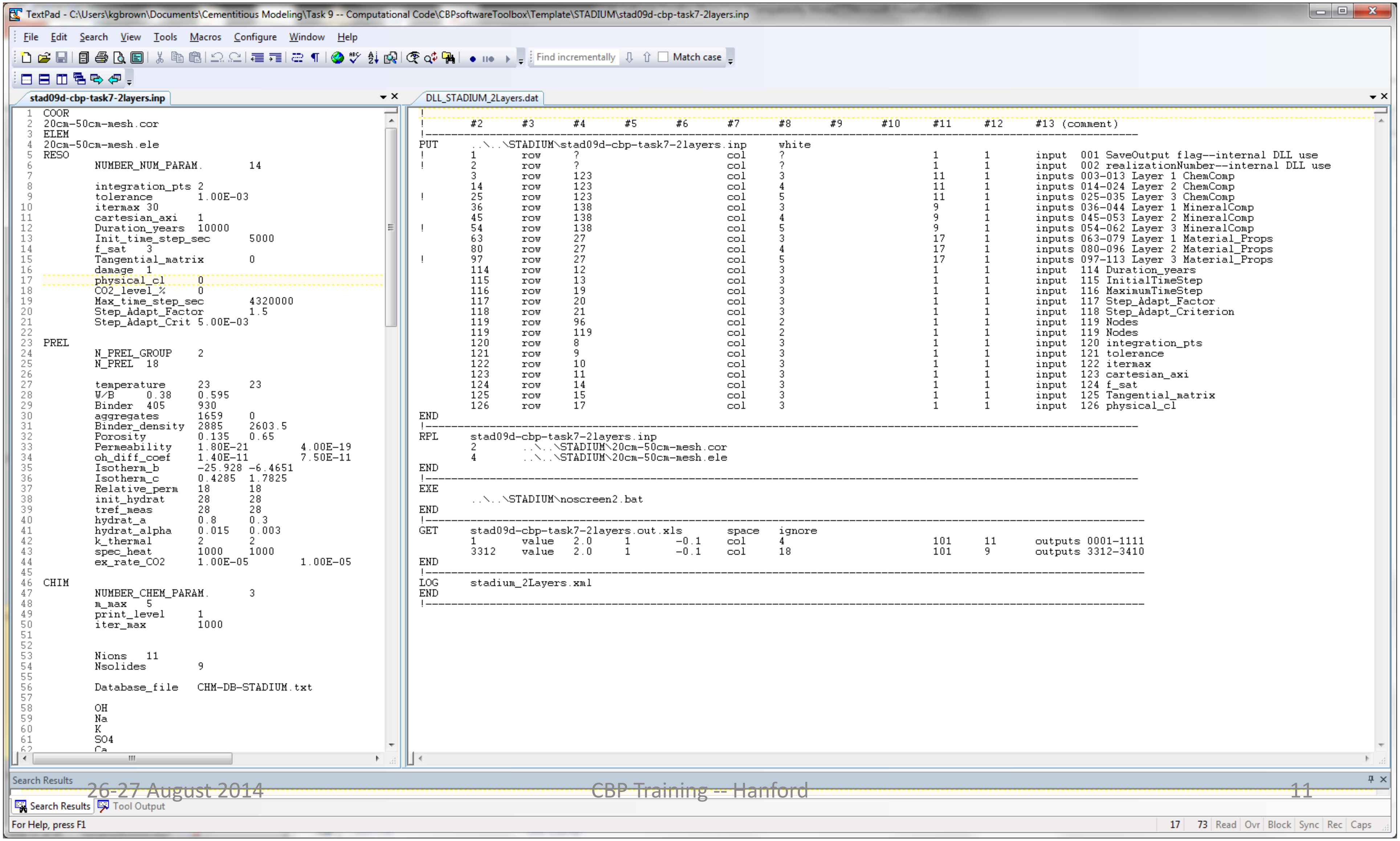
Simplified one-layer carbonation case ignoring steel liner with boundary condition representing gas ingress of CO_2 and O_2

Simplified one-layer percolation with radial diffusion case ignoring waste layer with boundary condition representing percolating water

CBP ToolBox—Develop Scenario



ToolBox—Define Model & Instructions Files



ToolBox—STADIUM Model & Instructions Files

stad09d-cbp-task7-2layers.inp

```
          Temperature      2      0      1      365     0      5      15
          101     365      0      5      15
    INIT
          external_file    0

          OH       400     670.08
          Na       282.1   4420
          K        138     120
          SO4      8       130.7
          Ca       0.5     0.41
          Al(OH)4  0.1     0.14
          Cl       5       9
          H2SiO4   0       9.7
          CO3      0       2.9
          NO3      0       2000
          NO2      0       1575
          Rel_Humidity     1      1
          Potential        0      0
          Temperature      23     23

```

DLL_STADIUM_2Layers.dat

```
!
!       #2      #3      #4      #5      #6      #7      #8      #9      #10     #11     #12     #13 (comment)
!-----------------------------------------------------------------------------------------------------------
PUT     ..\..\STADIUM\stad09d-cbp-task7-2layers.inp       white
!       1       row     ?                       col     ?                       1       1       input   001 SaveOutput flag--internal DLL use
!       2       row     ?                       col     ?                       1       1       input   002 realizationNumber internal DLL use
        3       row     123                     col     3                       11      1       inputs  003-013 Layer 1 ChemComp
        14      row     123                     col     4                       11      1       inputs  014-024 Layer 2 ChemComp
!       25      row     123                     col     5                       11      1       inputs  025-035 Layer 3 ChemComp
        36      row     138                     col     3                       9       1       inputs  036-044 Layer 1 MineralComp
        45      row     138                     col     4                       9       1       inputs  045-053 Layer 2 MineralComp
!       54      row     138                     col     5                       9       1       inputs  054-062 Layer 3 MineralComp
        63      row     27                      col     3                       17      1       inputs  063-079 Layer 1 Material_Props
        80      row     27                      col     4                       17      1       inputs  080-096 Layer 2 Material_Props
!       97      row     27                      col     5                       17      1       inputs  097-113 Layer 3 Material_Props
        114     row     12                      col     3                       1       1       input   114 Duration_years
        115     row     13                      col     3                       1       1       input   115 InitialTimeStep
        116     row     19                      col     3                       1       1       input   116 MaximumTimeStep
        117     row     20                      col     3                       1       1       input   117 Step_Adapt_Factor
        118     row     21                      col     3                       1       1       input   118 Step_Adapt_Criterion
        119     row     96                      col     2                       1       1       input   119 Nodes
        119     row     119                     col     2                       1       1       input   119 Nodes
        120     row     8                       col     3                       1       1       input   120 integration_pts
        121     row     9                       col     3                       1       1       input   121 tolerance
```

ToolBox—LXO Model & Instructions Files

leachxs_parameters.txt

```
@class: block_barrier_chemical()
The chemical parameters of the cement barrier.
{
Var:   pe  H+.kg Al+3.kg Ca+2.kg H2CO3.kg Fe+3.kg Mg+2.kg Na+.kg H4SiO4.kg SO4-2.kg
Data:   7.50000E+00   1.01078E-15   2.40868E-01   1.13290E+00   3.92855E-03   3.42400E-02   2.72040E-01   7.01721E-03   1.72373E-01   1.71214E-
Data:   7.50000E+00   1.01078E-15   2.40868E-01   1.13290E+00   3.92855E-03   3.42400E-02   2.72040E-01   7.01721E-03   1.72373E-01   1.71214E-
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Data:   7.50000E+00   1.01078E-15   2.40868E-01   1.13290E+00   3.92855E-03   3.42400E-02   2.72040E-01   7.01721E-03   1.72373E-01   1.71214E-
Data:   7.50000E+00   1.01078E-15   2.40868E-01   1.13290E+00   3.92855E-03   3.42400E-02   2.72040E-01   7.01721E-03   1.72373E-01   1.71214E-
Data:   7.50000E+00   1.01078E-15   2.40868E-01   1.13290E+00   3.92855E-03   3.42400E-02   2.72040E-01   7.01721E-03   1.72373E-01   1.71214E-
Data:   7.50000E+00   1.01078E-15   2.40868E-01   1.13290E+00   3.92855E-03   3.42400E-02   2.72040E-01   7.01721E-03   1.72373E-01   1.71214E-
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Data:   7.50000E+00   1.01078E-15   2.40868E-01   1.13290E+00   3.92855E-03   3.42400E-02   2.72040E-01   7.01721E-03   1.72373E-01   1.71214E-
```
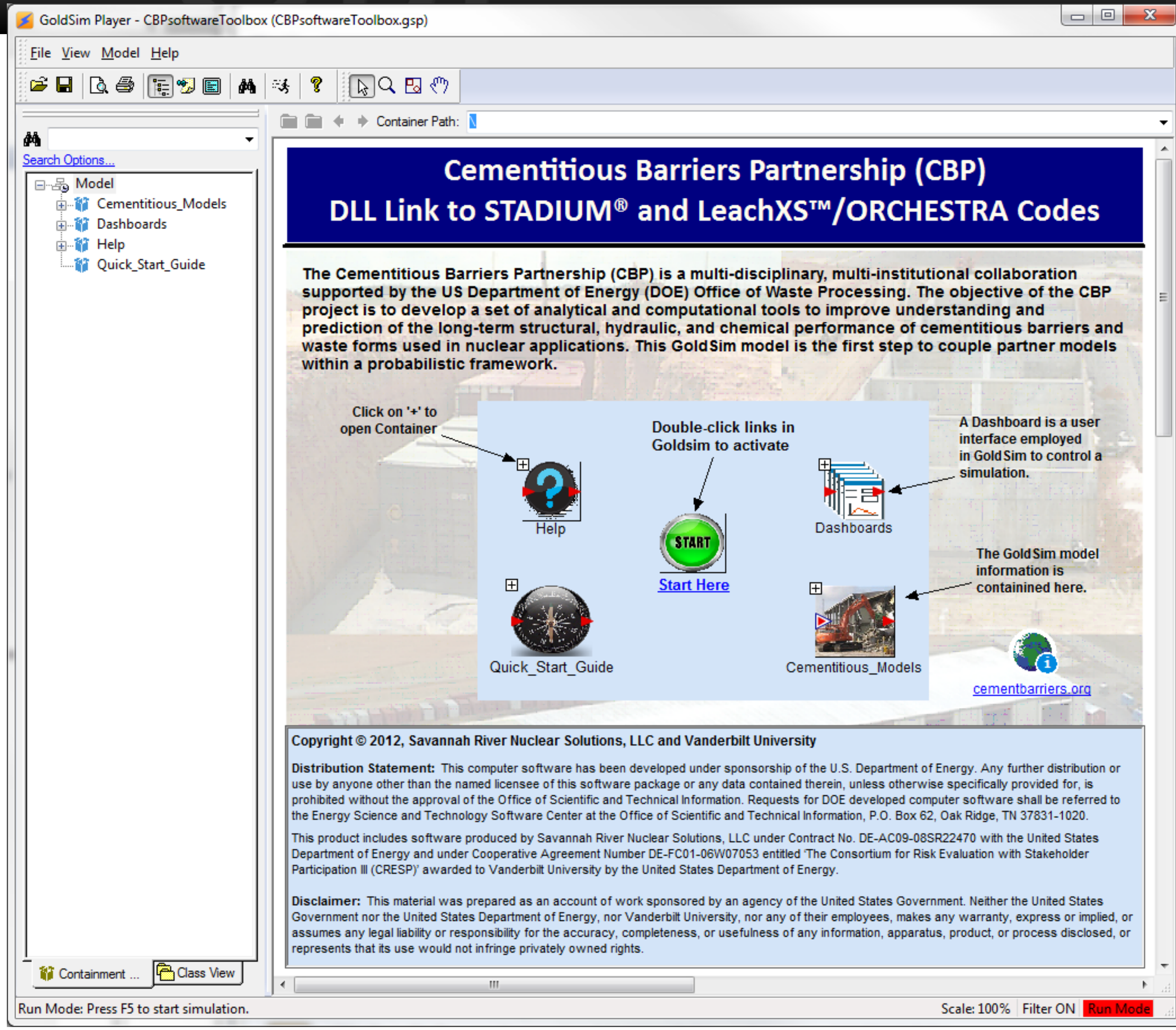

DLL_LXO_1Layer.dat

```
!----------------------------------------------------------------------------------------------------------
PUT     ..\..\LXO\CBPSulfateAttack_1Layer\Projects\CBPSulfateAttack\leachxs_parameters.txt      white   ignore
!       1       row     ?               col     N/A             1       1       input   001 SaveOutput flag--internal DLL use
!       2       row     2               col     5               1       1       input   002 realizationNumber
!       17804   row     7               col     2               1       1       input   17804 SimDuration_hr
!       17805   row     3               col     5               1       1       input   17805 CurrentDate
! Solid composition for Layer 1
!
! Solid composition for Layer 2
        44      row     260             heading Al+3.kg 259     |       100     1       input   044 Al+3 for Layer 1
        345     row     260             heading Ca+2.kg 259             100     1       input   345 Ca+2 for Layer 1
        646     row     260             heading H2CO3.kg        259             100     1       input   646 H2CO3 for Layer 1
        947     row     260             heading Fe+3.kg 259             100     1       input   947  Fe+3 for Layer 1
        1248    row     260             heading Mg+2.kg 259             100     1       input   1248 Mg+2 for Layer 1
        1549    row     260             heading Na+.kg  259             100     1       input   1549 na+ for Layer 1
        1850    row     260             heading H4SiO4.kg       259             100     1       input   1850 H4SiO4 for Layer 1
        2151    row     260             heading SO4-2.kg        259             100     1       input   2151 SO4-2 for Layer 1
        3957    row     260             heading H+.kg   259             100     1       input   3957 H+ for Layer 1
        14793   row     260             heading pe      259             100     1       input   14793 pe for Layer 1
!
! Solid composition for Layer 3
!
```


