Cementitious Barriers Partnership: Release of CBP Software ToolBox Phase I

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Richland, Washington
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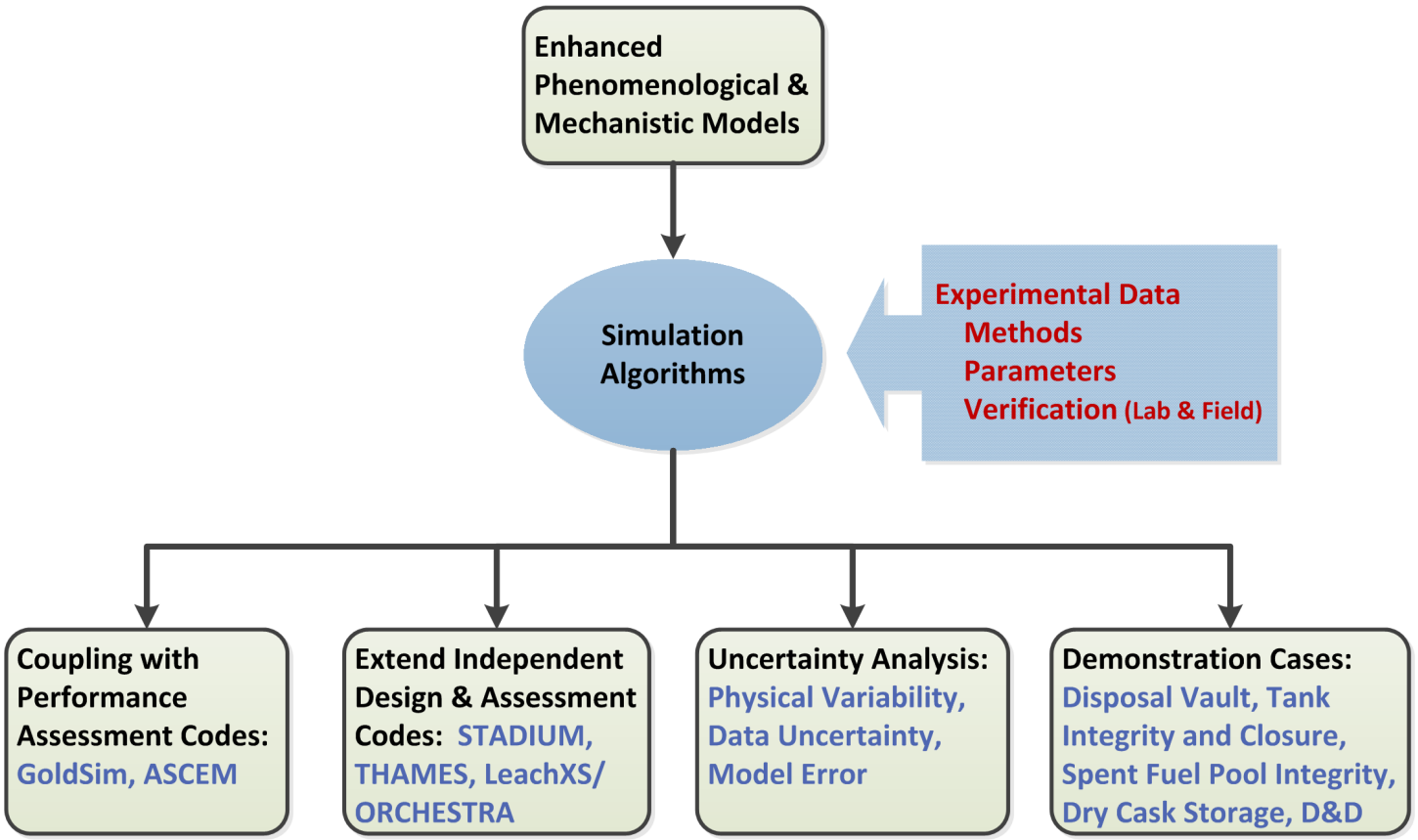
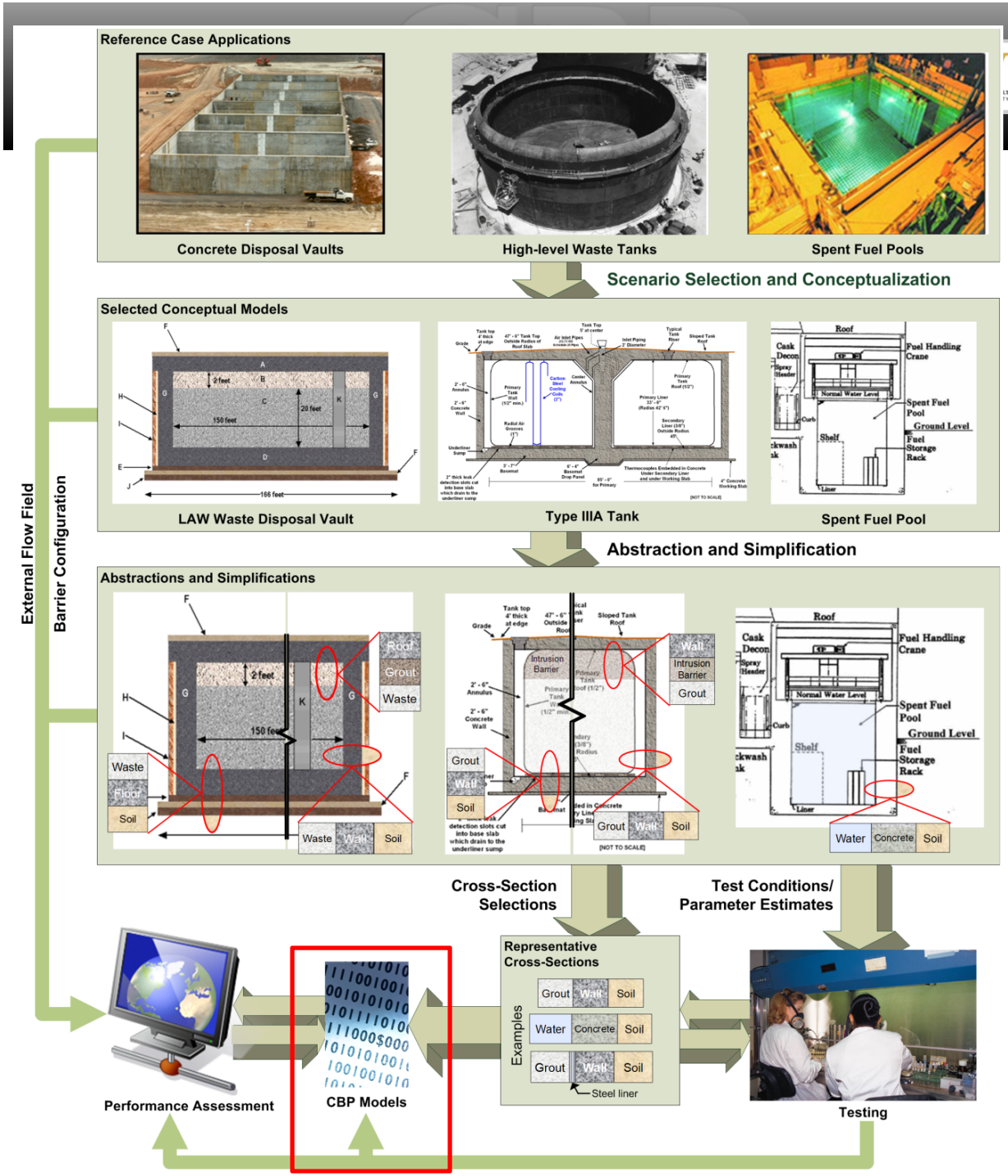
CBP
Cementitious Barriers Partnership

Workshop Summary

- CBP Software ToolBox Release (Phase 1)
  - Focus on sulfate ingress and attack / damage
  - Custom Dynamic-link library (DLL) developed (SRNL/VU)
  - GoldSim model → Probabilistic wrapper for partner codes
  - Custom DLL used to link to current partner codes
- Current Partner Codes
  - STADIUM® by SIMCO Technologies, Inc.
  - LeachXS™/ORCHESTRA by ECN/VU/DHI/NRG
  - THAMES (NIST) is pending
- Uncertainty Analyses using GoldSim functionality
- Future Plans for Software ToolBox (Phase II)