GoldSim Player - CBPsoftwareToolbox (CBPsoftwareToolbox.gsp)
File View Model Help
Search Options...
Model
Cementitious_Models
Dashboards
Help
Quick_Start_Guide
Containment ...
Class View
Container Path:
Cementitious Barriers Partnership (CBP)
DLL Link to STADIUM® and LeachXS™/ORCHESTRA Codes
The Cementitious Barriers Partnership (CBP) is a multi-disciplinary, multi-institutional collaboration supported by the US Department of Energy (DOE) Office of Waste Processing. The objective of the CBP project is to develop a set of analytical and computational tools to improve understanding and prediction of the long-term structural, hydraulic, and chemical performance of cementitious barriers and waste forms used in nuclear applications. This GoldSim model is the first step to couple partner models within a probabilistic framework.
Click on '+' to open Container
Double-click links in Goldsim to activate
A Dashboard is a user interface employed in GoldSim to control a simulation.
Help
START
Start Here
Dashboards
The GoldSim model information is containined here.
Quick_Start_Guide
Cementitious_Models
cementbarriers.org
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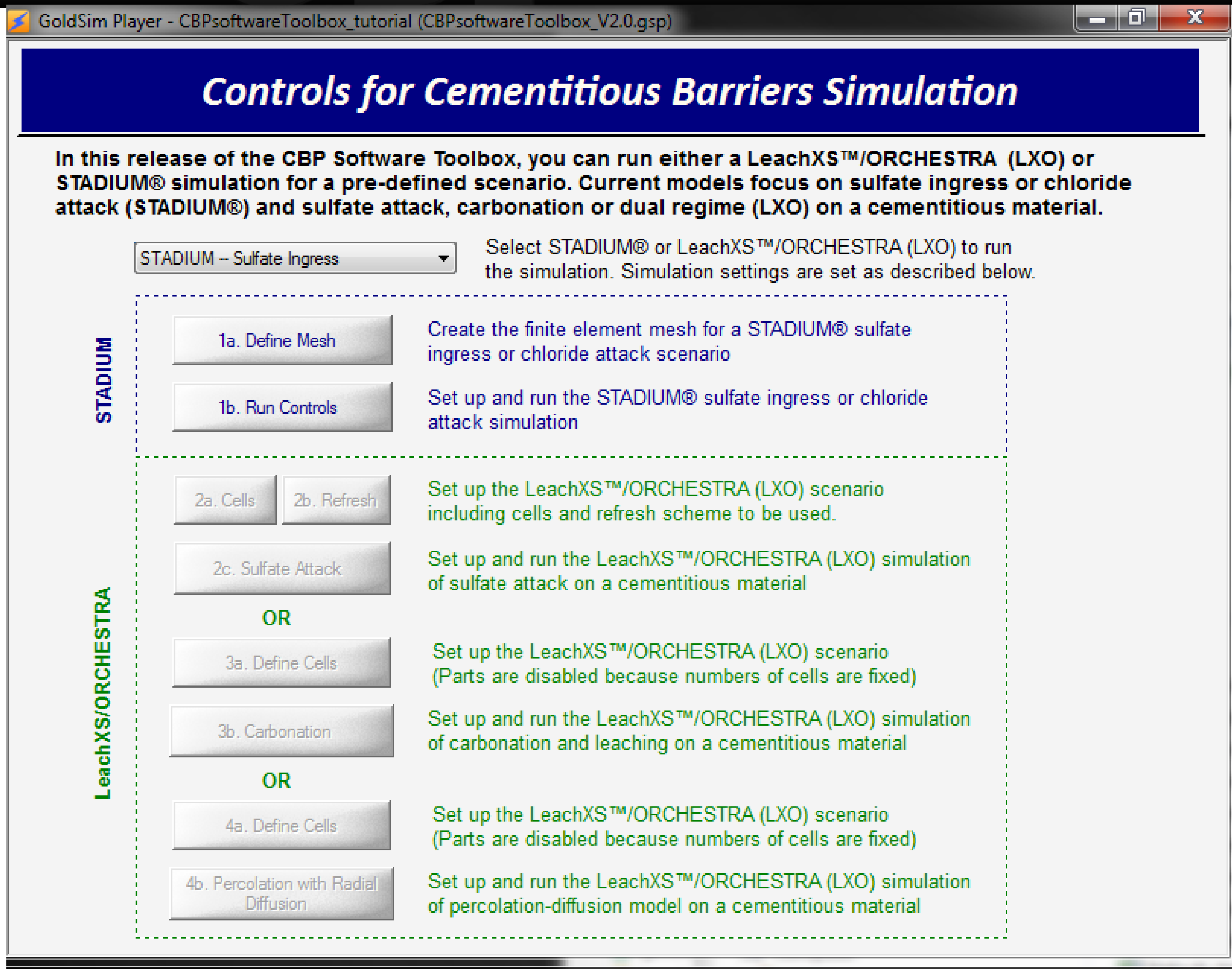
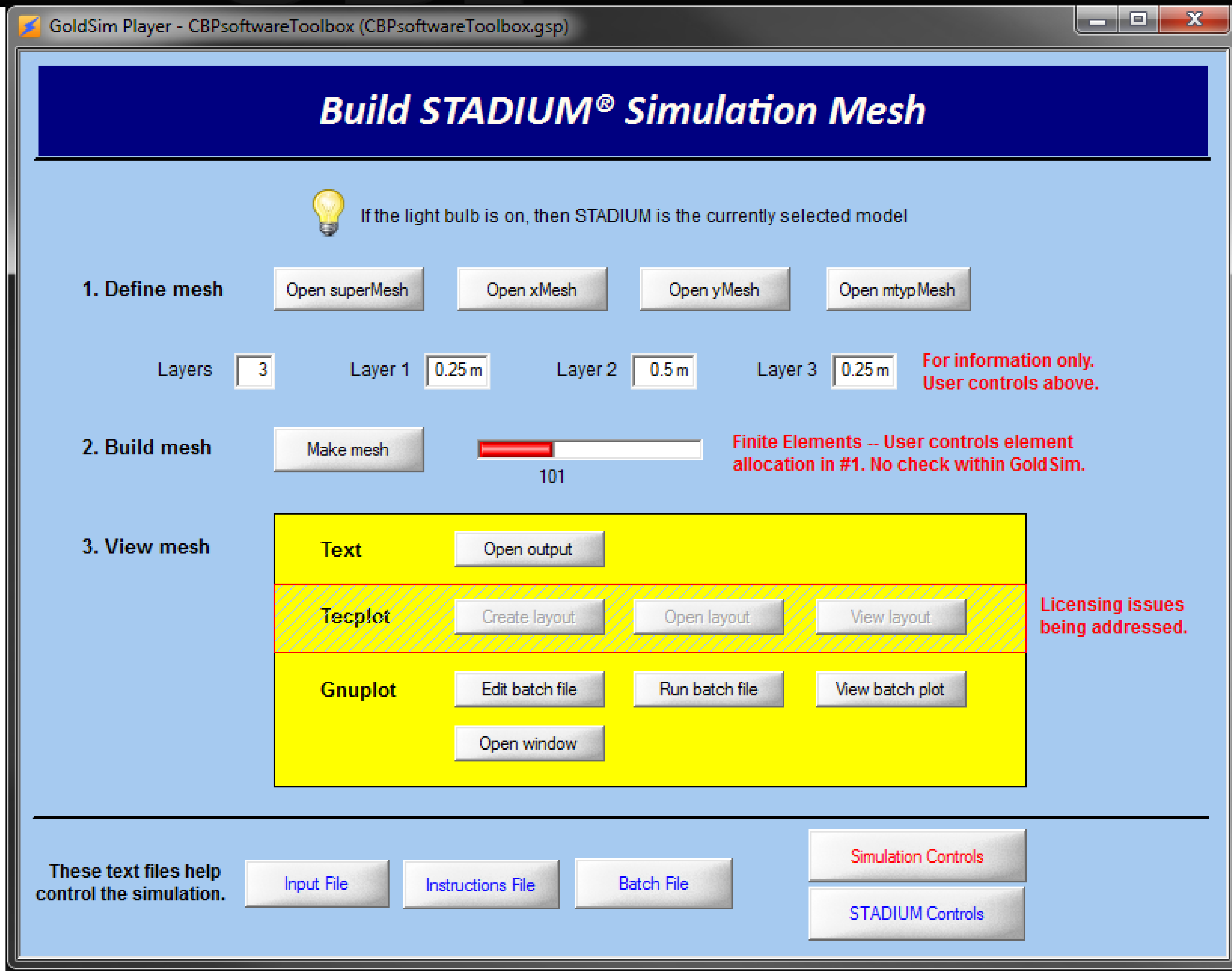
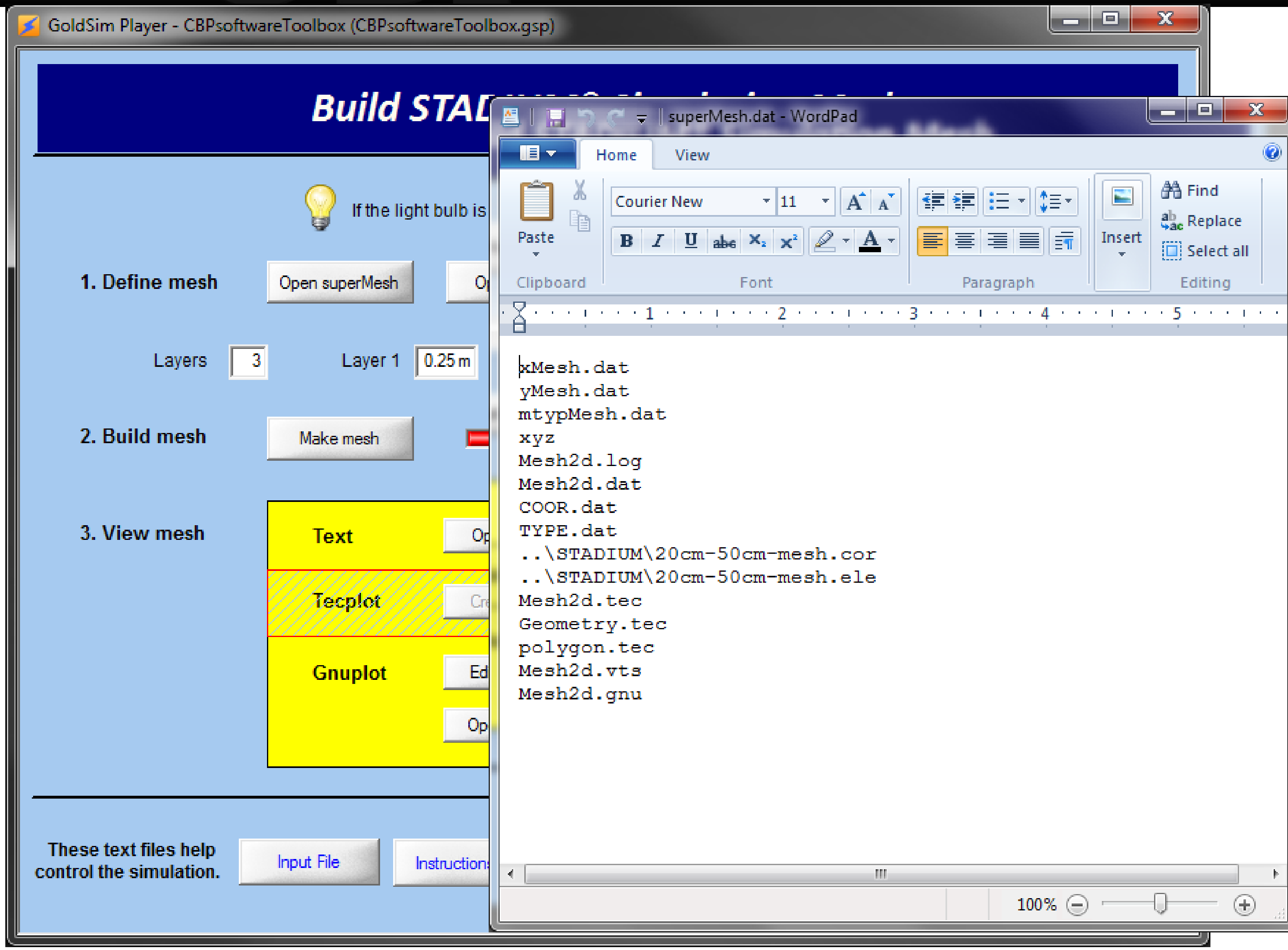
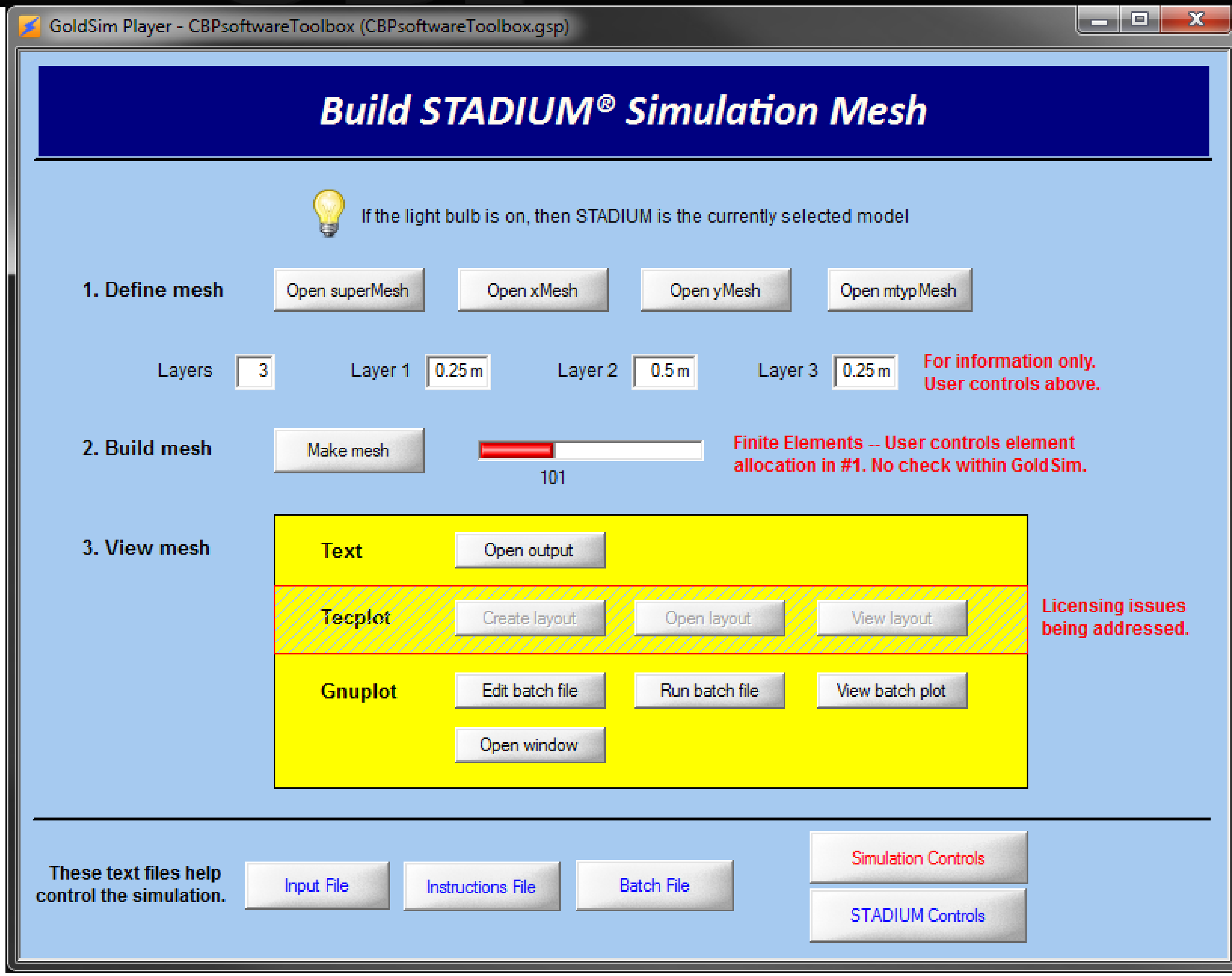
Run Mode: Press F5 to start simulation.
Scale: 100%
Filter ON
Run Mode


GoldSim Player - CBPsoftwareToolbox_tutorial (CBPsoftwareToolbox_V2.0.gsp)
Controls for Cementitious Barriers Simulation
In this release of the CBP Software Toolbox, you can run either a LeachXS™/ORCHESTRA (LXO) or STADIUM® simulation for a pre-defined scenario. Current models focus on sulfate ingress or chloride attack (STADIUM®) and sulfate attack, carbonation or dual regime (LXO) on a cementitious material.
STADIUM -- Sulfate Ingress
Select STADIUM® or LeachXS™/ORCHESTRA (LXO) to run the simulation. Simulation settings are set as described below.
STADIUM
1a. Define Mesh
Create the finite element mesh for a STADIUM® sulfate ingress or chloride attack scenario
1b. Run Controls
Set up and run the STADIUM® sulfate ingress or chloride attack simulation
LeachXS/ORCHESTRA
2a. Cells
2b. Refresh
Set up the LeachXS™/ORCHESTRA (LXO) scenario including cells and refresh scheme to be used.
2c. Sulfate Attack
Set up and run the LeachXS™/ORCHESTRA (LXO) simulation of sulfate attack on a cementitious material
OR
3a. Define Cells
Set up the LeachXS™/ORCHESTRA (LXO) scenario (Parts are disabled because numbers of cells are fixed)
3b. Carbonation
Set up and run the LeachXS™/ORCHESTRA (LXO) simulation of carbonation and leaching on a cementitious material
OR
4a. Define Cells
Set up the LeachXS™/ORCHESTRA (LXO) scenario (Parts are disabled because numbers of cells are fixed)
4b. Percolation with Radial Diffusion
Set up and run the LeachXS™/ORCHESTRA (LXO) simulation of percolation-diffusion model on a cementitious material


GoldSim Player - CBPsoftwareToolbox (CBPsoftwareToolbox.gsp)
Build STADIUM® Simulation Mesh
If the light bulb is on, then STADIUM is the currently selected model
1. Define mesh
Open superMesh
Open xMesh
Open yMesh
Open mtypMesh
Layers
3
Layer 1
0.25 m
Layer 2
0.5 m
Layer 3
0.25 m
For information only. User controls above.
2. Build mesh
Make mesh
101
Finite Elements -- User controls element allocation in #1. No check within GoldSim.
3. View mesh
Text
Open output
Tecplot
Create layout
Open layout
View layout
Licensing issues being addressed.
Gnuplot
Edit batch file
Run batch file
View batch plot
Open window
These text files help control the simulation.
Input File
Instructions File
Batch File
Simulation Controls
STADIUM Controls


GoldSim Player - CBPsoftwareToolbox (CBPsoftwareToolbox.gsp)
Build STAD
If the light bulb is
1. Define mesh
Open superMesh
Layers
3
Layer 1
0.25 m
2. Build mesh
Make mesh
3. View mesh
Text
Tecplot
Gnuplot
These text files help control the simulation.
Input File
superMesh.dat - WordPad
Home
View
Paste
Clipboard
Courier New
11
Font
Paragraph
Insert
Find
Replace
Select all
Editing
xMesh.dat
yMesh.dat
mtypMesh.dat
xyz
Mesh2d.log
Mesh2d.dat
COOR.dat
TYPE.dat
..\STADIUM\20cm-50cm-mesh.cor
..\STADIUM\20cm-50cm-mesh.ele
Mesh2d.tec
Geometry.tec
polygon.tec
Mesh2d.vts
Mesh2d.gnu
100%


GoldSim Player - CBPsoftwareToolbox (CBPsoftwareToolbox.gsp)
Build STADIUM® Simulation Mesh
If the light bulb is on, then STADIUM is the currently selected model
1. Define mesh
Open superMesh
Open xMesh
Open yMesh
Open mtypMesh
Layers
3
Layer 1
0.25 m
Layer 2
0.5 m
Layer 3
0.25 m
For information only.
User controls above.
2. Build mesh
Make mesh
101
Finite Elements -- User controls element allocation in #1. No check within GoldSim.
3. View mesh
Text
Open output
Tecplot
Create layout
Open layout
View layout
Licensing issues being addressed.
Gnuplot
Edit batch file
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These text files help control the simulation.
Input File
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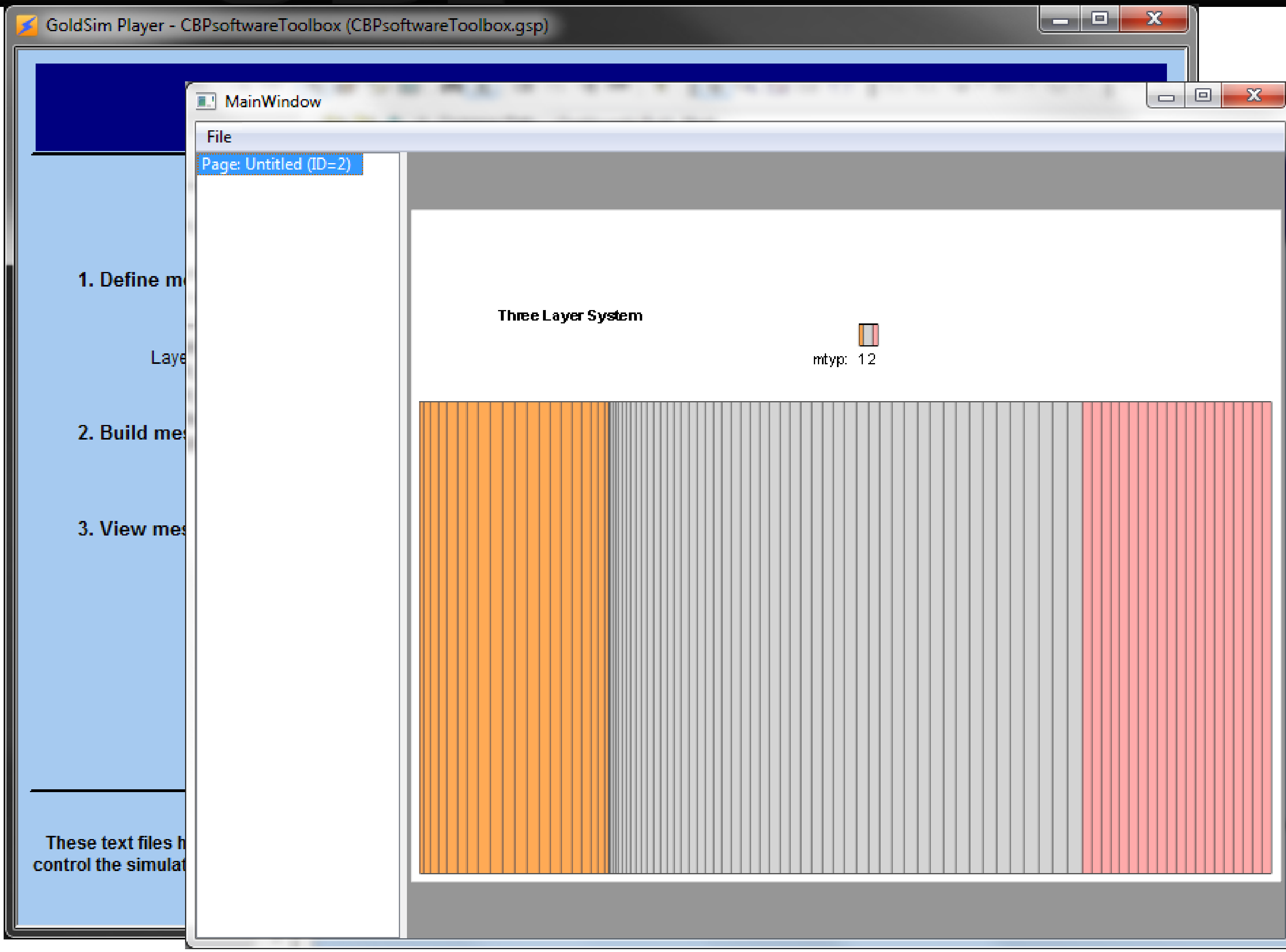
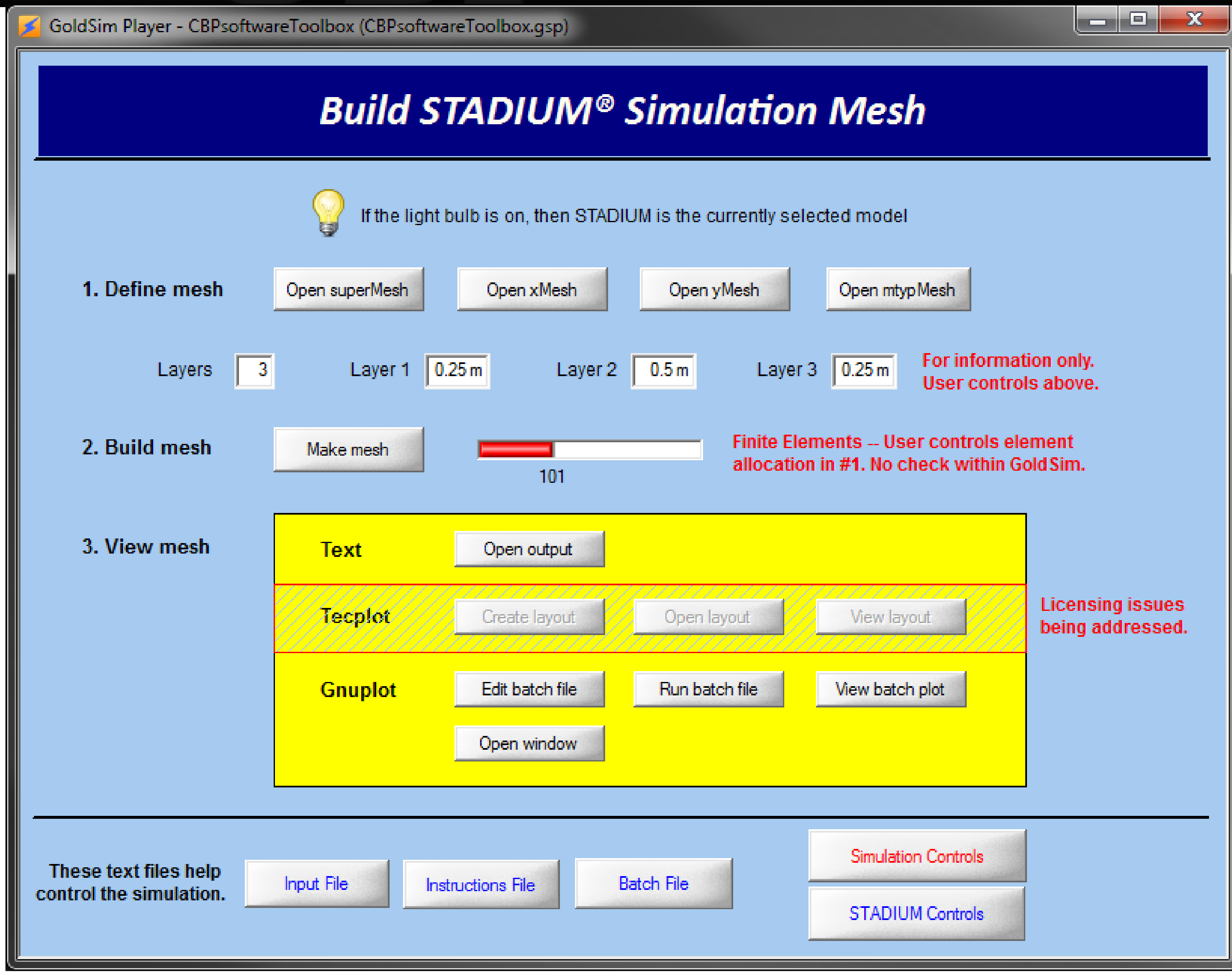
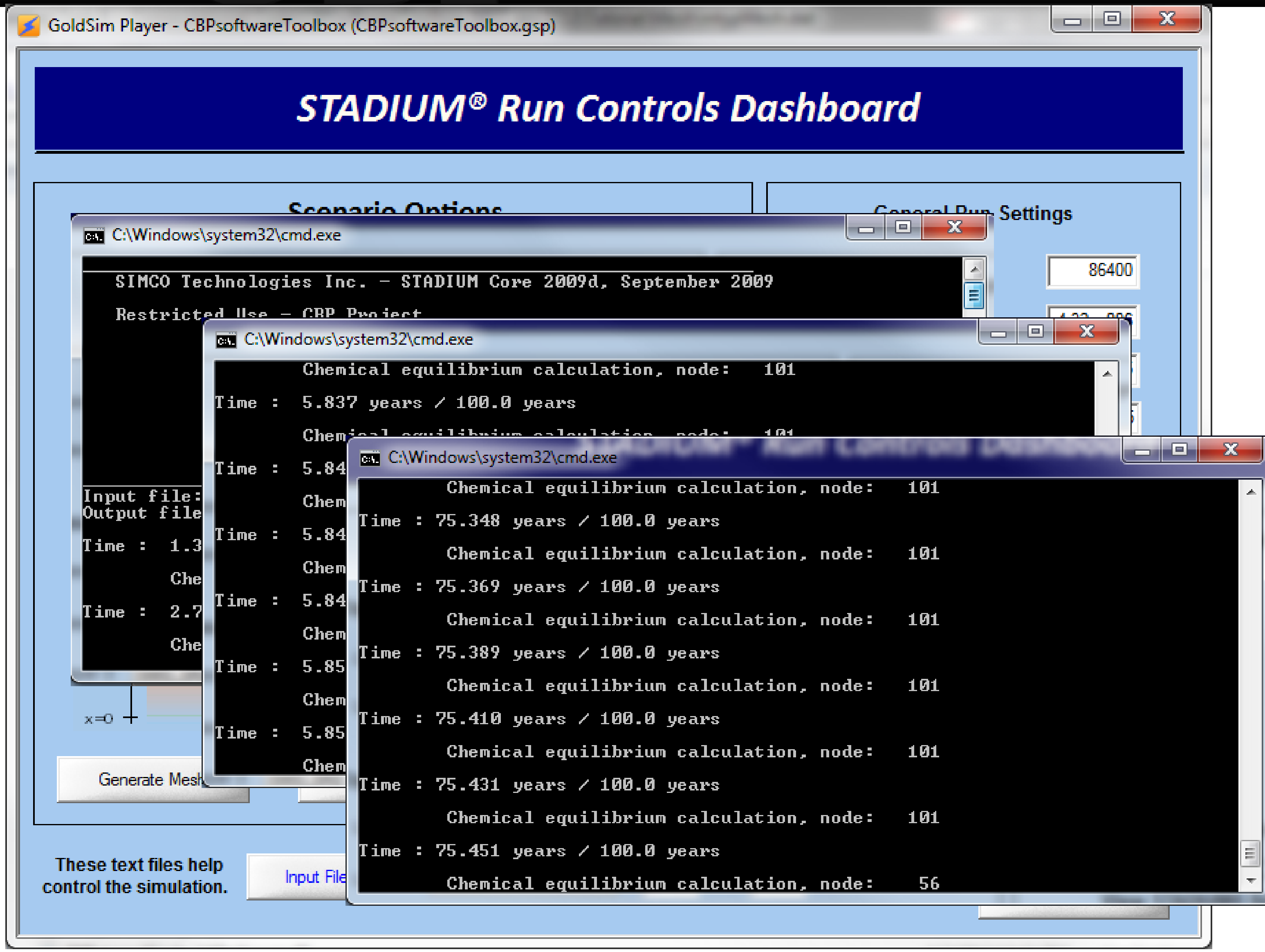
Simulation Controls
STADIUM Controls