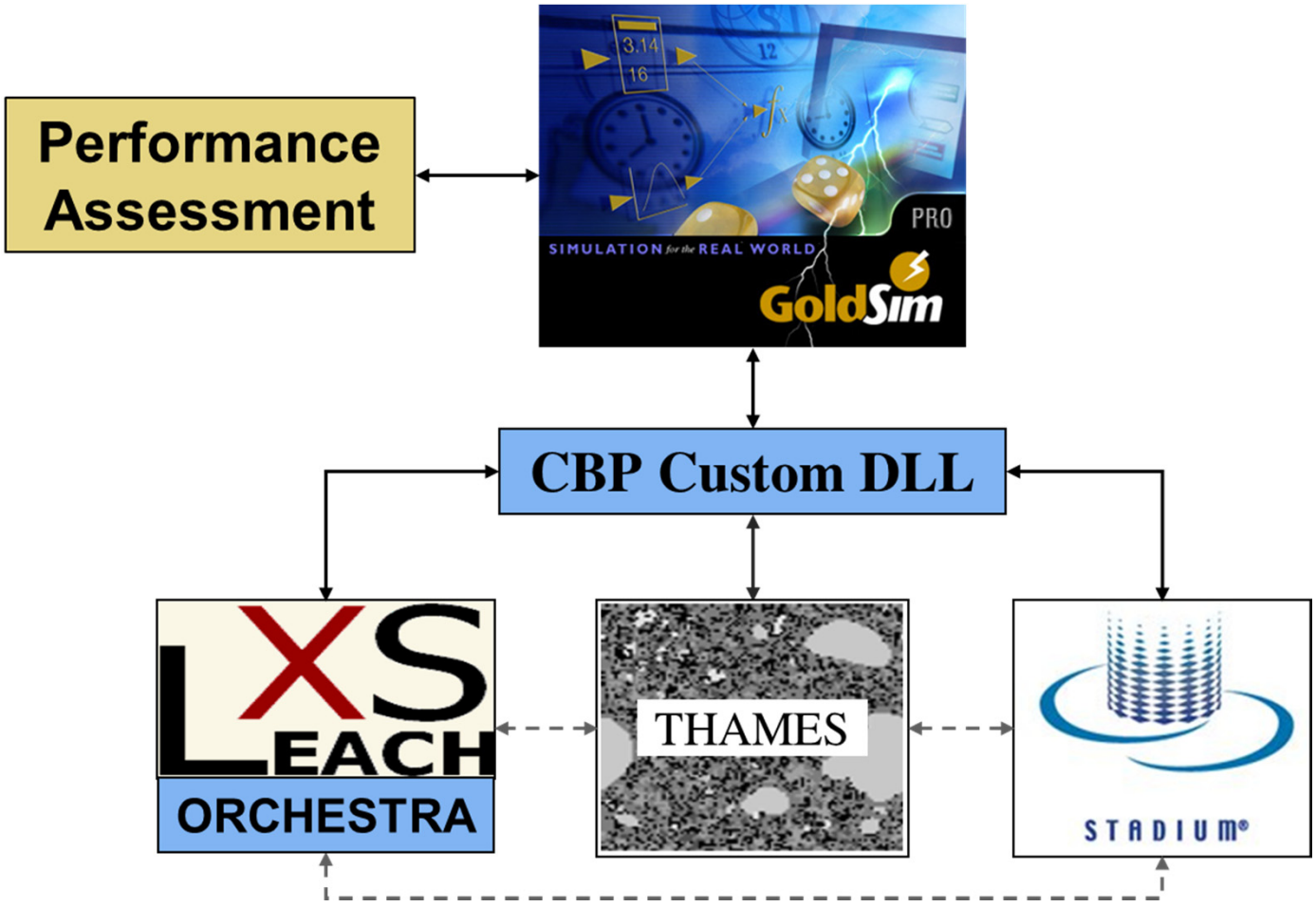
CBP Toolbox Development





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

General Integrated Model Concept



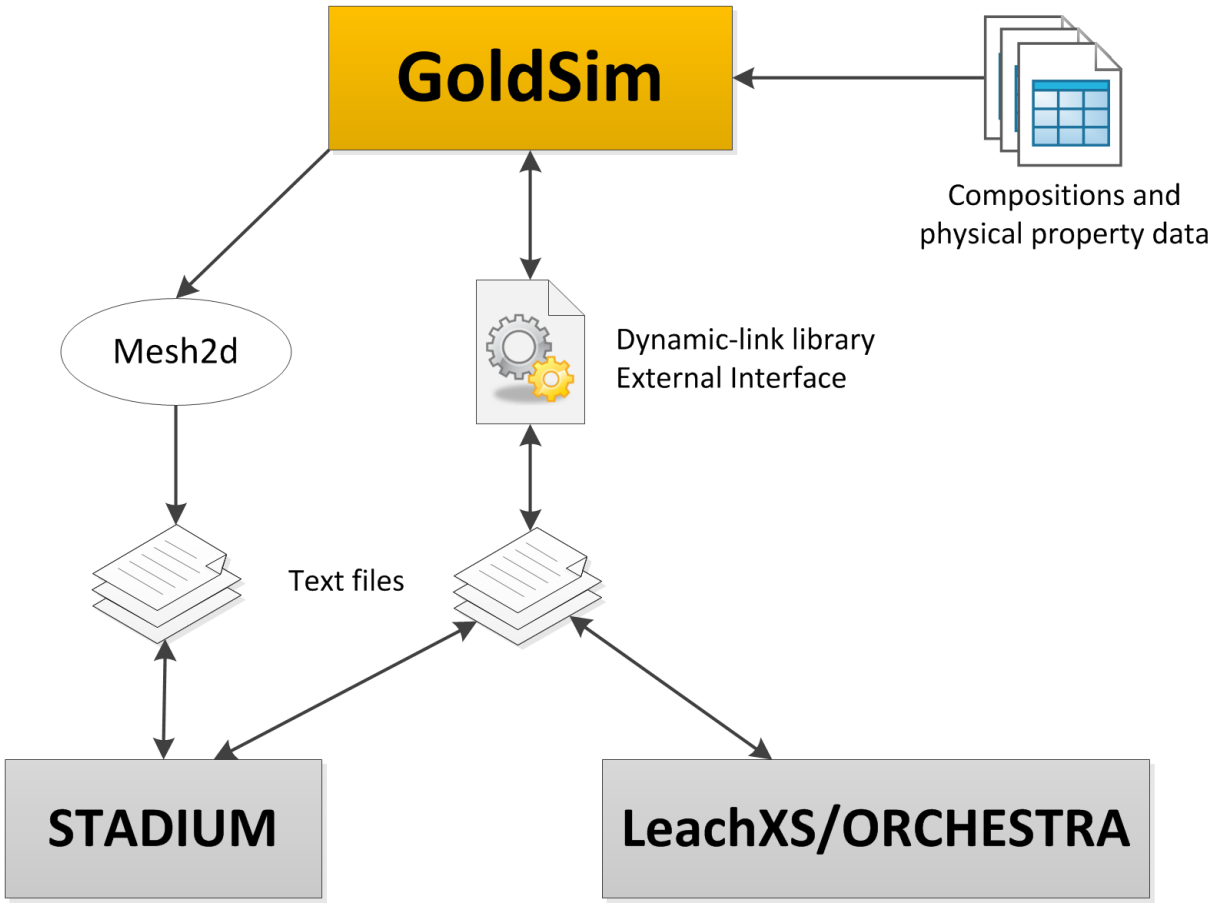
Software ToolBox General Design Principles

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

Phased CBP ToolBox Development

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

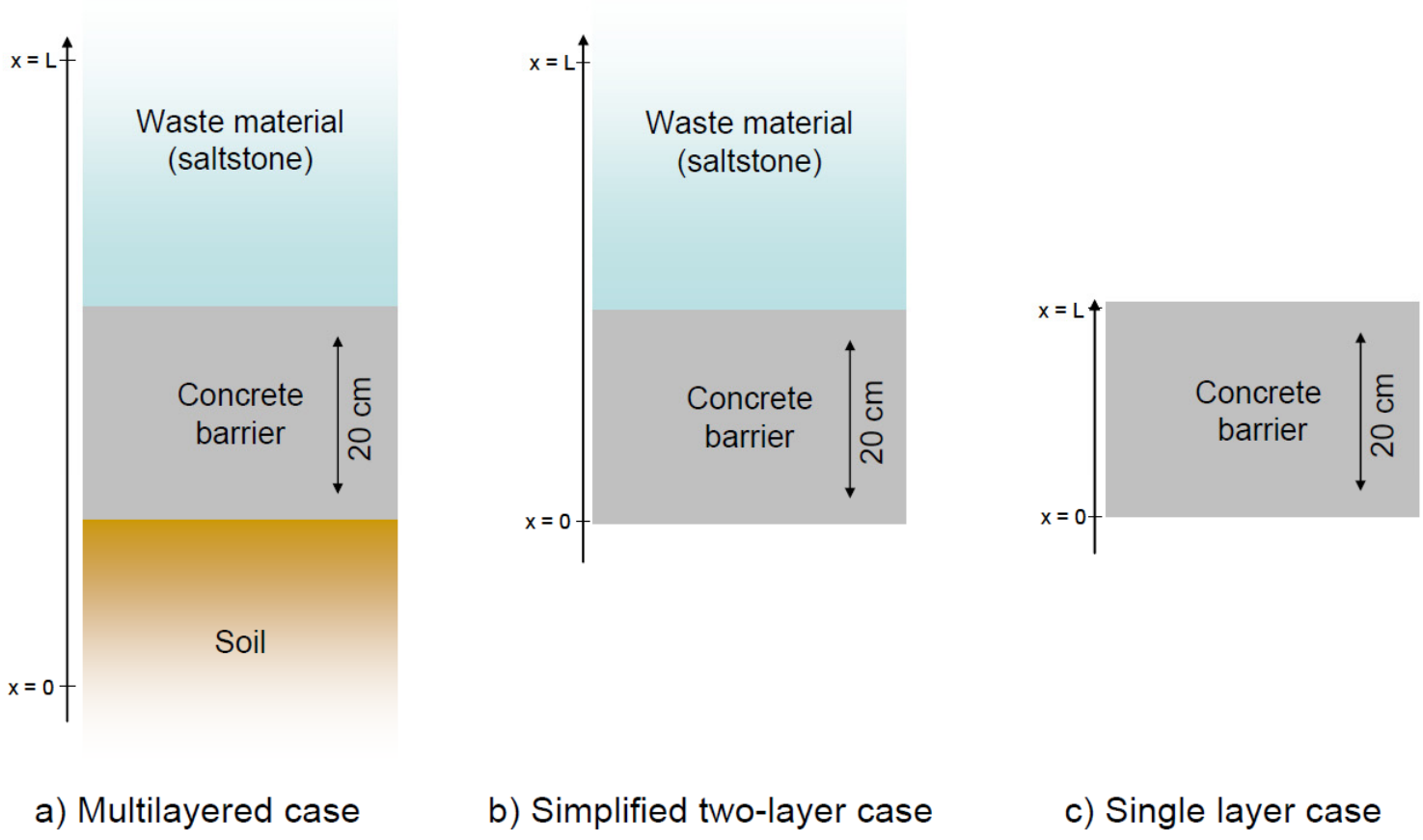
CBP Software ToolBox—Phase I



CBP ToolBox Development—Process

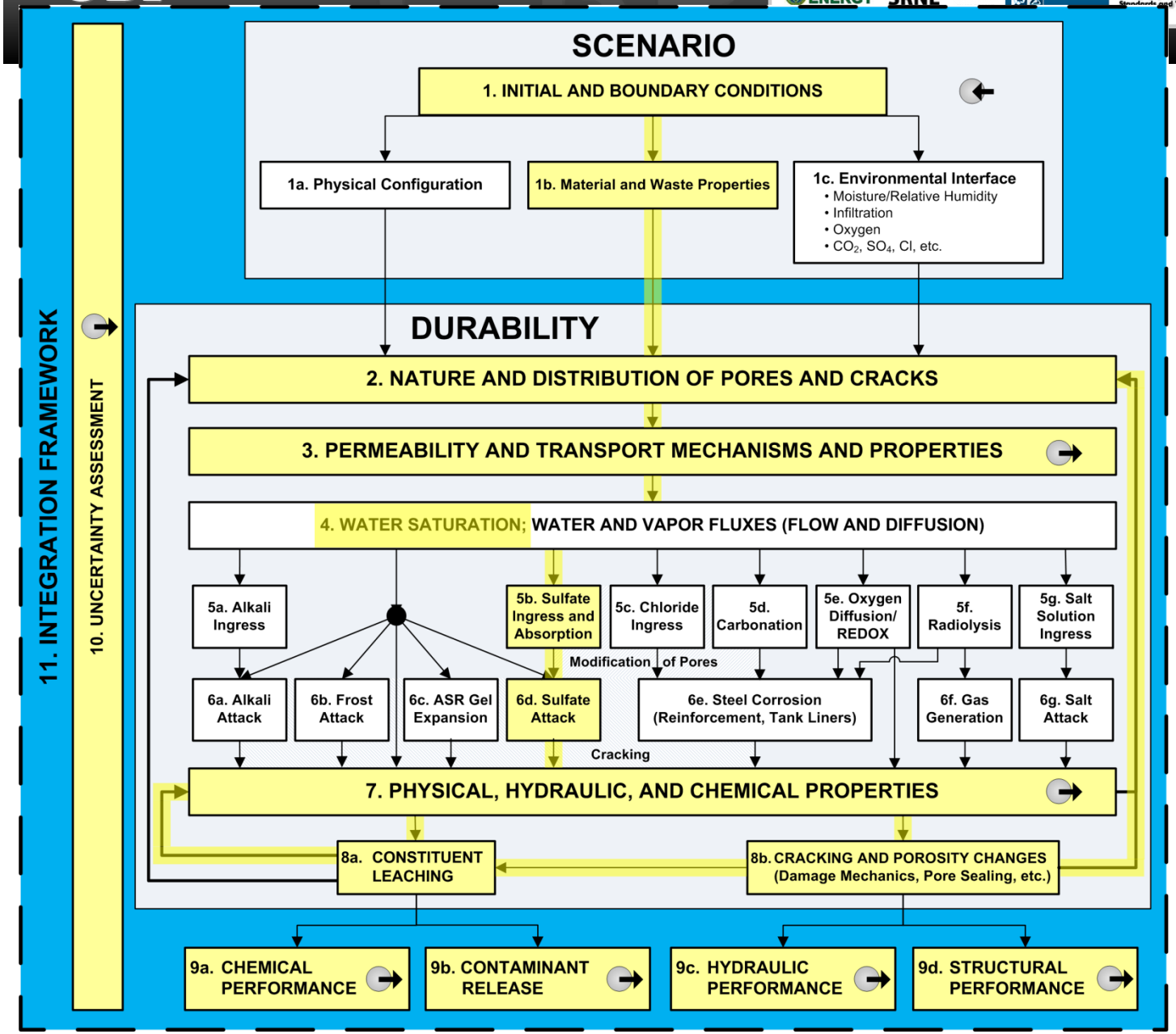
1. Conceptualize problem scenario and determine appropriate model and coupling, if needed
   - Need to consider availability of needed data
2. Develop scenario in appropriate partner code(s)
   - No coupling between LXO and STADIUM in Phase I
   - STADIUM → SIMCO Technologies, Inc.
   - LeachXS/ORCHESTRA (LXO) → LeachXS Lite
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



a) Multilayered case b) Simplified two-layer case c) Single layer case

Figure 1 – Schematic representation of demonstration cases



Sulfate Attack as a "Proof of Principle" for Coupling of Phenomena and Uncertainty Analysis

FROM PA systems modeling

TO PA systems modeling

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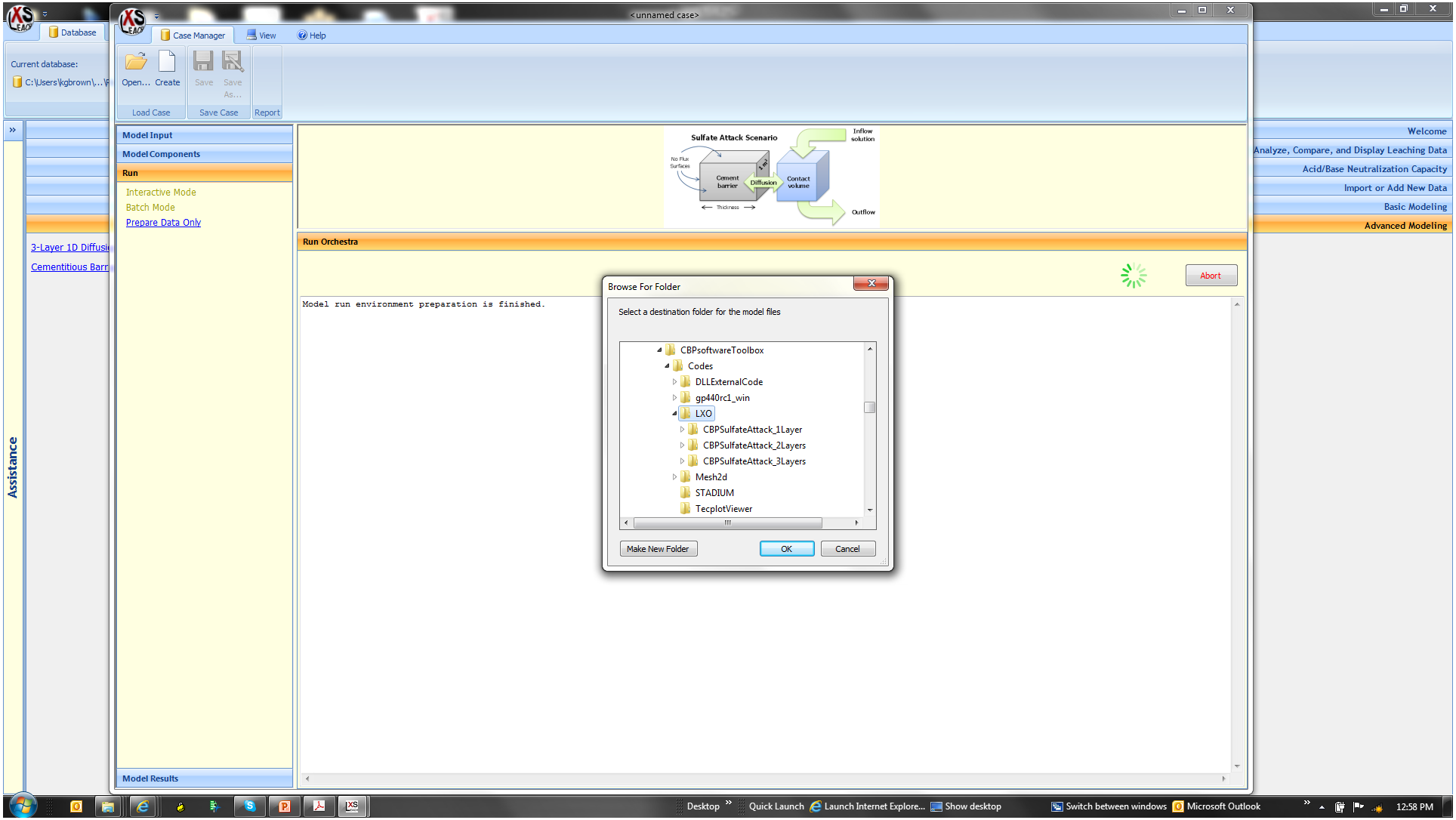
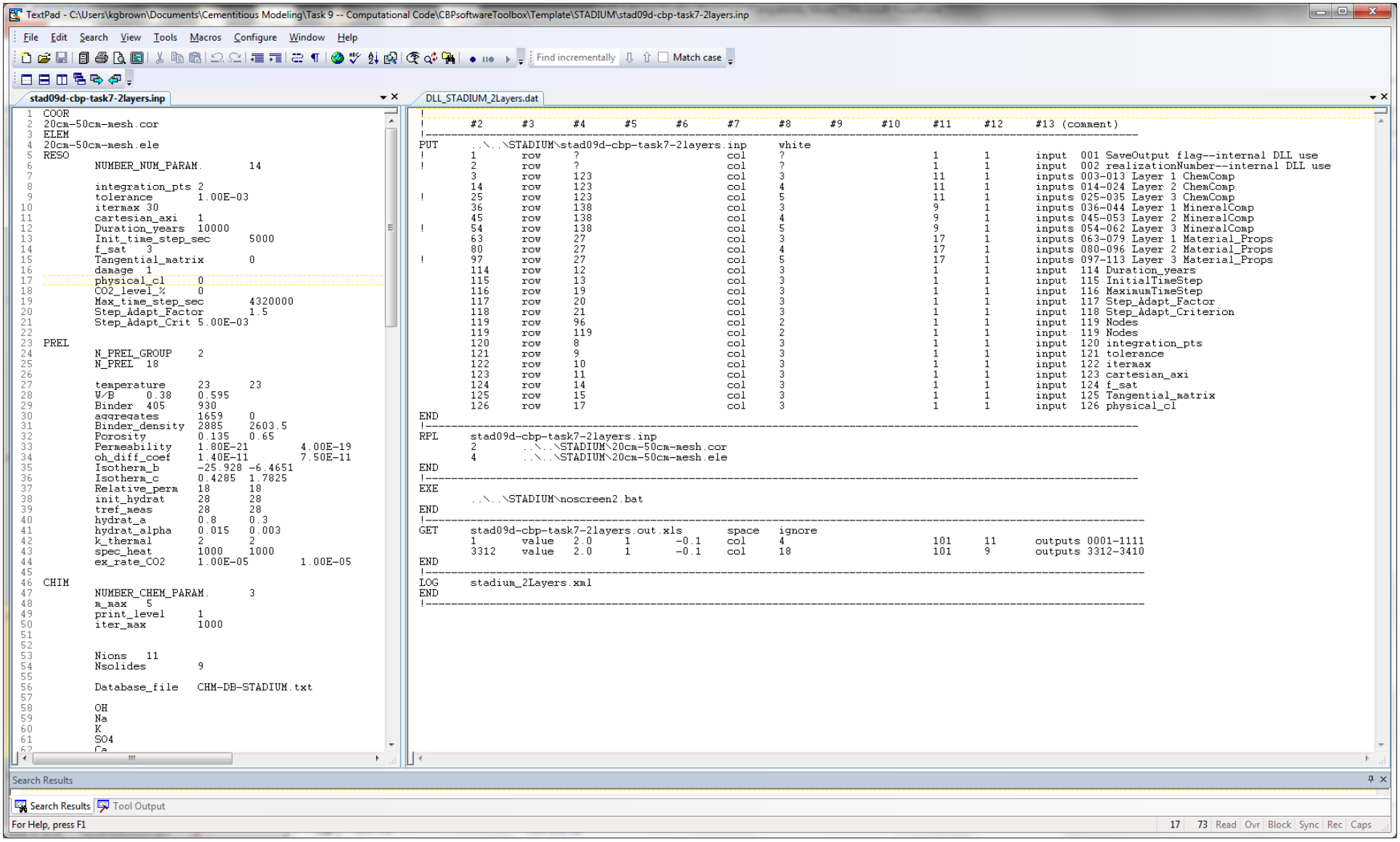
CBP ToolBox—Develop Scenario



ToolBox—Define Model & Instructions Files



ToolBox—STADIUM Model & Instructions Files

stad09d-cbp-task7-2layers.inp

```
118          Temperature      2        0        1        365      0        5        15
119          101      365     0        5        15
120  INIT
121          external_file    0
122
123          OH       400     670.08
124          Na       282.1   4420
125          K        138     120
126          SO4      8       130.7
127          Ca       0.5     0.41
128          Al(OH)4  0.1     0.14
129          Cl       5       9
130          H2SiO4   0       9.7
131          CO3      0       2.9
132          NO3      0       2000
133          NO2      0       1575
134          Rel_Humidity     1        1
135          Potential        0        0
136          Temperature      23       23
137
```