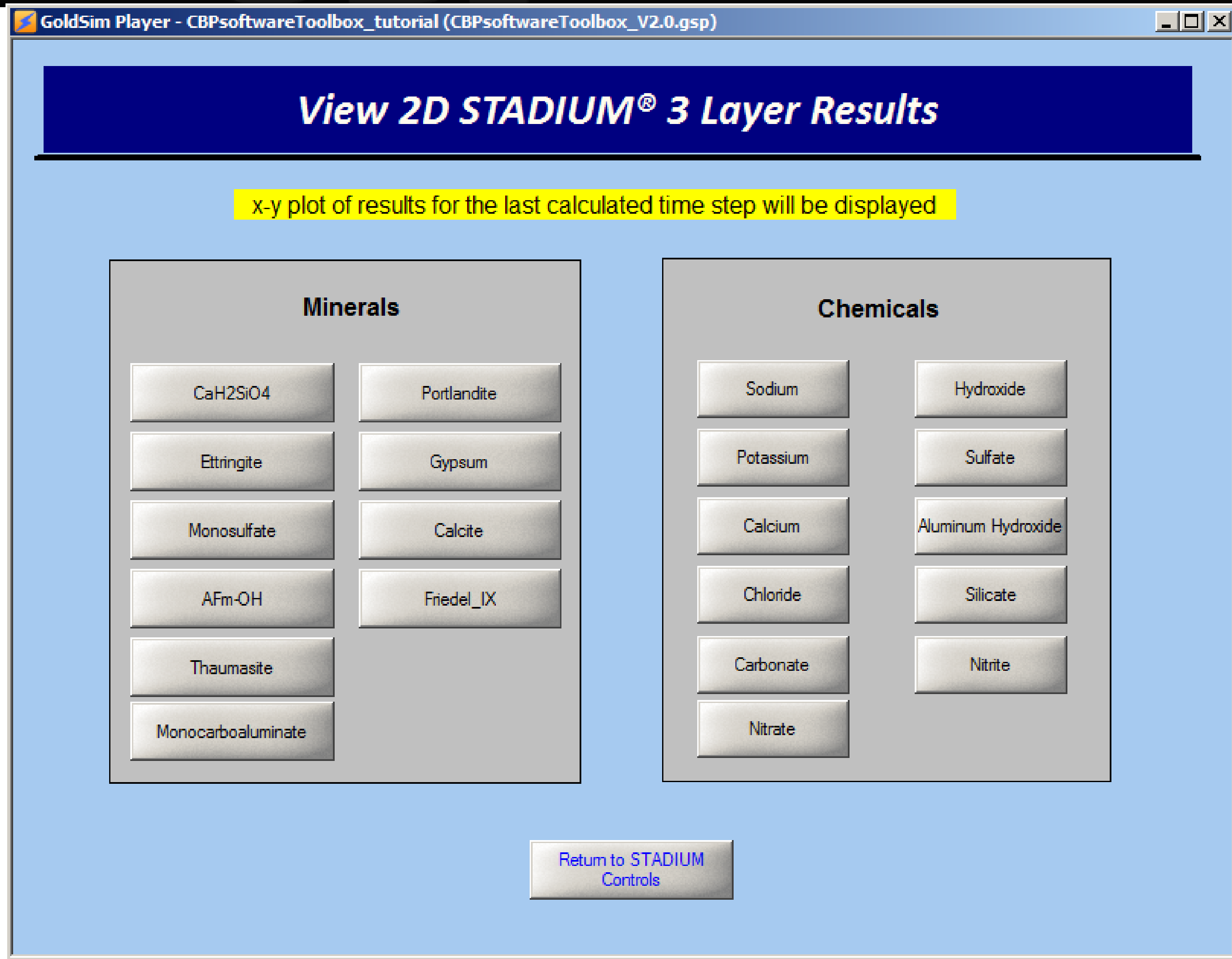

GoldSim Player - CBPsoftwareToolbox (CBPsoftwareToolbox.gsp)
MainWindow
File
Page: Untitled (ID=2)
Three Layer System
mtyp: 12

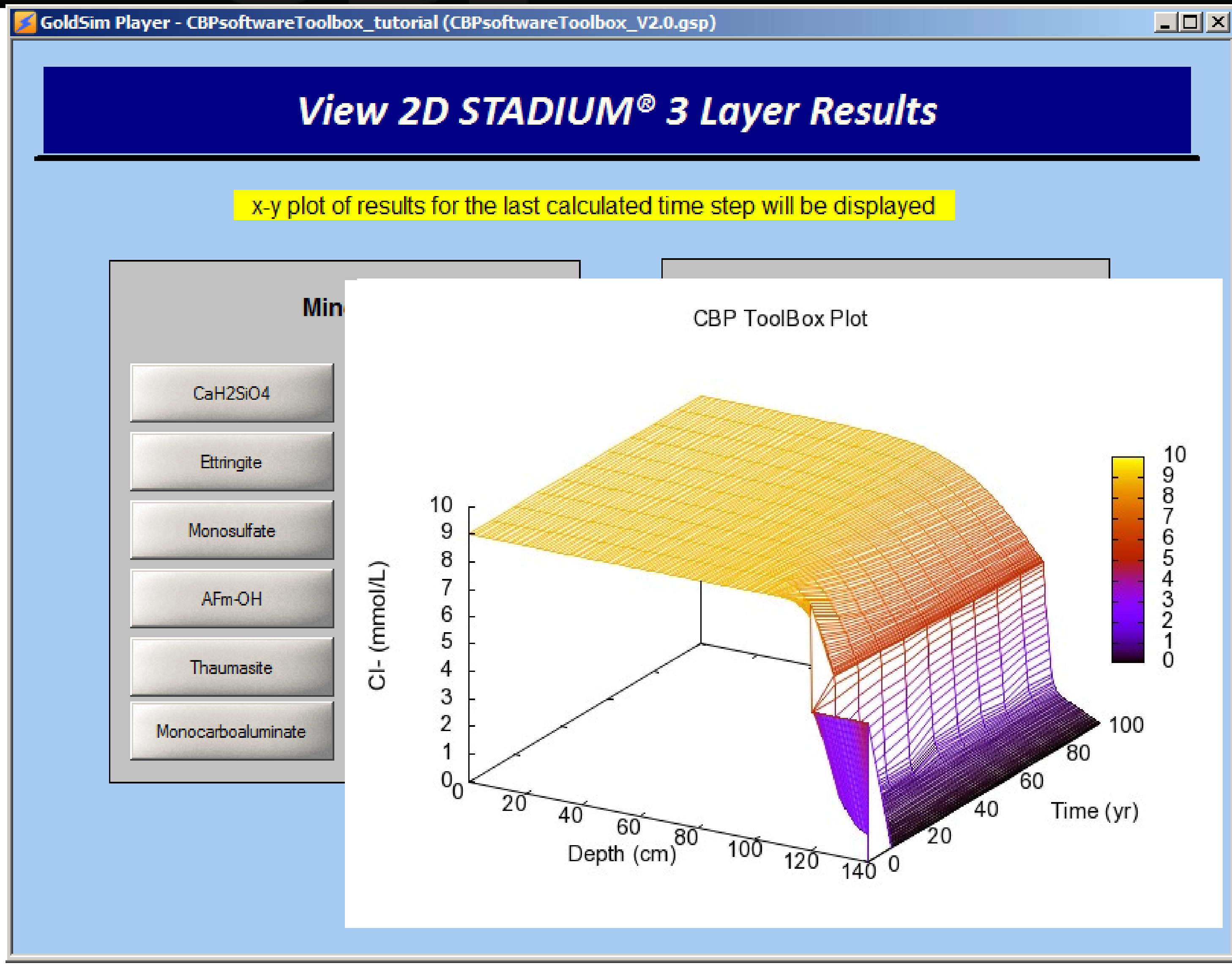
CBP
Cementitious Barriers Partnership



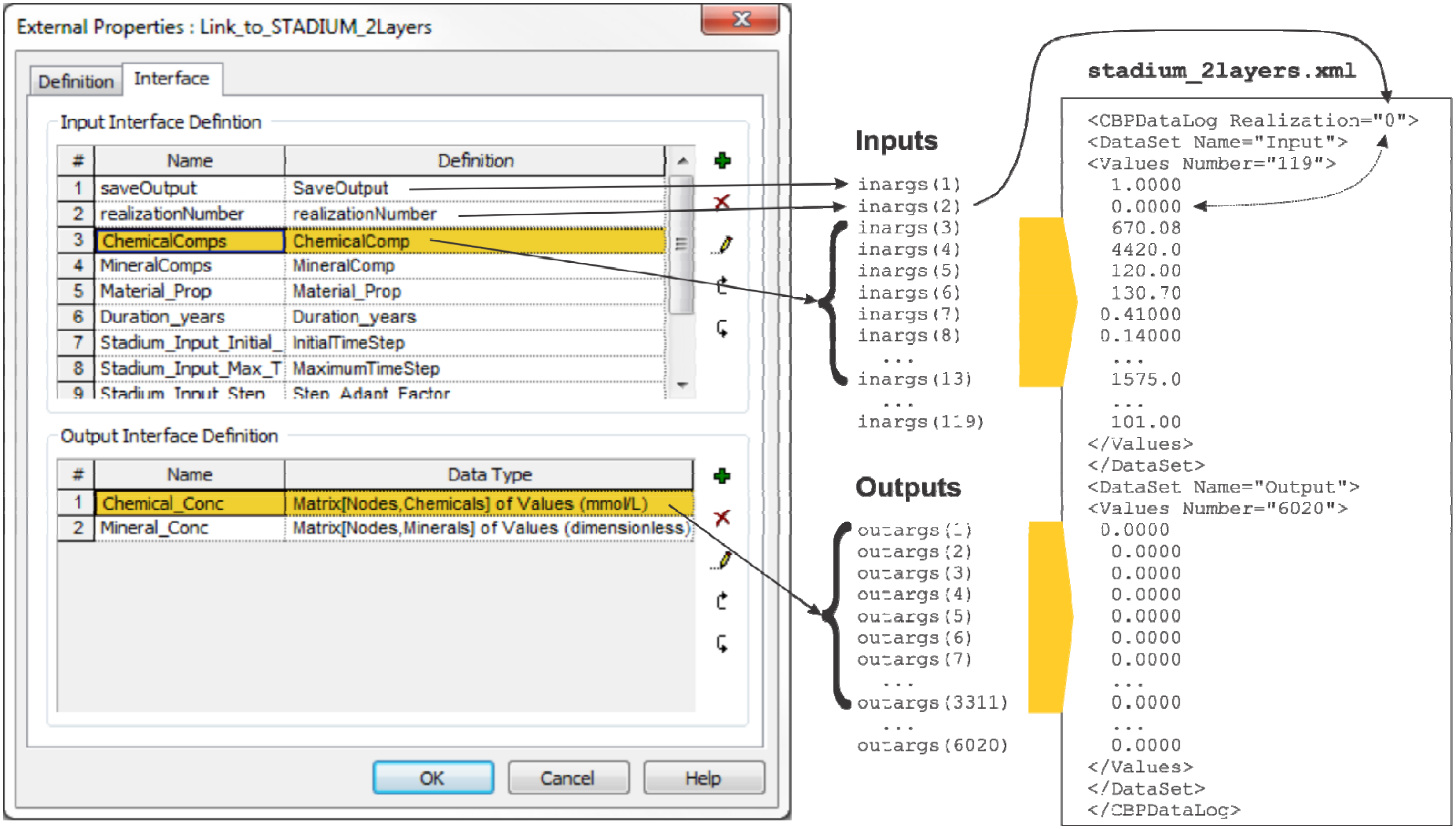

GoldSim Player - CBPsoftwareToolbox (CBPsoftwareToolbox.gsp)
STADIUM® Run Controls Dashboard
Scenario Options
If light bulb is on, then STADIUM is the currently selected model
Three Layer Model
Select the number of layers in the model
Width (m)
Conc. CoV
x=L
Layer 1:
Salt Waste Type 1
0.25
0.05
Layer 2:
Vault 1/4 (1)
0.5
0.05
width
Layer 3:
Soil Type 1
0.25
0.05
x=0
Generate Mesh
View Geometry
RESO Options
These text files help control the simulation.
Input File
Instructions File
Batch File
General Run Settings
Initial Time Step, sec
86400
Max Time Step, sec
4.32e+006
Step Adapt Factor
1.5
Step Adapt Criterion
0.005
Total number of nodes
101
Check to Save STADIUM® Output
View STADIUM® Results
View Inputs
View Results
Simulation Controls
Browse Model
Run Simulation (F5)
Simulation Settings (F2)
Simulation Controls
Exit GoldSim


GoldSim Player - CBPsoftwareToolbox (CBPsoftwareToolbox.gsp)
STADIUM® Run Controls Dashboard
General Run Settings
86400
C:\Windows\system32\cmd.exe
SIMCO Technologies Inc. - STADIUM Core 2009d, September 2009
Chemical equilibrium calculation, node: 101
Time : 5.837 years / 100.0 years
Time : 75.348 years / 100.0 years
Time : 75.369 years / 100.0 years
Time : 75.389 years / 100.0 years
Time : 75.410 years / 100.0 years
Time : 75.431 years / 100.0 years
Time : 75.451 years / 100.0 years
Chemical equilibrium calculation, node: 56
Input file:
Output file
x=0
Generate Mesh
These text files help control the simulation.
Input File


GoldSim Player - CBPsoftwareToolbox_tutorial (CBPsoftwareToolbox_V2.0.gsp)
View 2D STADIUM® 3 Layer Results
x-y plot of results for the last calculated time step will be displayed
Minerals
CaH2SiO4
Portlandite
Ettringite
Gypsum
Monosulfate
Calcite
AFm-OH
Friedel_IX
Thaumasite
Monocarboaluminate
Chemicals
Sodium
Hydroxide
Potassium
Sulfate
Calcium
Aluminum Hydroxide
Chloride
Silicate
Carbonate
Nitrite
Nitrate
Return to STADIUM Controls

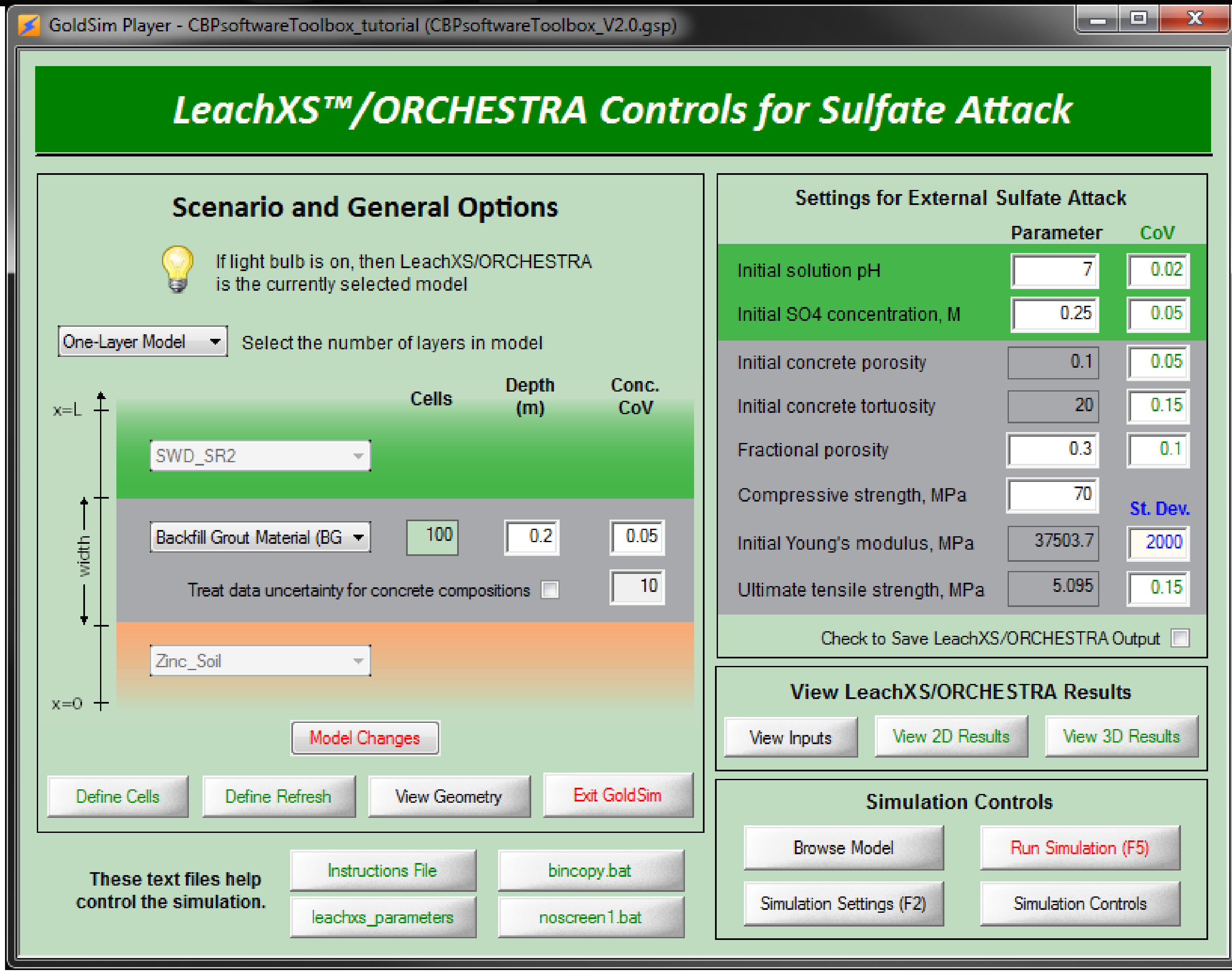

GoldSim Player - CBPsoftwareToolbox_tutorial (CBPsoftwareToolbox_V2.0.gsp)
View 2D STADIUM® 3 Layer Results
x-y plot of results for the last calculated time step will be displayed
Min
CaH2SiO4
Ettringite
Monosulfate
AFm-OH
Thaumasite
Monocarboaluminate
CBP ToolBox Plot
Cl- (mmol/L)
Depth (cm)
Time (yr)