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
```

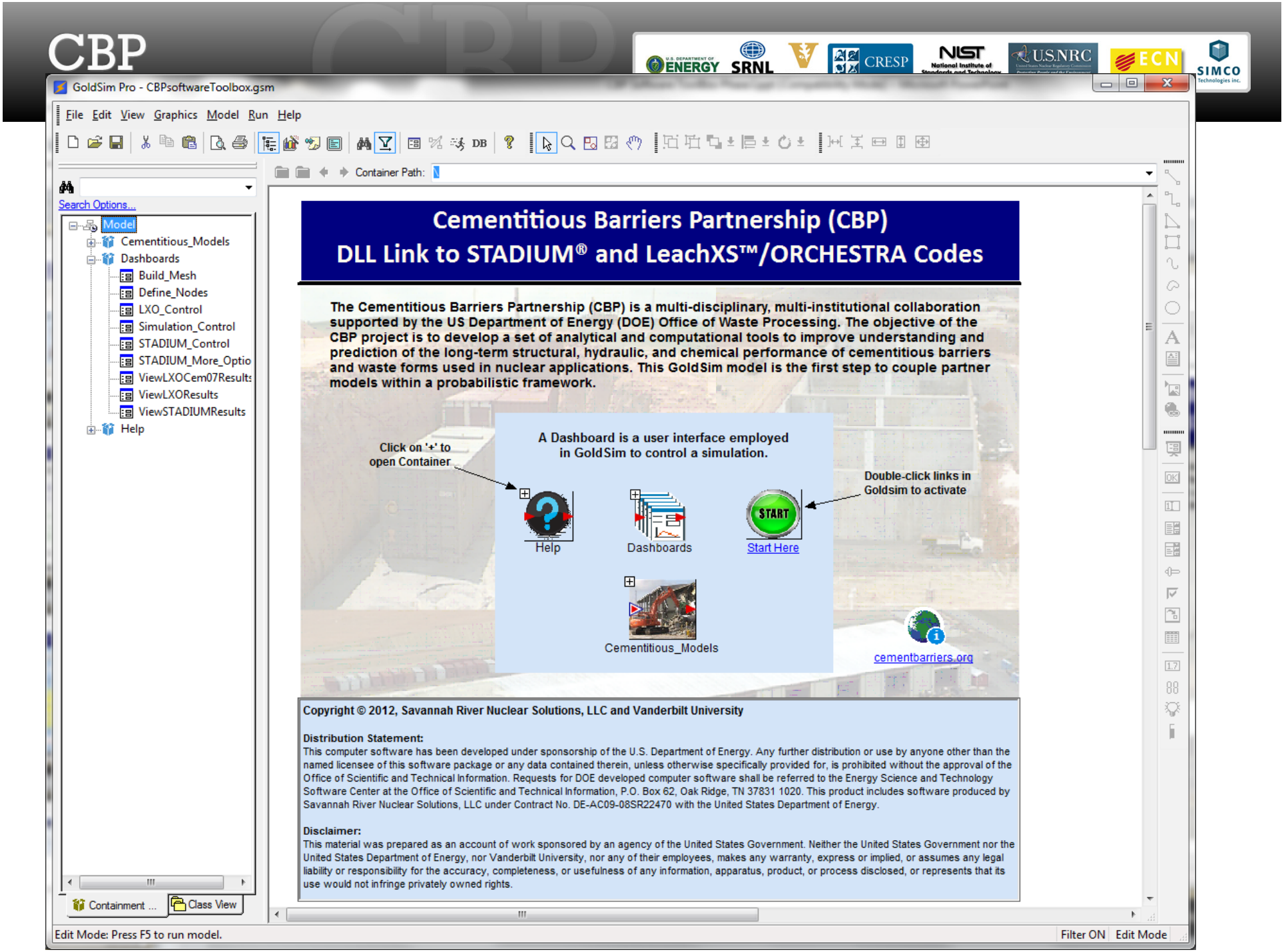
ToolBox—LXO Model & Instructions Files

leachxs_parameters.txt

```
256 @class: block_barrier_chemical()
257 The chemical parameters of the cement barrier.
258 {
259 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
260 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-
261 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-
262 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-
263 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-
264 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-
265 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-
266 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-
267 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-
268 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-
269 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-
270 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-
271 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-
272 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-
273 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-
274 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-
275 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-
276 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-
277 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
!
```


CBP
GoldSim Pro - CBPsoftwareToolbox.gsm
File Edit View Graphics Model Run Help
Container Path:
Search Options...
Model
Cementitious_Models
Dashboards
Build_Mesh
Define_Nodes
LXO_Control
Simulation_Control
STADIUM_Control
STADIUM_More_Optio
ViewLXOCem07Results
ViewLXOResults
ViewSTADIUMResults
Help
Containment ...
Class View
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.
A Dashboard is a user interface employed in GoldSim to control a simulation.
Click on '+' to open Container
Double-click links in Goldsim to activate
Help
Dashboards
START
Start Here
Cementitious_Models
cementbarriers.org
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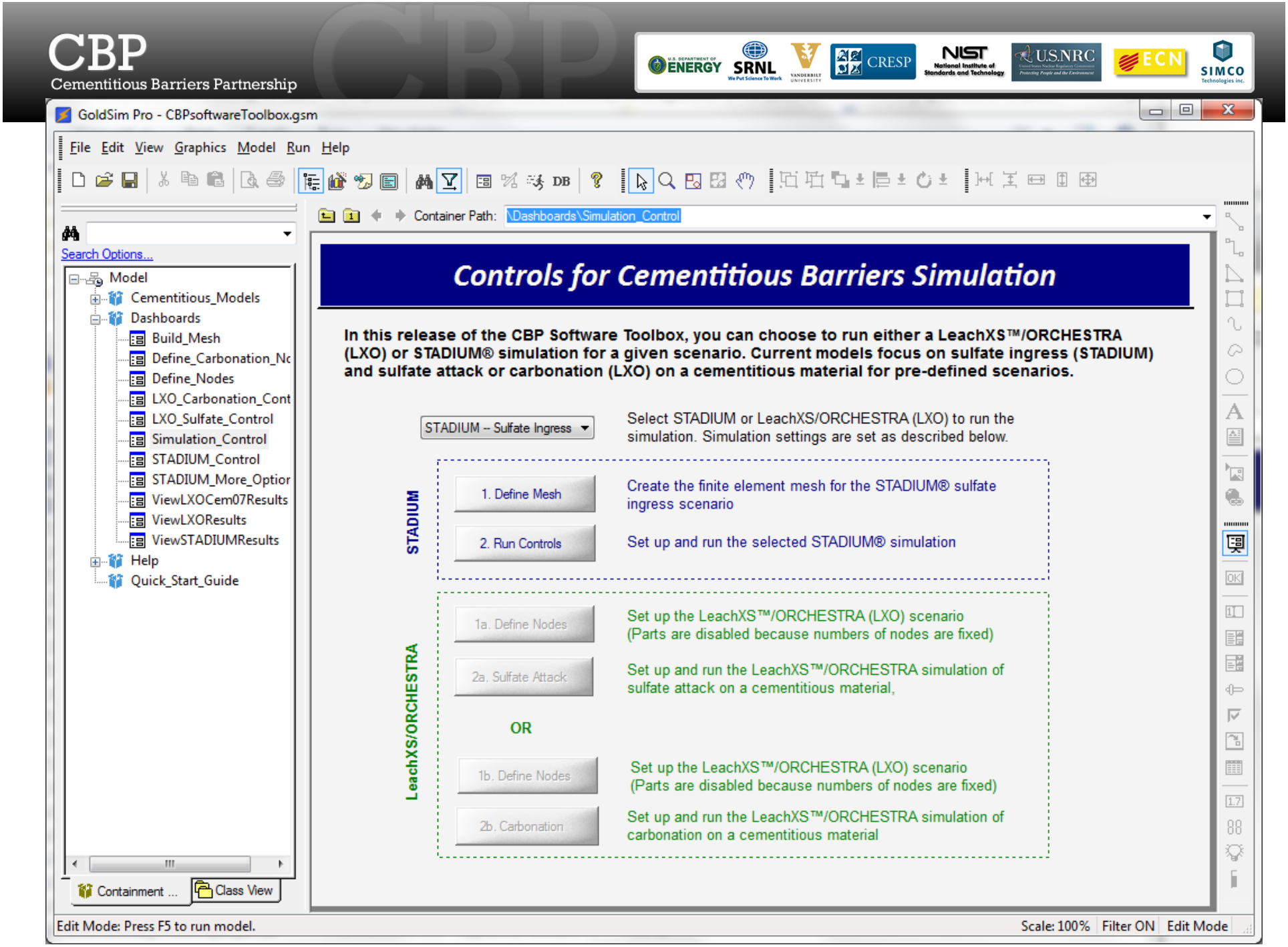
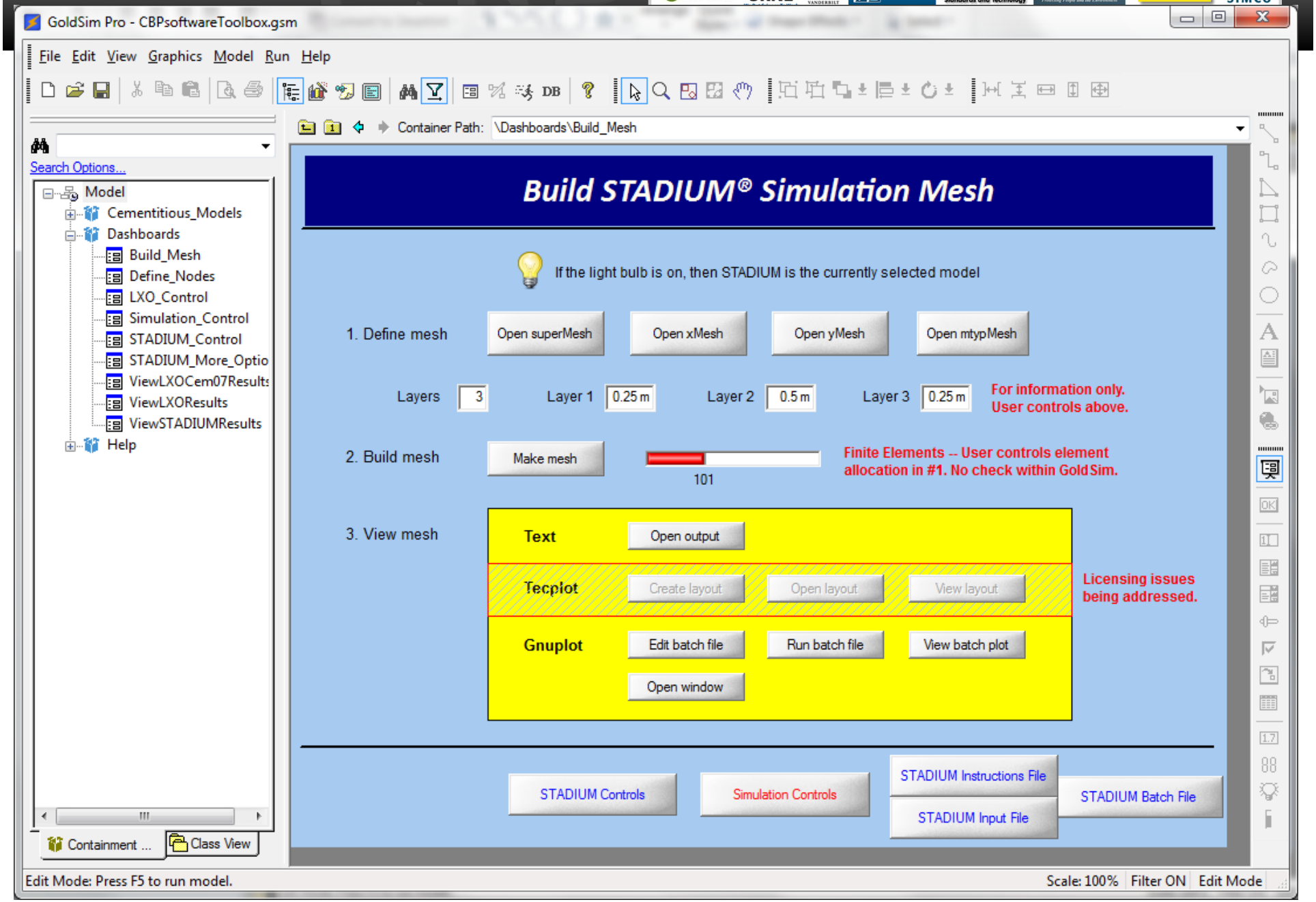
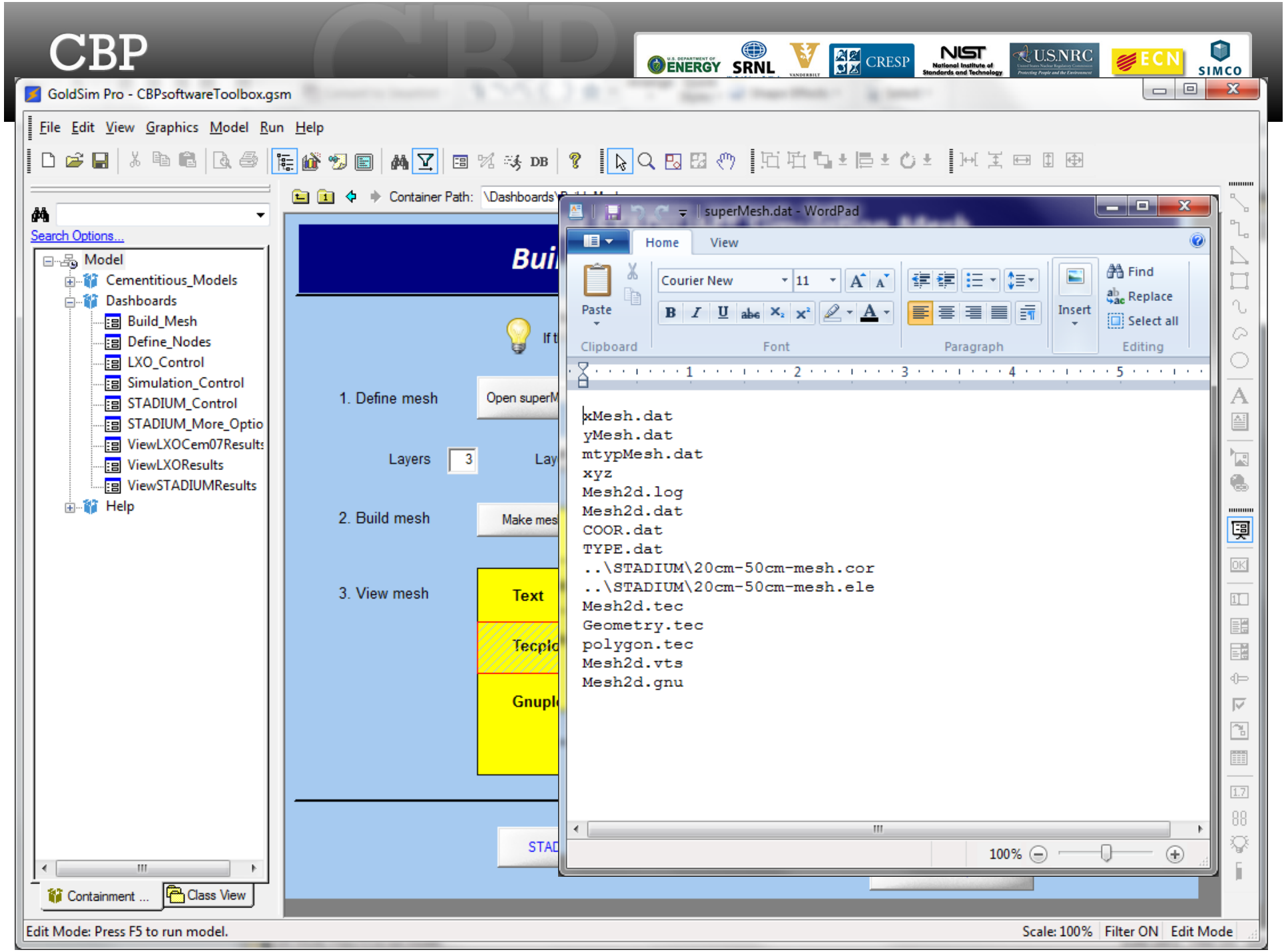
Edit Mode: Press F5 to run model.
Filter ON
Edit Mode

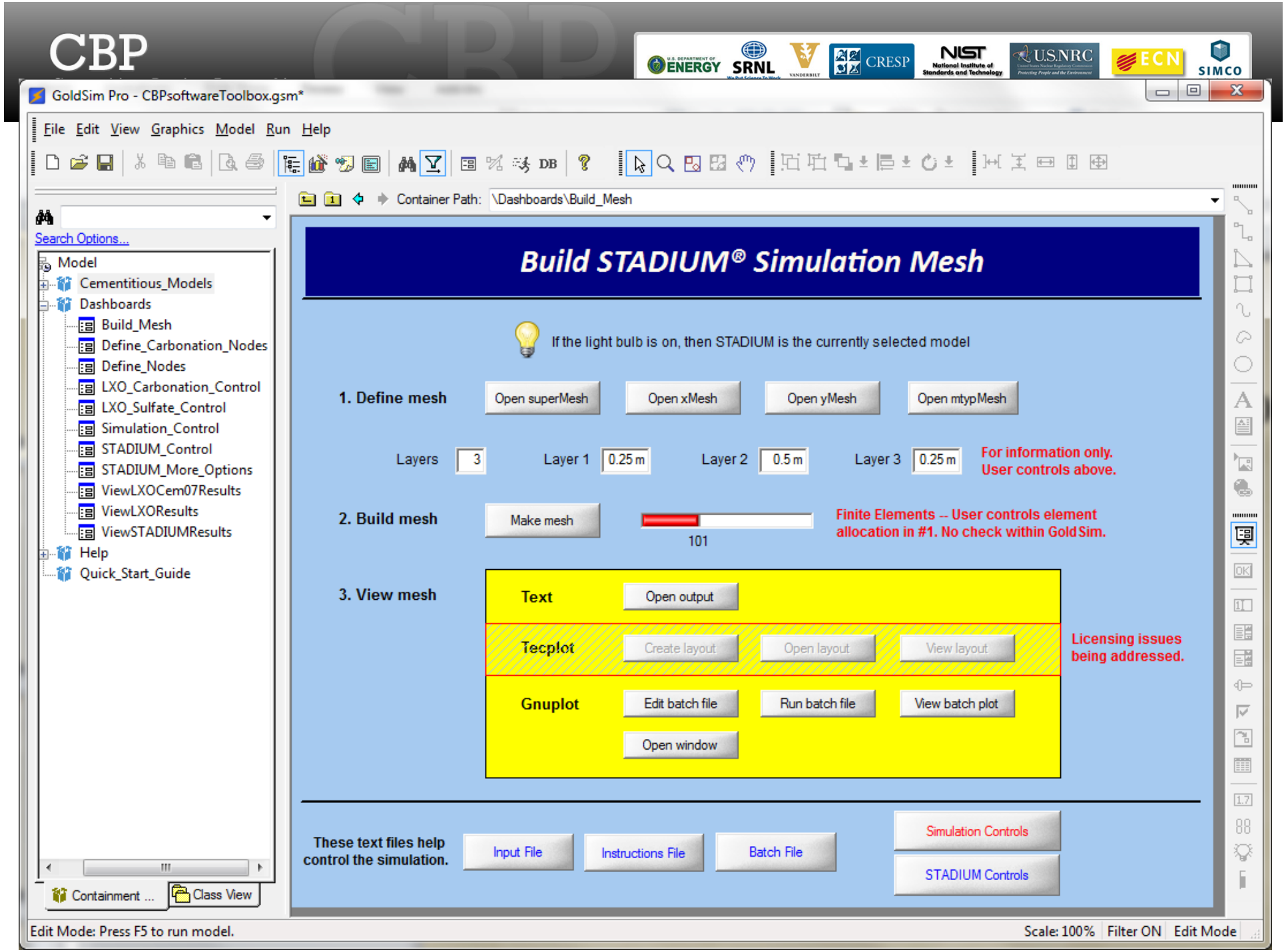

CBP
Cementitious Barriers Partnership
GoldSim Pro - CBPsoftwareToolbox.gsm
File Edit View Graphics Model Run Help
Container Path: \Dashboards\Simulation_Control
Search Options...
Model
Cementitious_Models
Dashboards
Build_Mesh
Define_Carbonation_Nc
Define_Nodes
LXO_Carbonation_Cont
LXO_Sulfate_Control
Simulation_Control
STADIUM_Control
STADIUM_More_Optior
ViewLXOCem07Results
ViewLXOResults
ViewSTADIUMResults
Help
Quick_Start_Guide