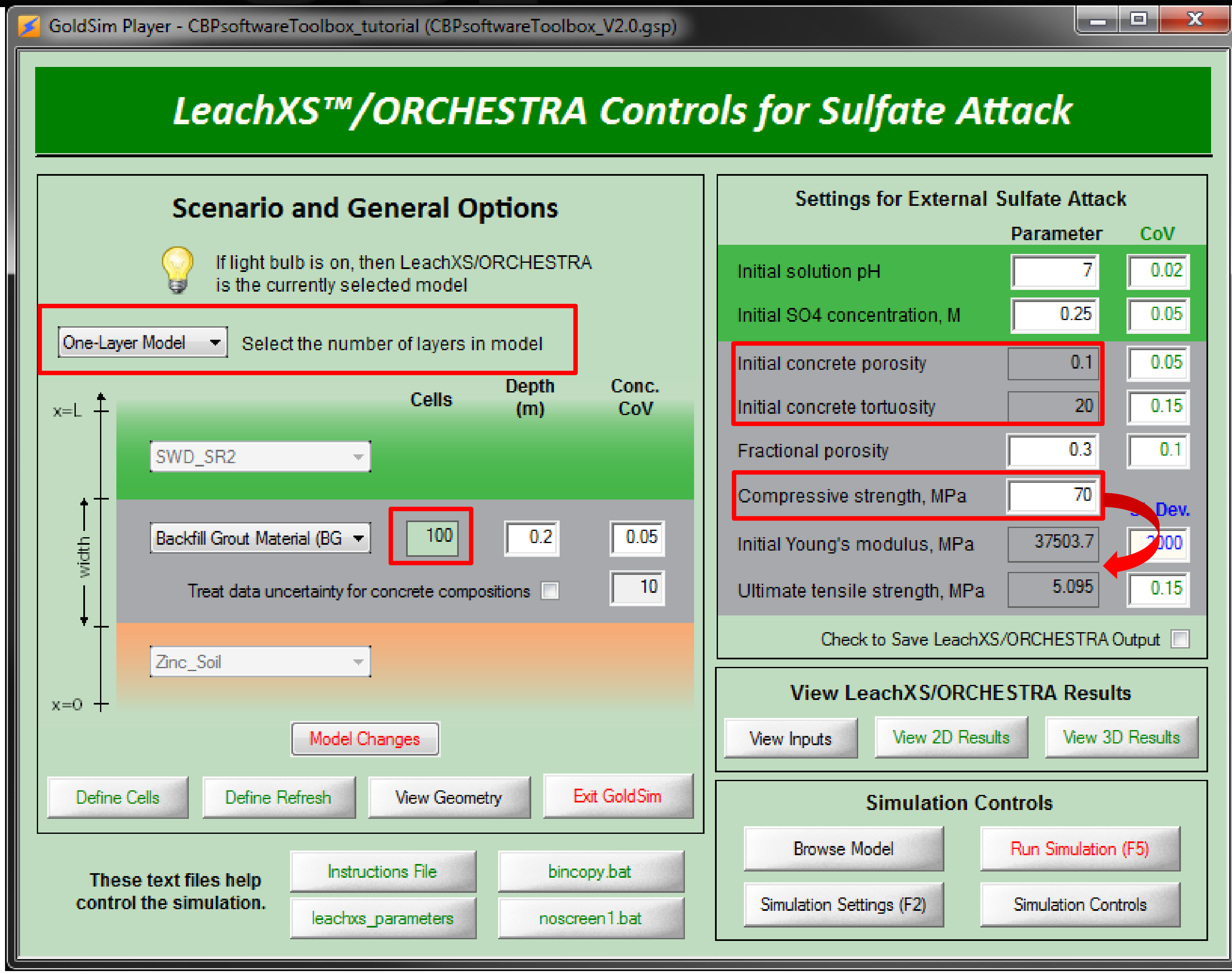
Summary of STADIUM External Linking



CBP Custom DLL Subroutine

- Avoid need for low-level programming by user
  - Put generic executable content in pre-compiled subroutine (Dynamic-link Library)
  - Put application content in an “instructions file” interpreted at run-time
  - Primary instructions: PUT (create input), EXE (execute file), GET (retrieve input), and LOG (record)
- Provide flexible, user-friendly access to partner code input and output files via instructions file
  - Row selection by number, label, value
  - Field selection by number
- Used to couple STADIUM and LeachXS/ORCHESTRA to GoldSim model


GoldSim Player - CBPsoftwareToolbox_tutorial (CBPsoftwareToolbox_V2.0.gsp)
LeachXS™/ORCHESTRA Controls for Sulfate Attack
Scenario and General Options
If light bulb is on, then LeachXS/ORCHESTRA is the currently selected model
One-Layer Model
Select the number of layers in model
x=L
Cells
Depth (m)
Conc. CoV
SWD_SR2
width
Backfill Grout Material (BG
100
0.2
0.05
Treat data uncertainty for concrete compositions
10
Zinc_Soil
x=0
Model Changes
Define Cells
Define Refresh
View Geometry
Exit GoldSim
These text files help control the simulation.
Instructions File
bincopy.bat
leachxs_parameters
noscreen1.bat
Settings for External Sulfate Attack
Parameter
CoV
Initial solution pH
7
0.02
Initial SO4 concentration, M
0.25
0.05
Initial concrete porosity
0.1
0.05
Initial concrete tortuosity
20
0.15
Fractional porosity
0.3
0.1
Compressive strength, MPa
70
St. Dev.
Initial Young's modulus, MPa
37503.7
2000
Ultimate tensile strength, MPa
5.095
0.15
Check to Save LeachXS/ORCHESTRA Output
View LeachXS/ORCHESTRA Results
View Inputs
View 2D Results
View 3D Results
Simulation Controls
Browse Model
Run Simulation (F5)
Simulation Settings (F2)
Simulation Controls


GoldSim Player - CBPsoftwareToolbox_tutorial (CBPsoftwareToolbox_V2.0.gsp)
LeachXS™/ORCHESTRA Controls for Sulfate Attack
Scenario and General Options
If light bulb is on, then LeachXS/ORCHESTRA is the currently selected model
One-Layer Model
Select the number of layers in model
x=L
Cells
Depth (m)
Conc. CoV
SWD_SR2
width
Backfill Grout Material (BG
100
0.2
0.05
Treat data uncertainty for concrete compositions
10
Zinc_Soil
x=0
Model Changes
Define Cells
Define Refresh
View Geometry
Exit GoldSim
These text files help control the simulation.
Instructions File
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Settings for External Sulfate Attack
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Compressive strength, MPa
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Dev.
Initial Young's modulus, MPa
37503.7
Ultimate tensile strength, MPa
5.095
0.15
Check to Save LeachXS/ORCHESTRA Output
View LeachXS/ORCHESTRA Results
View Inputs
View 2D Results
View 3D Results
Simulation Controls
Browse Model
Run Simulation (F5)
Simulation Settings (F2)
Simulation Controls

GoldSim Player - CBPsoftwareToolbox_tutorial (CBPsoftwareToolbox_V2.0.gsp)

Define LeachXS™/ORCHESTRA (LXO) Sulfate Attack Refresh

The refresh/renewal scheme is defined. There are two steps: 1) define the refresh interval and 2) define the external liquid volume to solid contact area ratio that also establishes the contact volume exchanged at each refresh interval. Note the ratio used to define the solution volume differs from the ratios used in related EPA and ASTM methods since only one face of the monolith is in contact with the external solution.

1. Refresh interval (d)

900

Extremely Dry (2 yr)

Relatively Dry (180d)

Moderately Humid (30d)

30

Frequent Rain (1-7d)

2. External Liquid Volume (L) to Solid Contact Area (m²)

constant external concentration B.C. (500)

500

EPA Method 1315 (100)

100

No external solution, "resting" case (1)

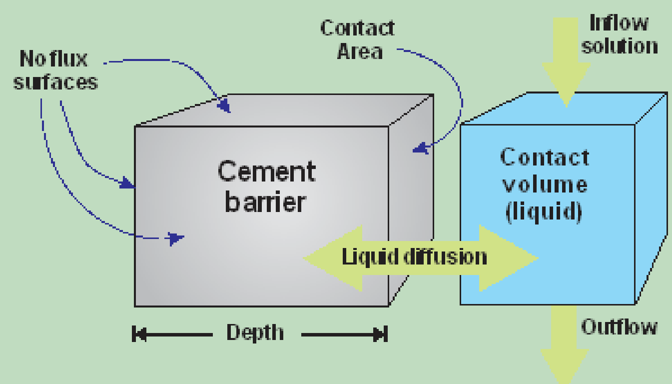
1

Note--you can select the slider and then use the keyboard arrows (▼▲) to increment/decrement