Containment ...
Class View
Controls for Cementitious Barriers Simulation
In this release of the CBP Software Toolbox, you can choose to run either a LeachXS™/ORCHESTRA (LXO) or STADIUM® simulation for a given scenario. Current models focus on sulfate ingress (STADIUM) and sulfate attack or carbonation (LXO) on a cementitious material for pre-defined scenarios.
STADIUM -- Sulfate Ingress
Select STADIUM or LeachXS/ORCHESTRA (LXO) to run the simulation. Simulation settings are set as described below.
STADIUM
1. Define Mesh
Create the finite element mesh for the STADIUM® sulfate ingress scenario
2. Run Controls
Set up and run the selected STADIUM® simulation
LeachXS/ORCHESTRA
1a. Define Nodes
Set up the LeachXS™/ORCHESTRA (LXO) scenario (Parts are disabled because numbers of nodes are fixed)
2a. Sulfate Attack
Set up and run the LeachXS™/ORCHESTRA simulation of sulfate attack on a cementitious material,
OR
1b. Define Nodes
Set up the LeachXS™/ORCHESTRA (LXO) scenario (Parts are disabled because numbers of nodes are fixed)
2b. Carbonation
Set up and run the LeachXS™/ORCHESTRA simulation of carbonation on a cementitious material
Edit Mode: Press F5 to run model.
Scale: 100%
Filter ON
Edit Mode

CBP


GoldSim Pro - CBPsoftwareToolbox.gsm
File Edit View Graphics Model Run Help
Container Path: \Dashboards\Build_Mesh
Search Options...
Model
Cementitious_Models
Dashboards
Build_Mesh
Define_Nodes
LXO_Control
Simulation_Control
STADIUM_Control
STADIUM_More_Optio
ViewLXOCem07Results
ViewLXOResults
ViewSTADIUMResults
Help
Containment ...
Class View
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
STADIUM Controls
Simulation Controls
STADIUM Instructions File
STADIUM Input File
STADIUM Batch File
Edit Mode: Press F5 to run model.
Scale: 100%
Filter ON
Edit Mode

CBP


GoldSim Pro - CBPsoftwareToolbox.gsm
File Edit View Graphics Model Run Help
Container Path:
Search Options...
Model
Cementitious_Models
Dashboards
Build_Mesh
Define_Nodes
LXO_Control
Simulation_Control
STADIUM_Control
STADIUM_More_Optio
ViewLXOCem07Results
ViewLXOResults
ViewSTADIUMResults
Help
Containment ...
Class View
1. Define mesh
Open superM
Layers
3
2. Build mesh
Make mes
3. View mesh
Text
Gnupl
STAD
Edit Mode: Press F5 to run model.
Scale: 100%
Filter ON
Edit Mode
superMesh.dat - WordPad
Home
View
Courier New
11
Paste
Clipboard
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%


CBP
GoldSim Pro - CBPsoftwareToolbox.gsm*
File Edit View Graphics Model Run Help
Container Path: \Dashboards\Build_Mesh
Search Options...
Model
Cementitious_Models
Dashboards
Build_Mesh
Define_Carbonation_Nodes
Define_Nodes
LXO_Carbonation_Control
LXO_Sulfate_Control
Simulation_Control
STADIUM_Control
STADIUM_More_Options
ViewLXOCem07Results
ViewLXOResults
ViewSTADIUMResults
Help
Quick_Start_Guide
Containment ...
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Layer 1 0.25 m
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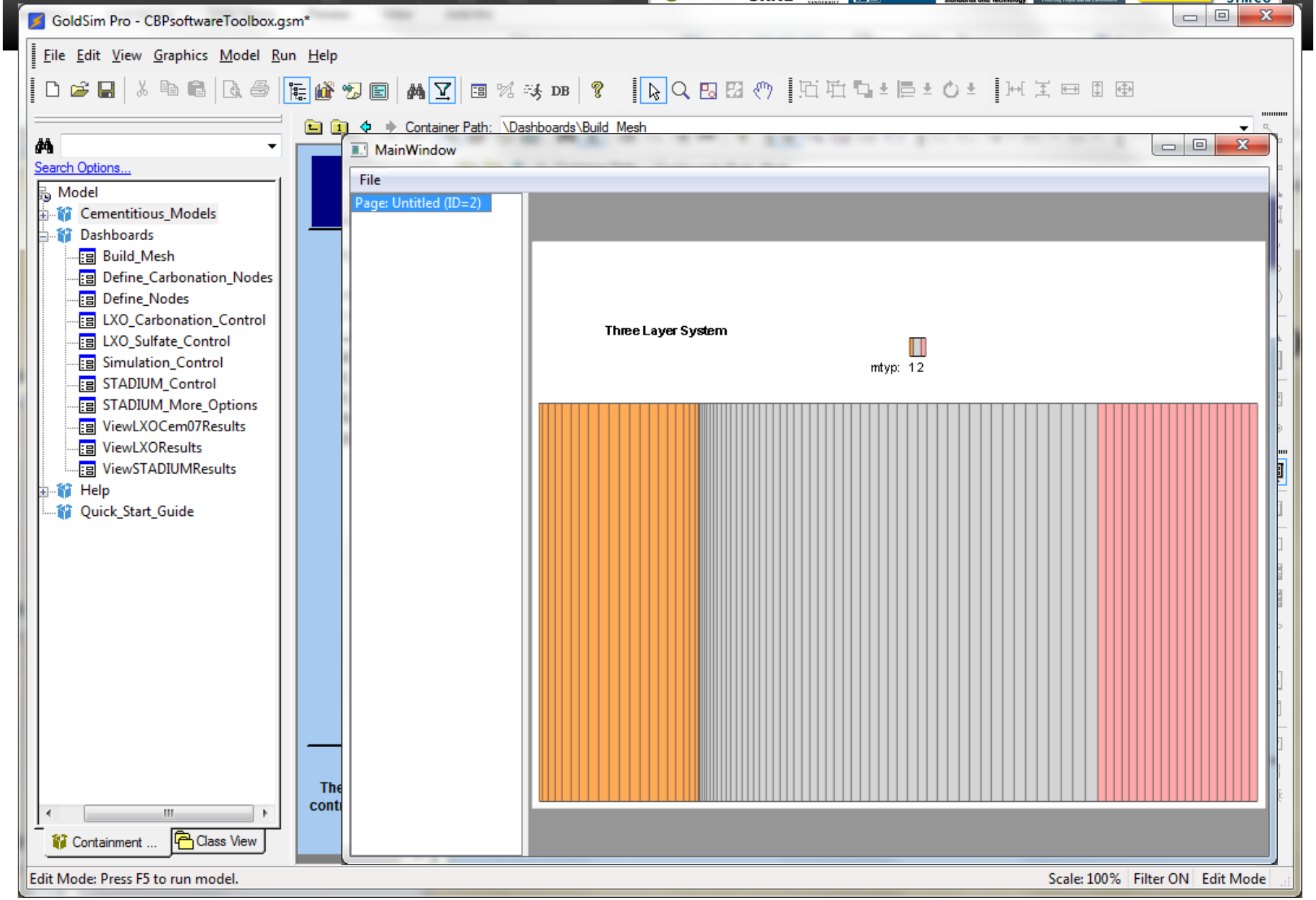
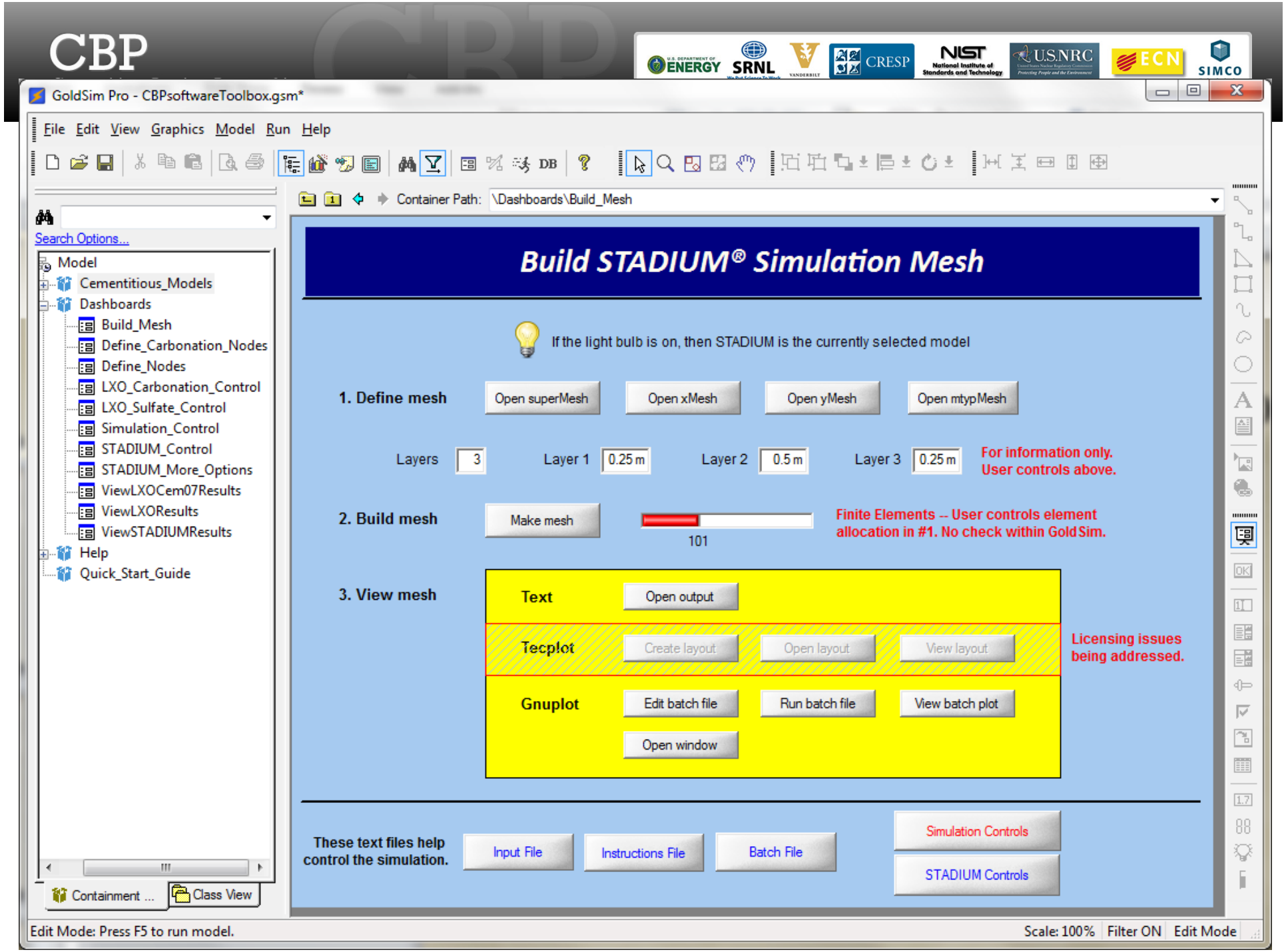
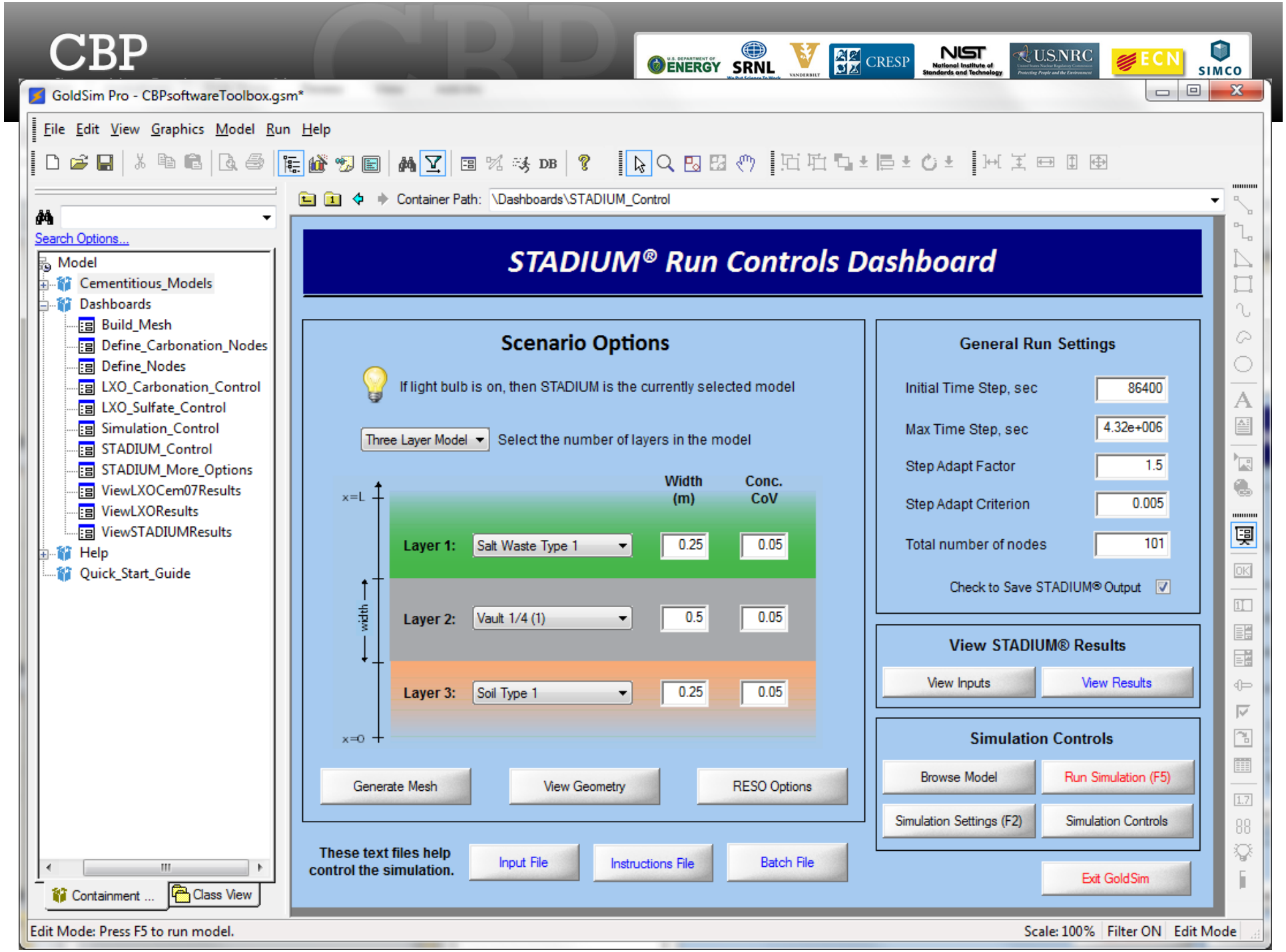
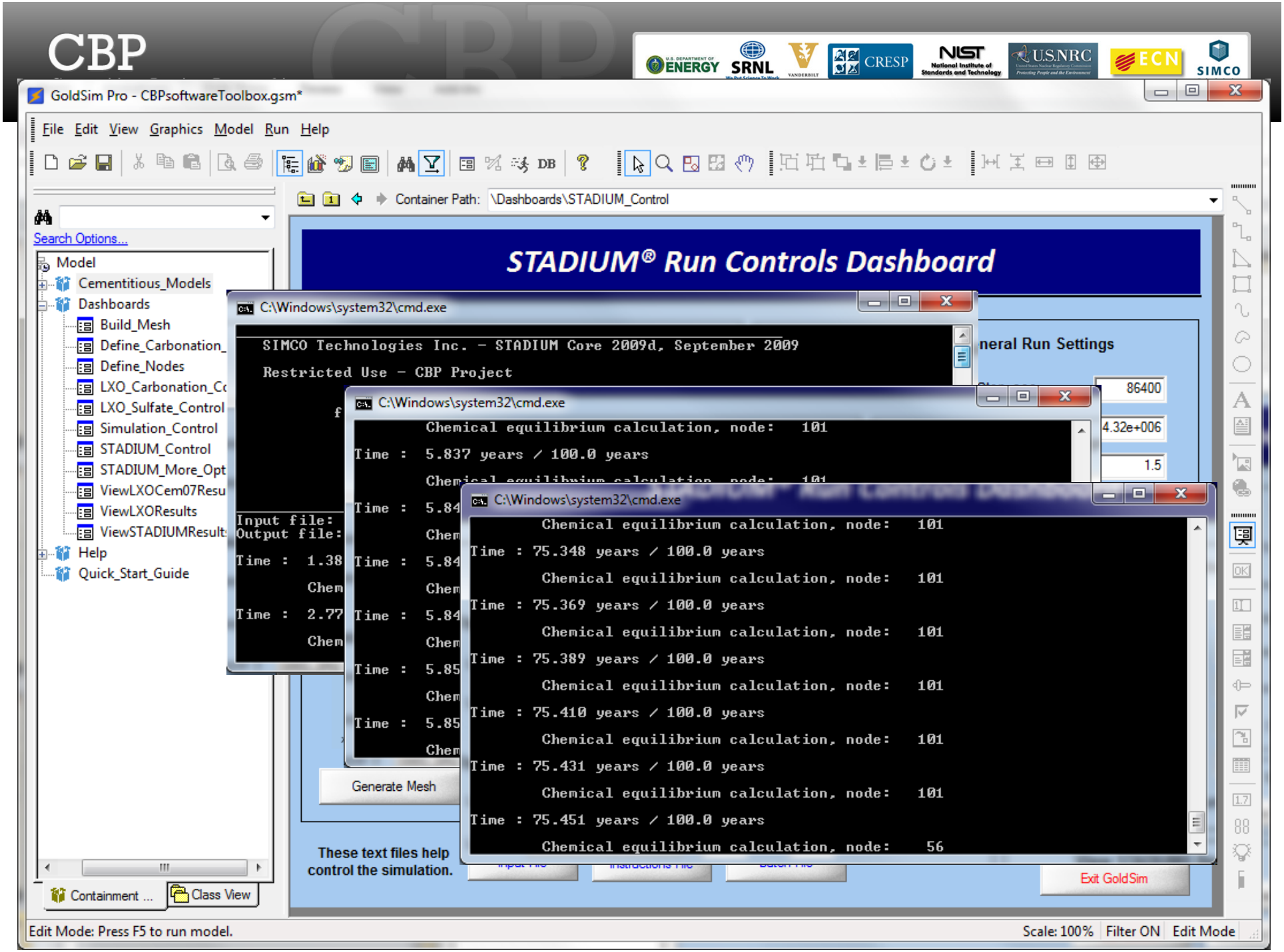
For information only.
User controls above.
2. Build mesh
Make mesh
101
Finite Elements -- User controls element allocation in #1. No check within GoldSim.
3. View mesh
Text
Open output
Tecplot
Create layout
Open layout
View layout
Licensing issues being addressed.
Gnuplot
Edit batch file
Run batch file
View batch plot
Open window
These text files help control the simulation.
Input File
Instructions File
Batch File
Simulation Controls
STADIUM Controls
Edit Mode: Press F5 to run model.
Scale: 100%
Filter ON
Edit Mode

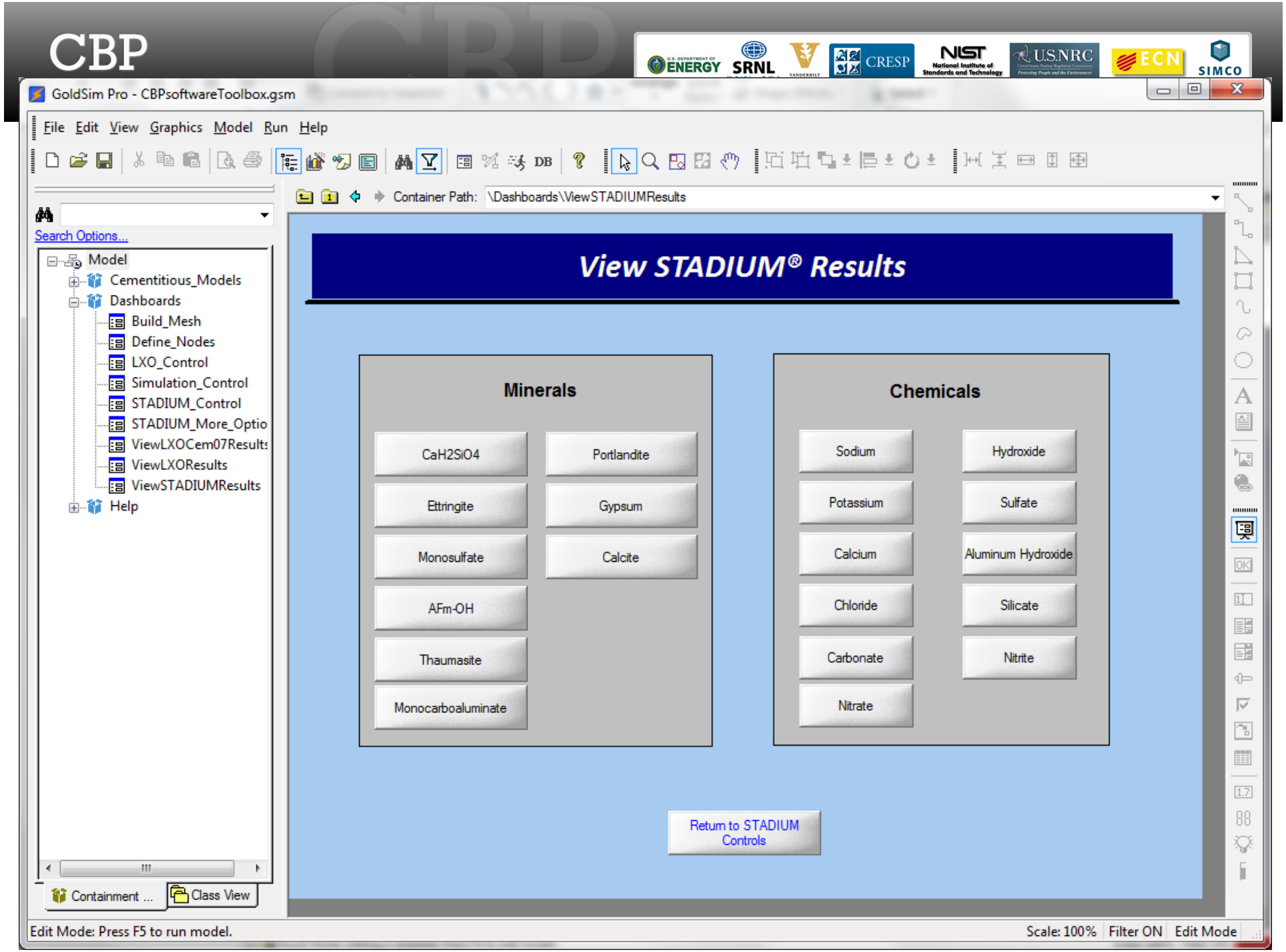
CBP


GoldSim Pro - CBPsoftwareToolbox.gsm*
File Edit View Graphics Model Run Help
Container Path: \Dashboards\Build_Mesh
Search Options...
Model
Cementitious_Models
Dashboards
Build_Mesh
Define_Carbonation_Nodes
Define_Nodes
LXO_Carbonation_Control
LXO_Sulfate_Control
Simulation_Control
STADIUM_Control
STADIUM_More_Options
ViewLXOCem07Results
ViewLXOResults
ViewSTADIUMResults
Help
Quick_Start_Guide
Containment ...
Class View
MainWindow
File
Page: Untitled (ID=2)
Three Layer System
mtyp: 1 2
Edit Mode: Press F5 to run model.
Scale: 100%
Filter ON
Edit Mode


CBP
GoldSim Pro - CBPsoftwareToolbox.gsm*
File Edit View Graphics Model Run Help
Container Path: \Dashboards\Build_Mesh
Search Options...
Model
Cementitious_Models
Dashboards
Build_Mesh
Define_Carbonation_Nodes
Define_Nodes
LXO_Carbonation_Control
LXO_Sulfate_Control
Simulation_Control
STADIUM_Control
STADIUM_More_Options
ViewLXOCem07Results
ViewLXOResults
ViewSTADIUMResults
Help
Quick_Start_Guide
Containment ...
Class View
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
Edit Mode: Press F5 to run model.
Scale: 100%
Filter ON
Edit Mode


CBP
GoldSim Pro - CBPsoftwareToolbox.gsm*
File Edit View Graphics Model Run Help
Container Path: \Dashboards\STADIUM_Control
Search Options...
Model
Cementitious_Models
Dashboards
Build_Mesh
Define_Carbonation_Nodes
Define_Nodes
LXO_Carbonation_Control
LXO_Sulfate_Control
Simulation_Control