Monolith (Layer2) Properties

Depth	Contact Area	Volume
0.2 m	1 m2	0.004 m3

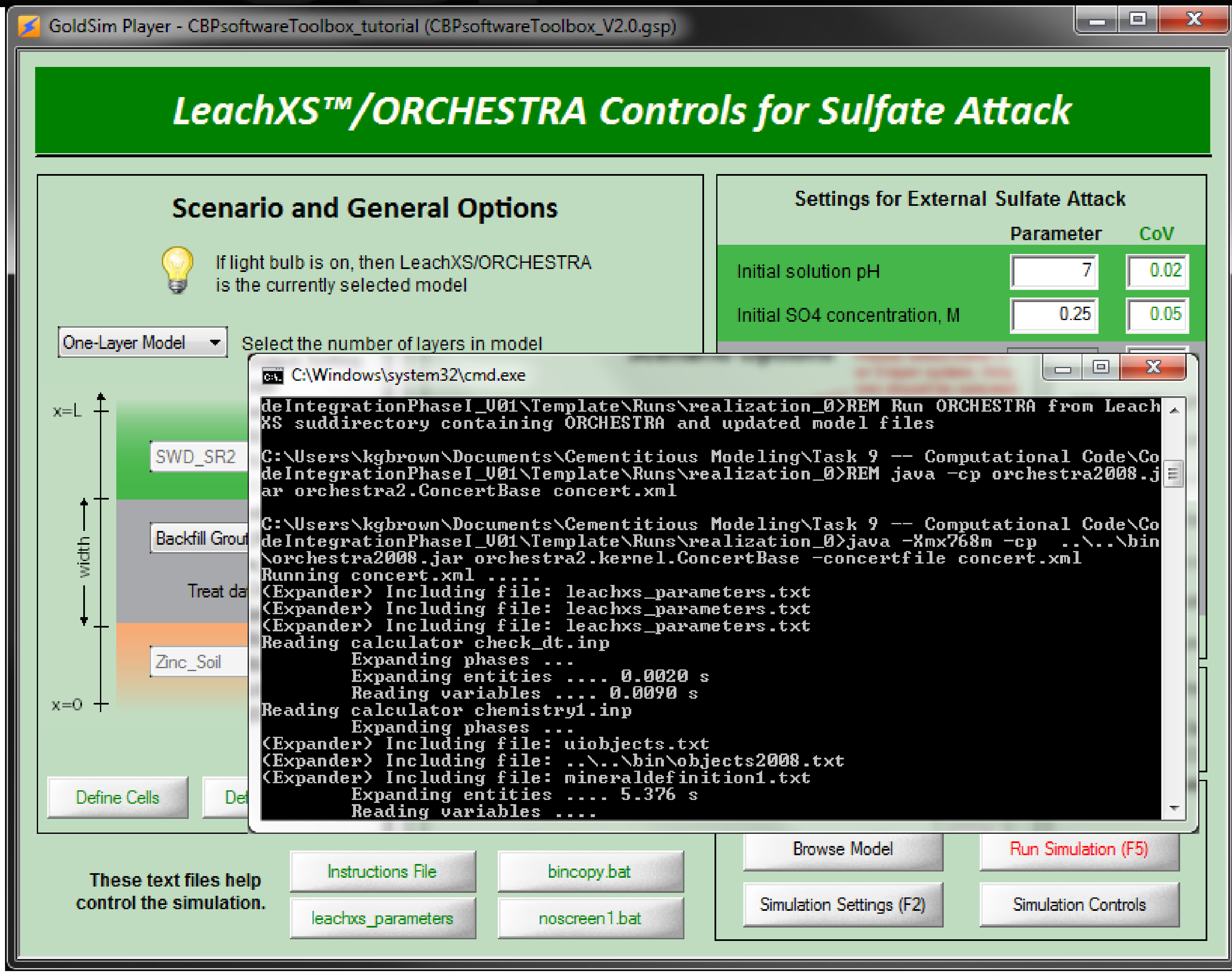
100 L External Contact Solution Volume



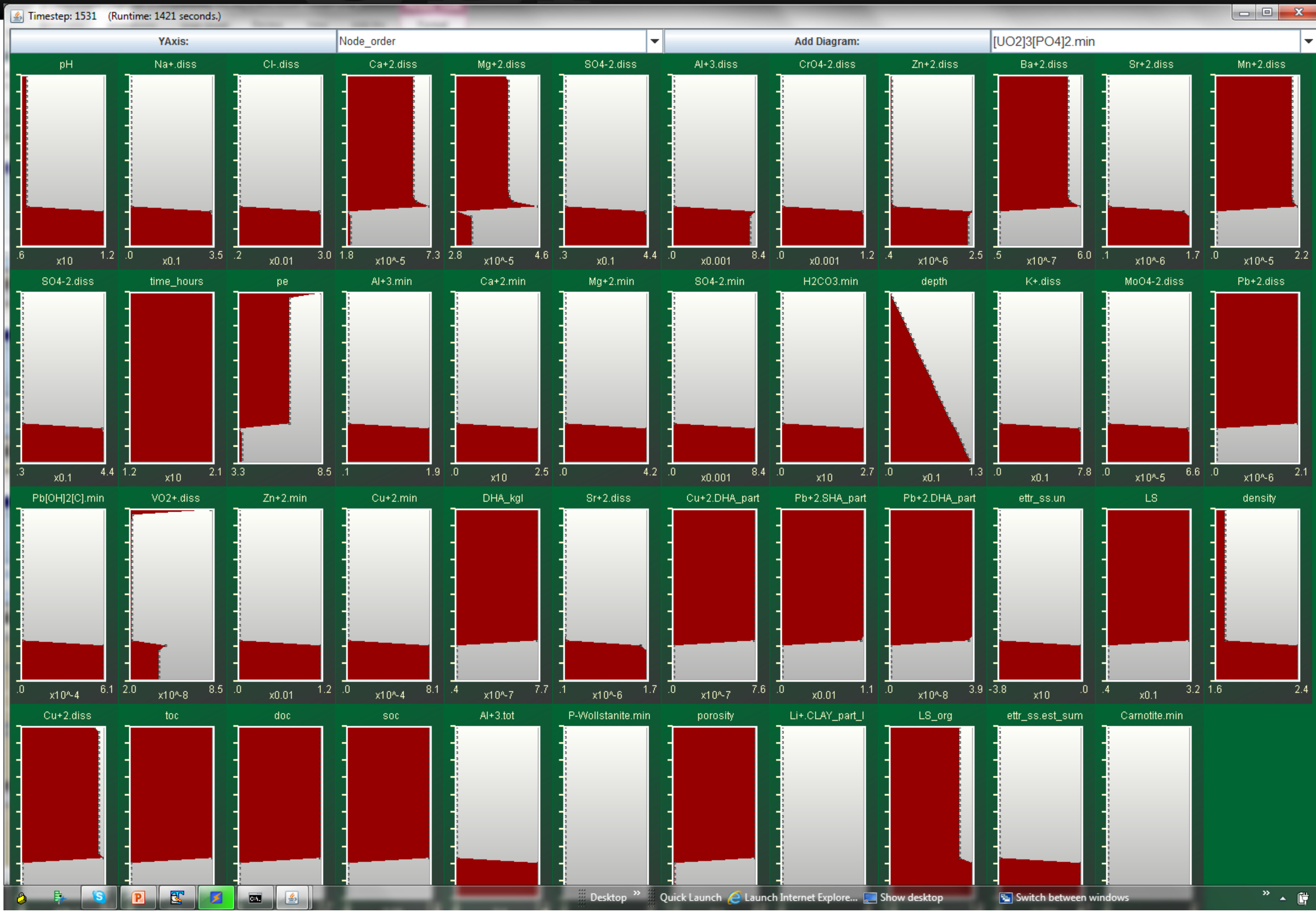
These text files help control the simulation.

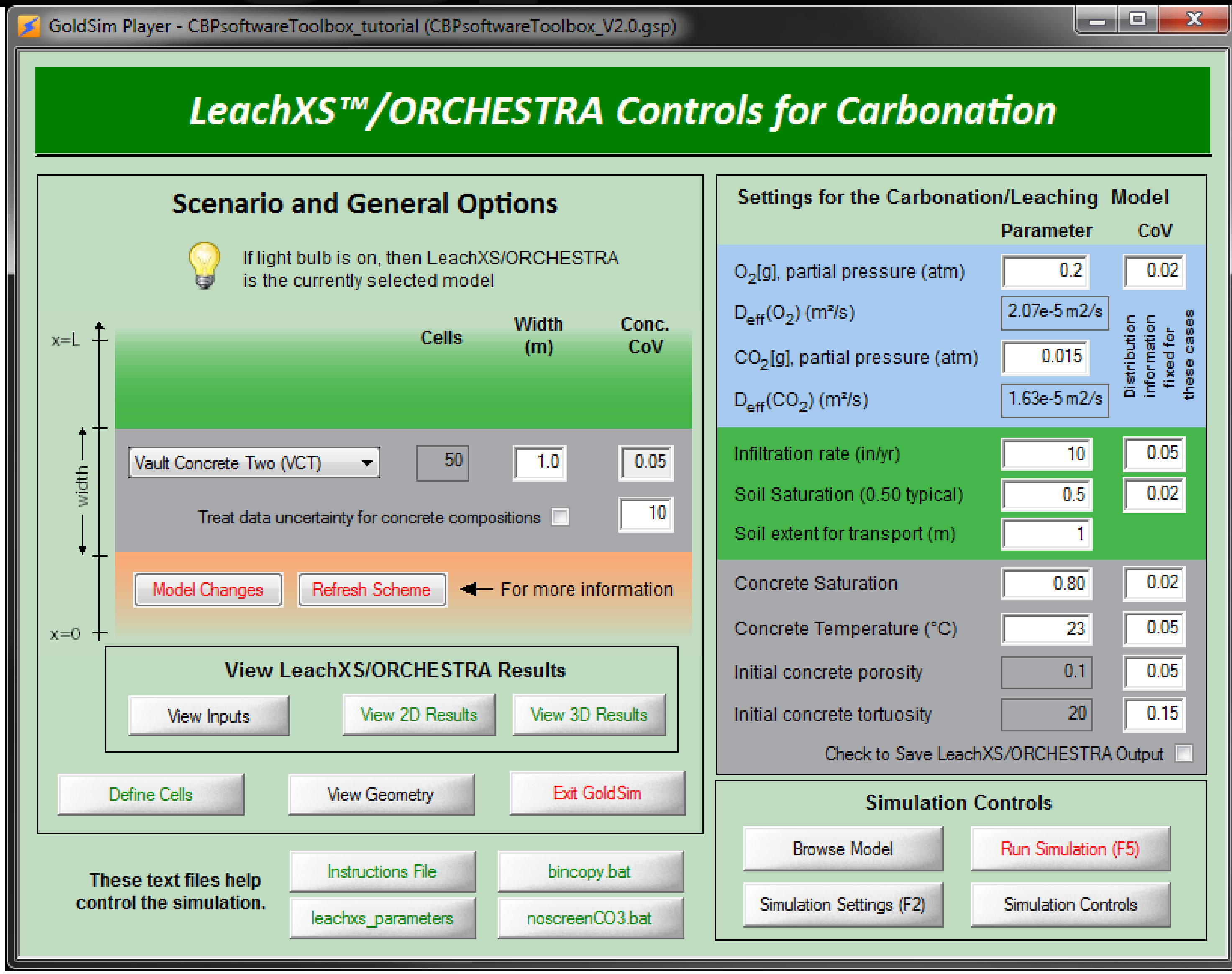
Instructions File | bincopy.bat | leachxs_parameters | noscreen1.bat

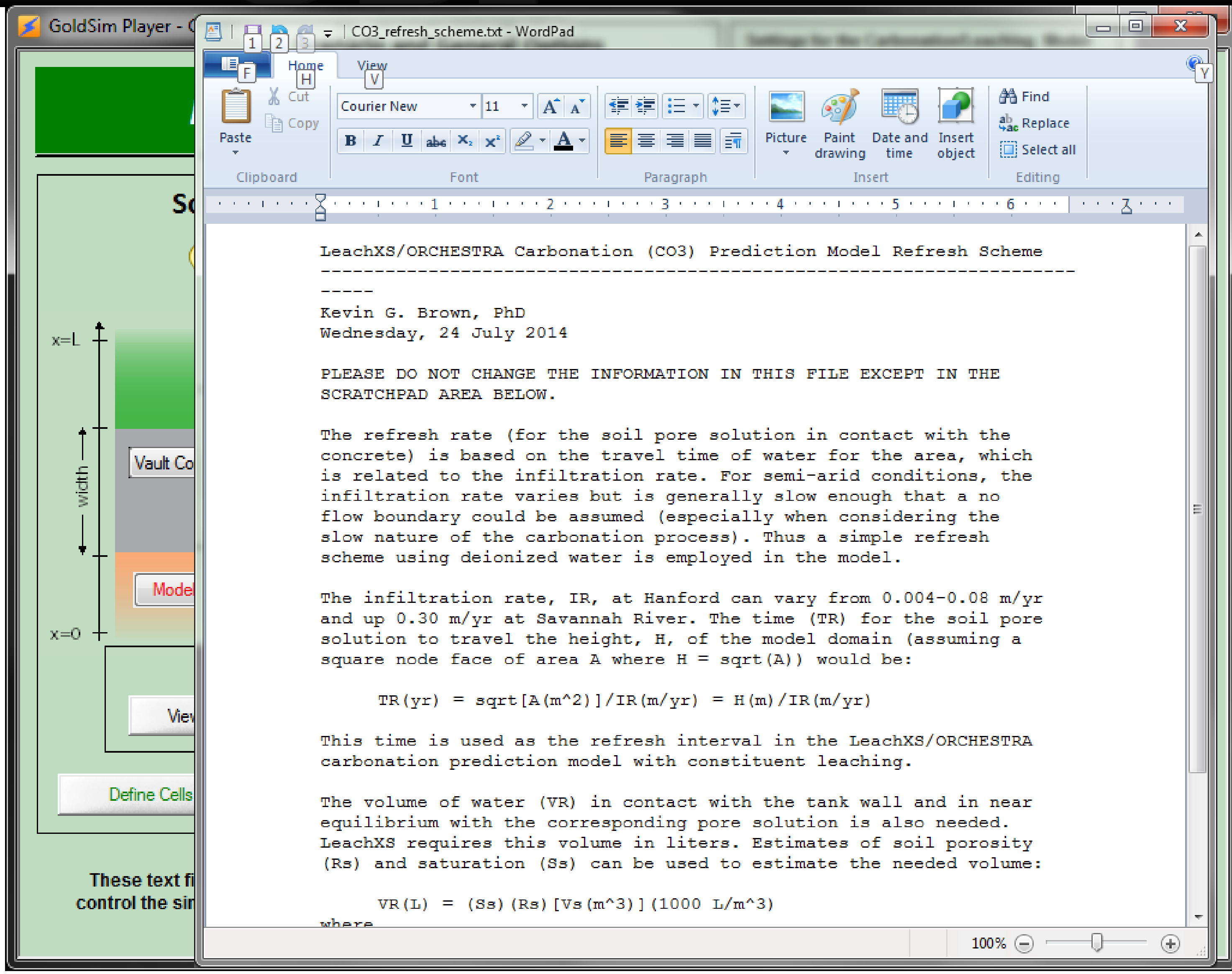
LXO Sulfate Attack Controls | Define Cells for Model | Simulation Controls


GoldSim Player - CBPsoftwareToolbox_tutorial (CBPsoftwareToolbox_V2.0.gsp)
LeachXS™/ORCHESTRA Controls for Sulfate Attack
Scenario and General Options
If light bulb is on, then LeachXS/ORCHESTRA is the currently selected model
One-Layer Model
Select the number of layers in model
x=L
SWD_SR2
Backfill Grout
width
Treat da
Zinc_Soil
x=0
Define Cells
Settings for External Sulfate Attack
Parameter
CoV
Initial solution pH
7
0.02
Initial SO4 concentration, M
0.25
0.05
C:\Windows\system32\cmd.exe
deIntegrationPhaseI_V01\Template\Runs\realization_0>REM Run ORCHESTRA from LeachXS suddirectory containing ORCHESTRA and updated model files
C:\Users\kgbrown\Documents\Cementitious Modeling\Task 9 -- Computational Code\CodeIntegrationPhaseI_V01\Template\Runs\realization_0>REM java -cp orchestra2008.jar orchestra2.ConcertBase concert.xml
C:\Users\kgbrown\Documents\Cementitious Modeling\Task 9 -- Computational Code\CodeIntegrationPhaseI_V01\Template\Runs\realization_0>java -Xmx768m -cp ..\..\bin\orchestra2008.jar orchestra2.kernel.ConcertBase -concertfile concert.xml
Running concert.xml .....
<Expander> Including file: leachxs_parameters.txt
<Expander> Including file: leachxs_parameters.txt
<Expander> Including file: leachxs_parameters.txt
Reading calculator check_dt.inp
Expanding phases ...
Expanding entities .... 0.0020 s
Reading variables .... 0.0090 s
Reading calculator chemistry1.inp
Expanding phases ...
<Expander> Including file: uiobjects.txt
<Expander> Including file: ..\..\bin\objects2008.txt
<Expander> Including file: mineraldefinition1.txt
Expanding entities .... 5.376 s
Reading variables ....
These text files help control the simulation.
Instructions File
bincopy.bat
leachxs_parameters
noscreen1.bat
Browse Model
Run Simulation (F5)
Simulation Settings (F2)
Simulation Controls

CBP
Cementitious Barriers Partnership




GoldSim Player - CBPsoftwareToolbox_tutorial (CBPsoftwareToolbox_V2.0.gsp)
LeachXS™/ORCHESTRA Controls for Carbonation
Scenario and General Options
If light bulb is on, then LeachXS/ORCHESTRA is the currently selected model
x=L
Cells
Width (m)
Conc. CoV
width
Vault Concrete Two (VCT)
50
1.0
0.05
Treat data uncertainty for concrete compositions
10
Model Changes
Refresh Scheme
For more information
x=0
View LeachXS/ORCHESTRA Results
View Inputs
View 2D Results
View 3D Results
Define Cells
View Geometry
Exit GoldSim
These text files help control the simulation.
Instructions File
bincopy.bat
leachxs_parameters
noscreenCO3.bat
Settings for the Carbonation/Leaching Model
Parameter
CoV
O_2[g], partial pressure (atm)
0.2
0.02
$D_{eff}(O_2)$ (m²/s)
2.07e-5 m2/s
CO_2[g], partial pressure (atm)
0.015
$D_{eff}(CO_2)$ (m²/s)
1.63e-5 m2/s
Distribution information fixed for these cases
Infiltration rate (in/yr)
10
0.05
Soil Saturation (0.50 typical)
0.5
0.02
Soil extent for transport (m)
1
Concrete Saturation
0.80
0.02
Concrete Temperature (°C)
23
0.05
Initial concrete porosity
0.1
0.05
Initial concrete tortuosity
20
0.15
Check to Save LeachXS/ORCHESTRA Output
Simulation Controls
Browse Model
Run Simulation (F5)
Simulation Settings (F2)
Simulation Controls



LeachXS/ORCHESTRA Carbonation (CO3) Prediction Model Refresh Scheme
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Kevin G. Brown, PhD
Wednesday, 24 July 2014

PLEASE DO NOT CHANGE THE INFORMATION IN THIS FILE EXCEPT IN THE SCRATCHPAD AREA BELOW.

The refresh rate (for the soil pore solution in contact with the concrete) is based on the travel time of water for the area, which is related to the infiltration rate. For semi-arid conditions, the infiltration rate varies but is generally slow enough that a no flow boundary could be assumed (especially when considering the slow nature of the carbonation process). Thus a simple refresh scheme using deionized water is employed in the model.

The infiltration rate, IR, at Hanford can vary from 0.004-0.08 m/yr and up 0.30 m/yr at Savannah River. The time (TR) for the soil pore solution to travel the height, H, of the model domain (assuming a square node face of area A where H = sqrt(A)) would be:

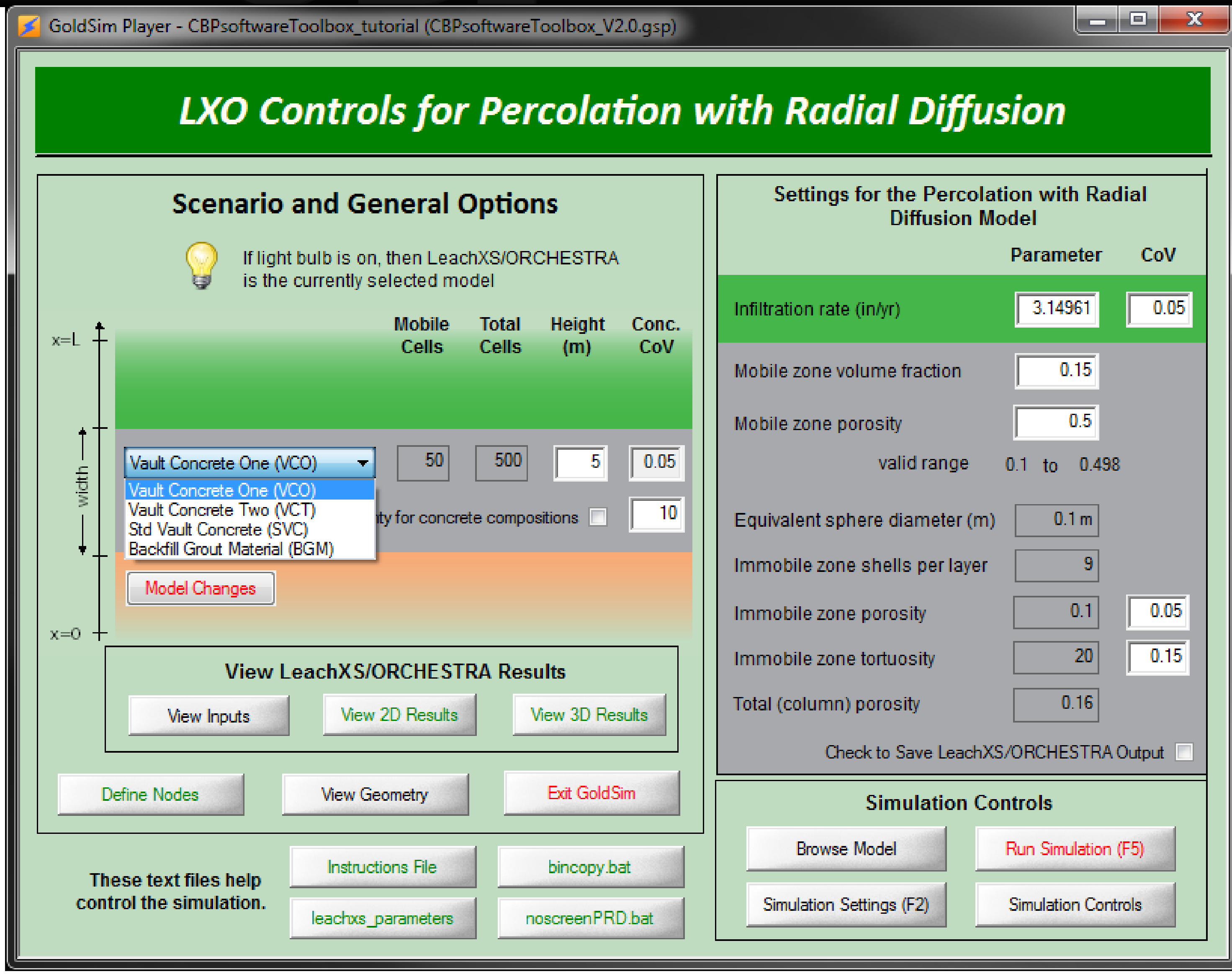
TR(yr) = sqrt[A(m^2)]/IR(m/yr) = H(m)/IR(m/yr)

This time is used as the refresh interval in the LeachXS/ORCHESTRA carbonation prediction model with constituent leaching.

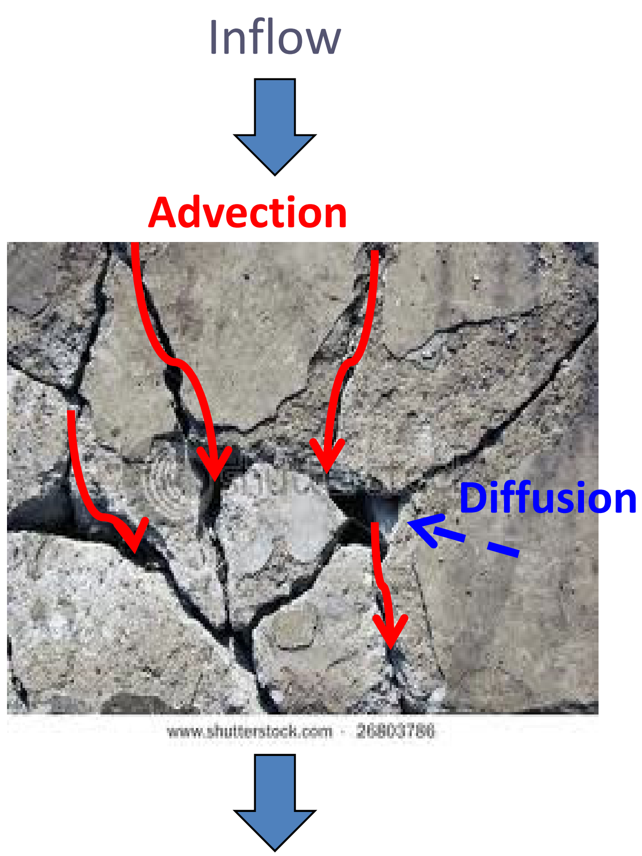
The volume of water (VR) in contact with the tank wall and in near equilibrium with the corresponding pore solution is also needed. LeachXS requires this volume in liters. Estimates of soil porosity (Rs) and saturation (Ss) can be used to estimate the needed volume:

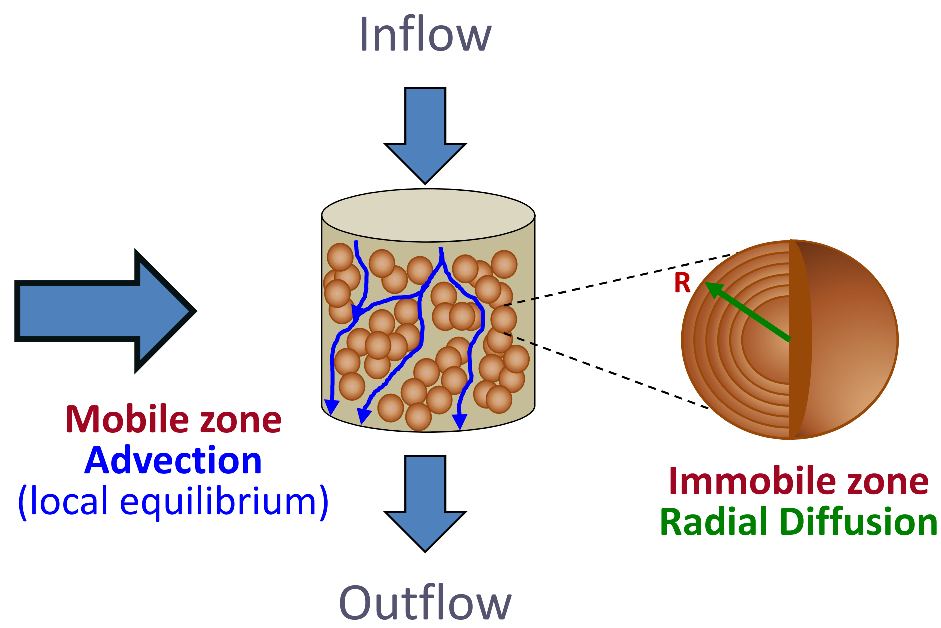
VR(L) = (Ss)(Rs)[Vs(m^3)](1000 L/m^3)

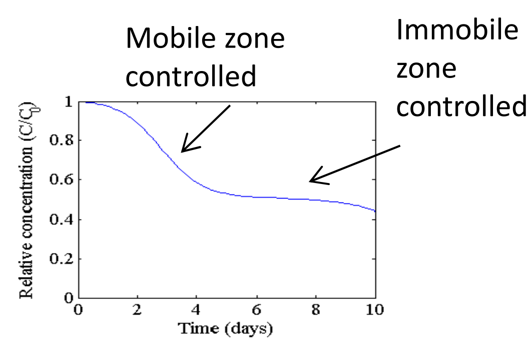
where


GoldSim Player - CBPsoftwareToolbox_tutorial (CBPsoftwareToolbox_V2.0.gsp)
LXO Controls for Percolation with Radial Diffusion
Scenario and General Options
If light bulb is on, then LeachXS/ORCHESTRA is the currently selected model
x=L
x=0
width
Mobile Cells
Total Cells
Height (m)
Conc. CoV
Vault Concrete One (VCO)
50
500
5
0.05
Vault Concrete One (VCO)
Vault Concrete Two (VCT)
Std Vault Concrete (SVC)
Backfill Grout Material (BGM)
ty for concrete compositions
10
Model Changes
View LeachXS/ORCHESTRA Results
View Inputs
View 2D Results
View 3D Results
Define Nodes
View Geometry
Exit GoldSim
These text files help control the simulation.
Instructions File
bincopy.bat
leachxs_parameters
noscreenPRD.bat
Settings for the Percolation with Radial Diffusion Model
Parameter
CoV
Infiltration rate (in/yr)
3.14961
0.05
Mobile zone volume fraction
0.15
Mobile zone porosity
0.5
valid range
0.1
to
0.498
Equivalent sphere diameter (m)
0.1 m
Immobile zone shells per layer
9
Immobile zone porosity
0.1
0.05
Immobile zone tortuosity
20
0.15
Total (column) porosity
0.16
Check to Save LeachXS/ORCHESTRA Output
Simulation Controls
Browse Model
Run Simulation (F5)
Simulation Settings (F2)
Simulation Controls

Advection – radial diffusion approach





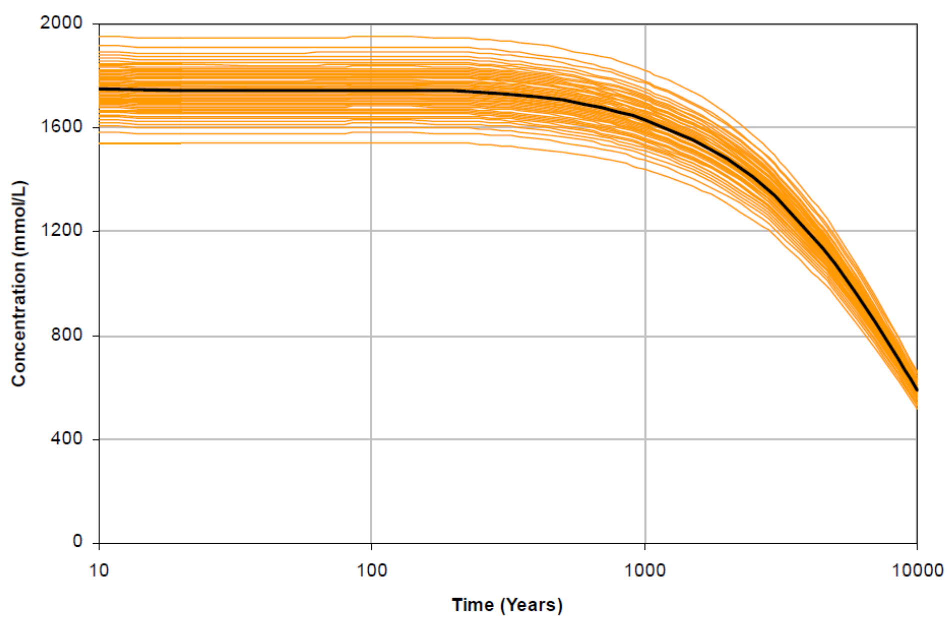


- Refined mobile-immobile approach
- Can capture micro-macro pore and particle size distributions

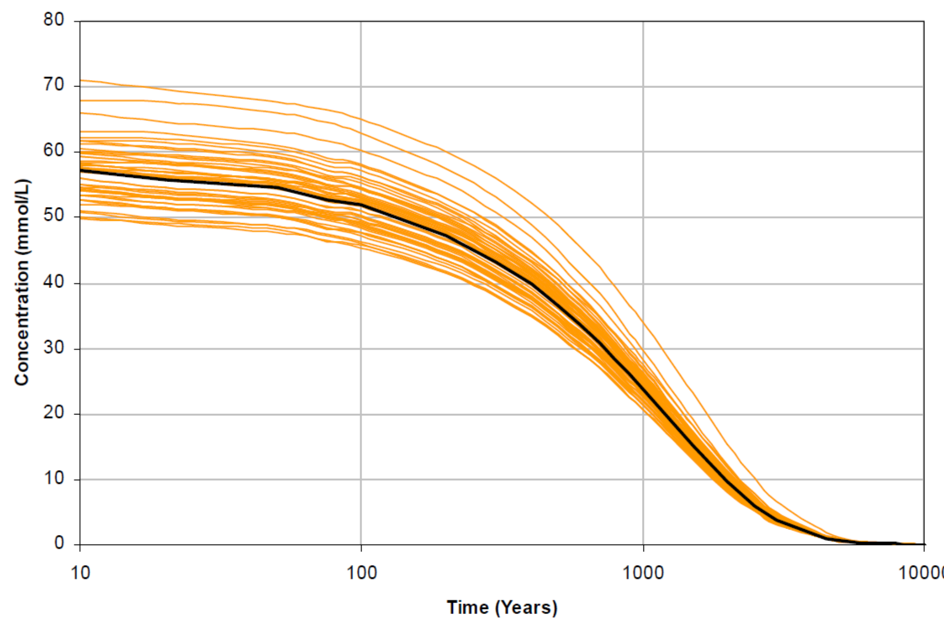
Uncertainty Analysis

- Sources of uncertainty
  - Inherent variability
  - Data uncertainty
  - Model uncertainty
- Approaches to uncertainty management
  - GoldSim has sensitivity and uncertainty analysis capabilities
  - GoldSim SubModel elements can be used to separate variability and uncertainty, if wanted
  - More advanced capabilities are being developed to evaluate model uncertainty impacts

Probabilistic STADIUM Results from GoldSim
Ion Concentrations at Saltstone-Concrete Interface



Nitrate



Sulfate

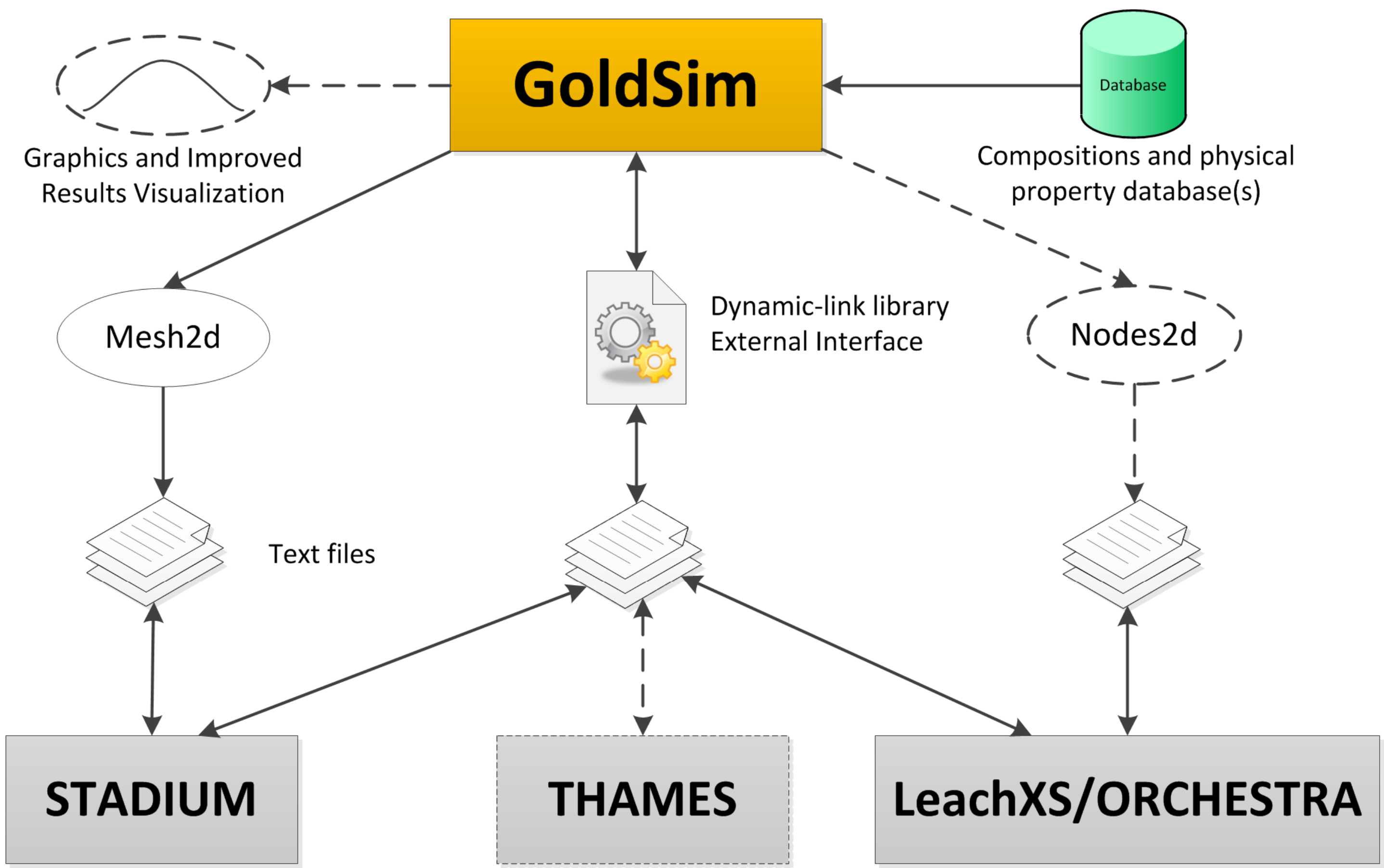
Summary of Uncertainty Analysis

- Uncertainties due to physical variability, data uncertainty, and model uncertainty considered
- Several methods available for uncertainty propagation through computational models
- Methods for model uncertainty and error quantification currently under study
- Bayesian framework appears attractive for managing various uncertainties
- Methods for epistemic uncertainty under investigation
- Application to large problems (time-dependent, complicated multi-physics) needs investigation (accuracy, computational effort, uncertainty quantification, confidence assessment)

CBP Software ToolBox – Phase II

- Items to be addressed in Phase II include:
  - *Improve DLL interface to include additional text handling capabilities and enhanced error trapping*
  - *Add improved data visualization capabilities to the CBP ToolBox using a direct interface*
  - Develop and link a "common" composition / material property database to GoldSim
  - Couple the NIST THAMES code to GoldSim using the DLL interface
  - Couple CBP partner codes for important phenomena (e.g., cracking) to reduce prediction uncertainty

CBP Software ToolBox – Phase II



Additional Overheads

CBP Goal

Develop a reasonable and credible set of tools to predict the structural, hydraulic and chemical performance of cement barriers used in nuclear applications over extended time frames (e.g., up to or >100 years for operating facilities and > 1000 years for waste management).

- Cementitious waste form in concrete disposal vault with cap (↔ Landfills Partnership)
- Grouted high-level waste (HLW) tank closure
- Spent nuclear fuel pool integrity
- Nuclear processing facilities closure / D&D
- Grouted vadose zone to immobilize contamination
- **Materials** – surrogate low-activity waste (LAW) cementitious waste form, reducing grout, reinforced concrete (historical) and reinforced concrete (future)

Example Uses and Reference Cases

Long-term Structural, Hydraulic & Chemical **Performance** of Cementitious Materials & Barriers

Mechanistic / Phenomenological Basis

Parameter Estimation and Measurement

Boundary Conditions (physical, chemical interfaces)

Uncertainty Characterization

Basic Elements of the Performance Evaluation

Being Completed

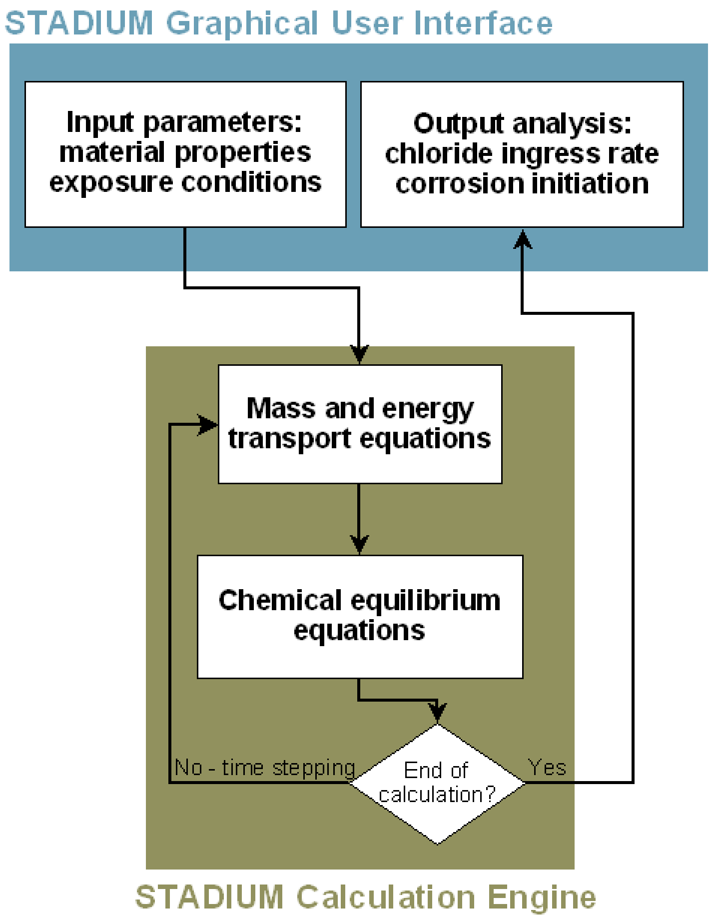
CBP Coordinated Experimental and Computational Program

- Develop and improve conceptual models
- Define test methods and estimate important parameters
- Calibrate and validate models and perform probabilistic analyses

STADIUM® (SIMCO Technologies)

- Simulates ionic transport in saturated/unsaturated, isothermal/non-isothermal cementitious materials
  - Simulates contaminant ingress, ionic leaching in pore solution, and modifications to microstructure of cementitious material
  - Accounts for electrical coupling between ions and activity gradients and dissolution/precipitation due to the high paste reactivity
  - Main components: ionic transport, electrodiffusion potential conservation, moisture transport, and energy conservation
  - Test results and methods available that relate directly to model predictions and validation
- Planned model improvements
  - Model damage due to sulfate exposure
  - Model effect of pore solution viscosity
  - Model effect of pore solution density of highly concentrated solutions
  - Model carbonation and acid exposure and resulting secondary species

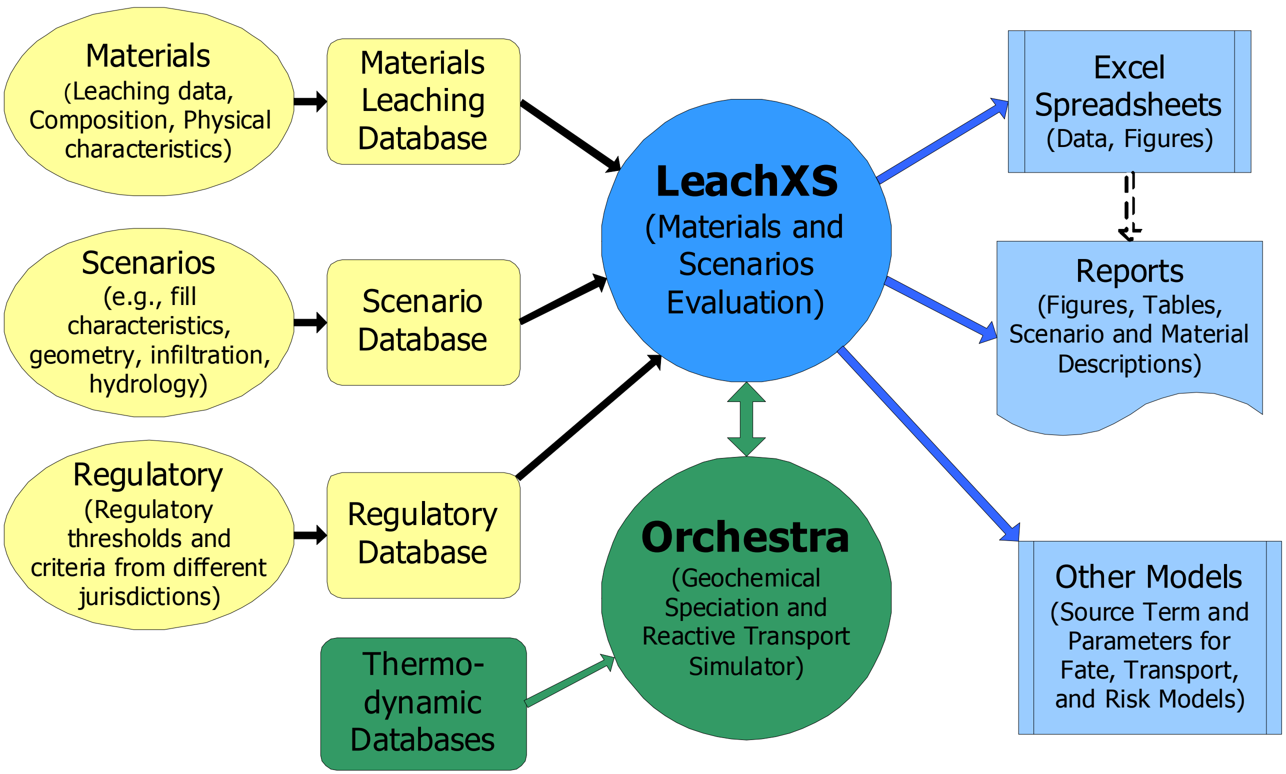
STADIUM® Overview



LeachXS™/ORCHESTRA (ECN)

- LeachXS is a database/expert decision support system for characterization and environmental impact assessment
  - Includes leaching results for 600+ materials (cements, concretes, stabilized wastes, soils), scenarios, and regulations
  - Assists evaluation and lab guidance, data management/evaluation, source term description, impact evaluation, and decision analysis
  - Geochemical speciation and chemical reaction/transport modeling integrated into LeachXS using the ORCHESTRA model
- Planned model improvements
  - Parallelize LeachXS/ORCHESTRA equilibrium module calculations
  - Incorporate radionuclides and decay in LeachXS/ORCHESTRA
  - Evaluate chemical model performance by comparing with pH dependent solubility and diffusion data
  - Account for chemical model uncertainty on transport predictions
  - Account for impact of variable saturation and intermittent wetting
  - Account for effects of physical and chemical heterogeneity

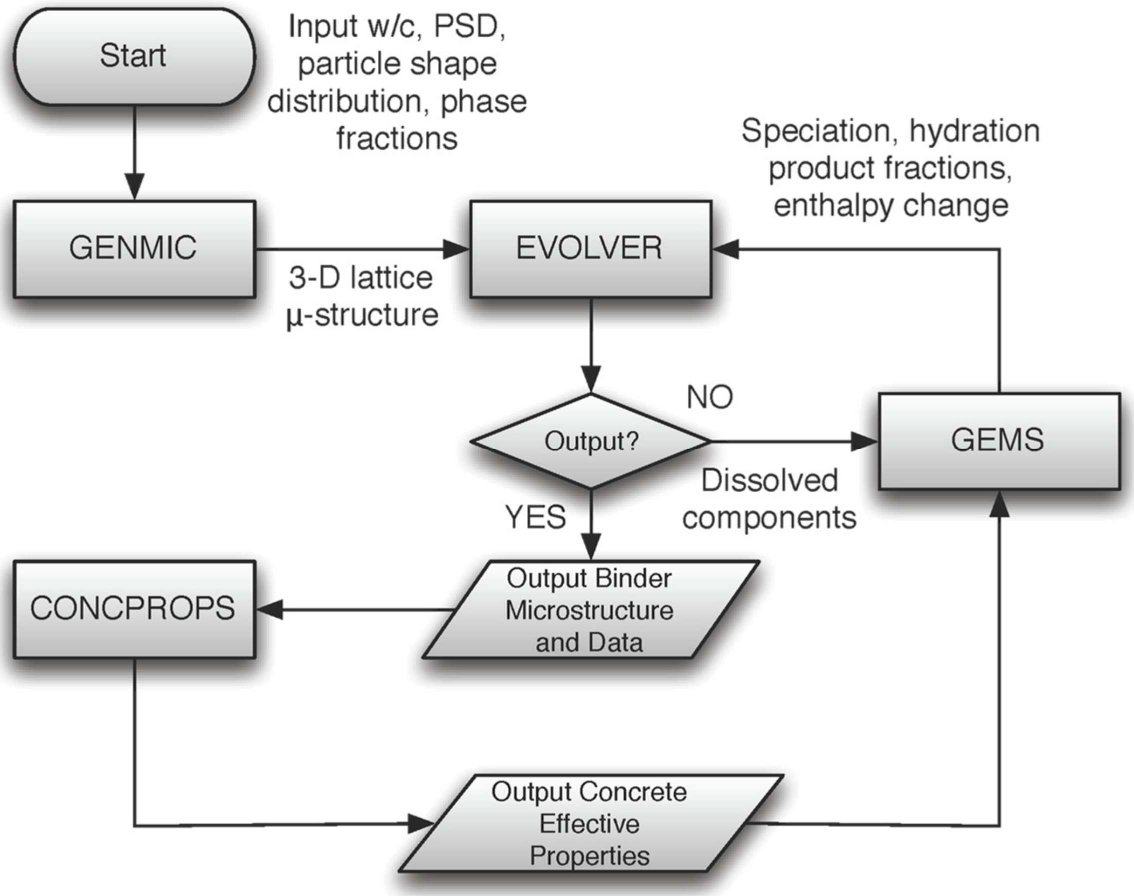
LeachXS™/ORCHESTRA Overview



THAMES (NIST)

- Virtual “micro-probe” of microstructure
  - Constructs time-dependent 3-D virtual microstructures of a cementitious binder during hydration or degradation
  - Computes important engineering properties of a concrete made from a binder at prescribed times
- Planned model improvements
  - Embed geochemical modeling code (GEMS) into microstructure module
  - Improve hydration microstructure growth rules
  - Parallelize THAMES code
  - Incorporate microstructure impact on GEMS boundary conditions
  - Incorporate degradation reactions and effects on microstructure
  - Improve predictions for more complex systems

THAMES Overview



Coupling Decisions and Software Integration