STADIUM_Control
STADIUM_More_Options
ViewLXOCem07Results
ViewLXOResults
ViewSTADIUMResults
Help
Quick_Start_Guide
Containment ...
Class View
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
width
Layer 2:
Vault 1/4 (1)
0.5
0.05
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
Edit Mode: Press F5 to run model.
Scale: 100%
Filter ON
Edit Mode


CBP
GoldSim Pro - CBPsoftwareToolbox.gsm*
File Edit View Graphics Model Run Help
Container Path: \Dashboards\STADIUM_Control
STADIUM® Run Controls Dashboard
Search Options...
Model
Cementitious_Models
Dashboards
Build_Mesh
Define_Carbonation_
Define_Nodes
LXO_Carbonation_Cc
LXO_Sulfate_Control
Simulation_Control
STADIUM_Control
STADIUM_More_Opt
ViewLXOCem07Resu
ViewLXOResults
ViewSTADIUMResult
Help
Quick_Start_Guide
C:\Windows\system32\cmd.exe
SIMCO Technologies Inc. - STADIUM Core 2009d, September 2009
Restricted Use - CBP Project
Input file:
Output file:
Time : 1.38
Time : 2.77
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
neral Run Settings
86400
4.32e+006
1.5
Generate Mesh
These text files help control the simulation.
Exit GoldSim
Containment ...
Class View
Edit Mode: Press F5 to run model.
Scale: 100%
Filter ON
Edit Mode


CBP
GoldSim Pro - CBPsoftwareToolbox.gsm
File Edit View Graphics Model Run Help
Container Path: \Dashboards\ViewSTADIUMResults
Search Options...
Model
Cementitious_Models
Dashboards
Build_Mesh
Define_Nodes
LXO_Control
Simulation_Control
STADIUM_Control
STADIUM_More_Optio
ViewLXOCem07Results
ViewLXOResults
ViewSTADIUMResults
Help
Containment ...
Class View
View STADIUM® Results
Minerals
CaH2SiO4
Portlandite
Ettringite
Gypsum
Monosulfate
Calcite
AFm-OH
Thaumasite
Monocarboaluminate
Chemicals
Sodium
Hydroxide
Potassium
Sulfate
Calcium
Aluminum Hydroxide
Chloride
Silicate
Carbonate
Nitrite
Nitrate
Return to STADIUM Controls
Edit Mode: Press F5 to run model.
Scale: 100%
Filter ON
Edit Mode

CBP

GoldSim Pro - CBPsoftwareToolbox.gsm

File Edit View Graphics Model Run Help

Container Path: \Dashboards\ViewSTADIUMResults

Search Options...

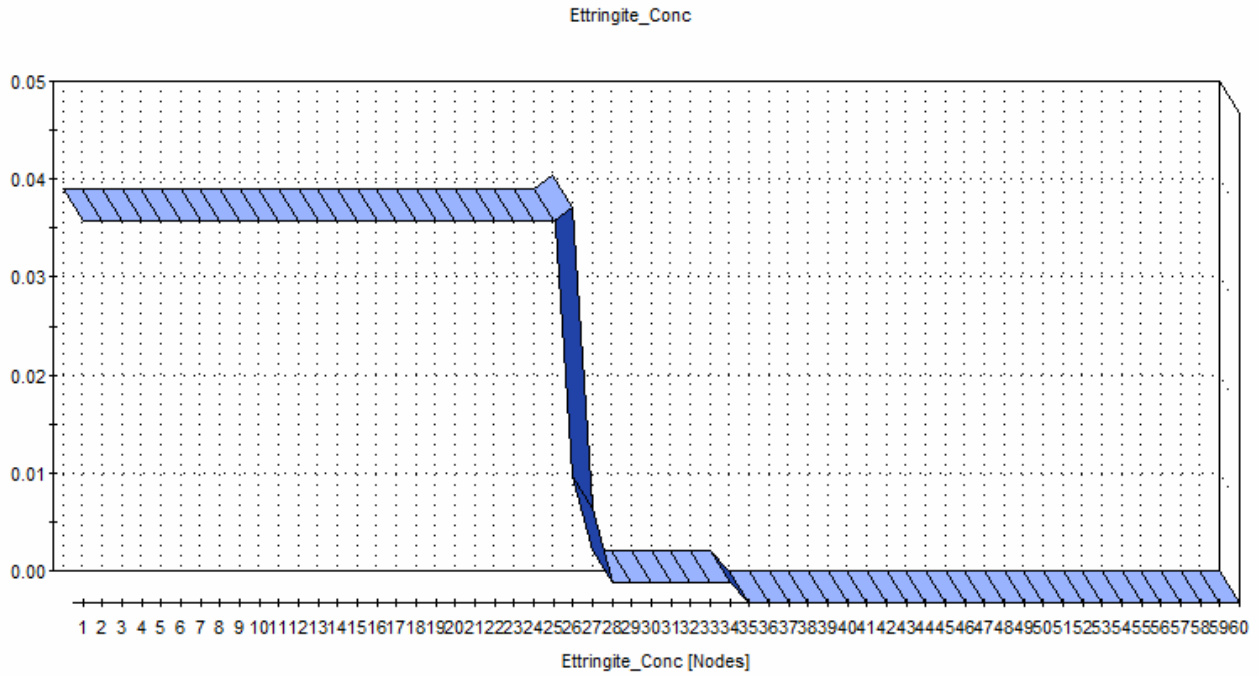
- Model
  - Cementitious_Models
  - Dashboards
    - Build_Mesh
    - Define_Nodes
    - LXO_Control
    - Simulation_Control
    - STADIUM_Control
    - STADIUM_More_Optio
    - ViewLXOCem07Results
    - ViewLXOResults
    - ViewSTADIUMResults
  - Help

Containment ... | Class View

View STADIUM® Results

Array Chart: Ettringite_Conc

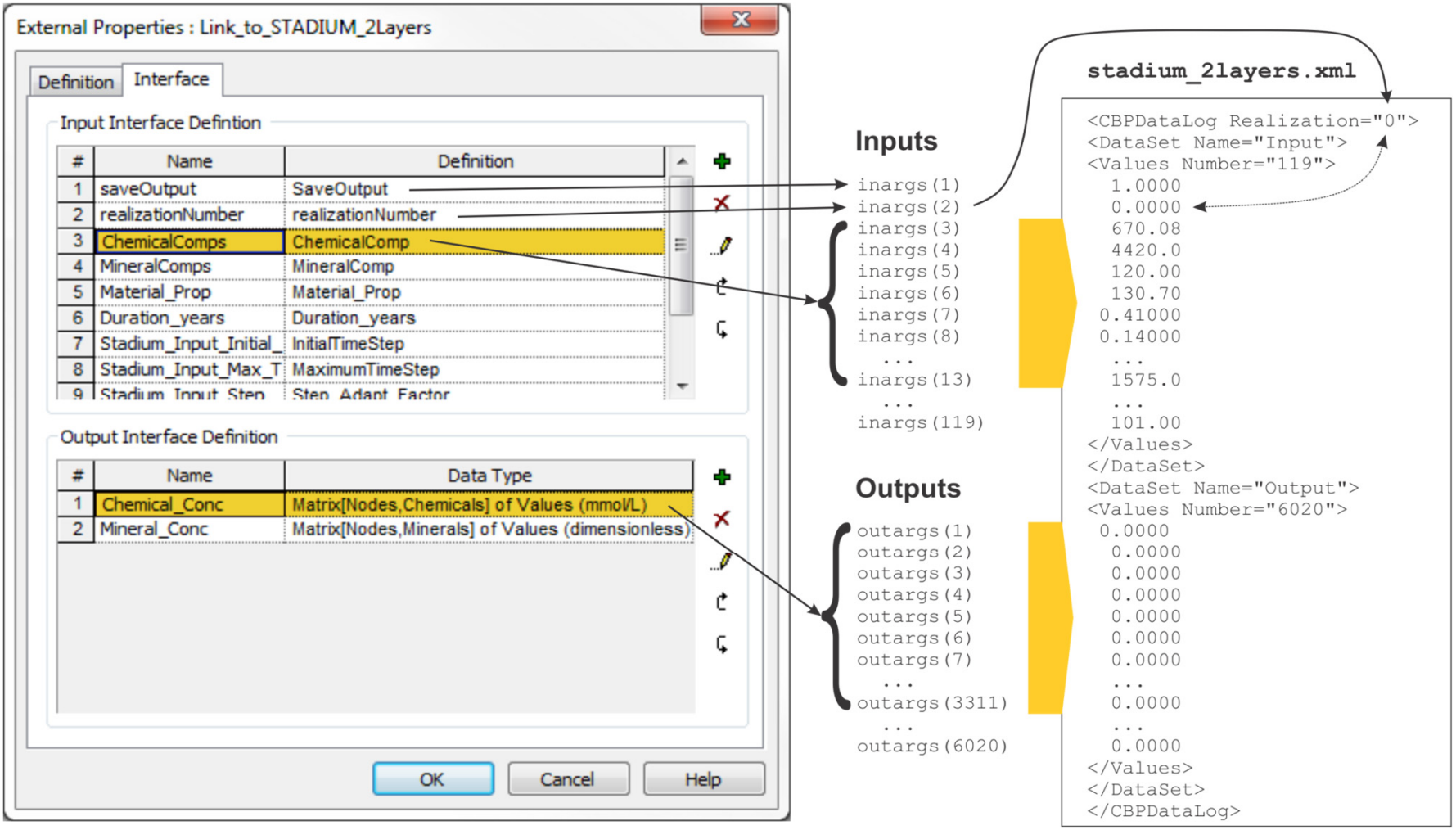
Realization: 12



Edit Mode: Press F5 to run model.

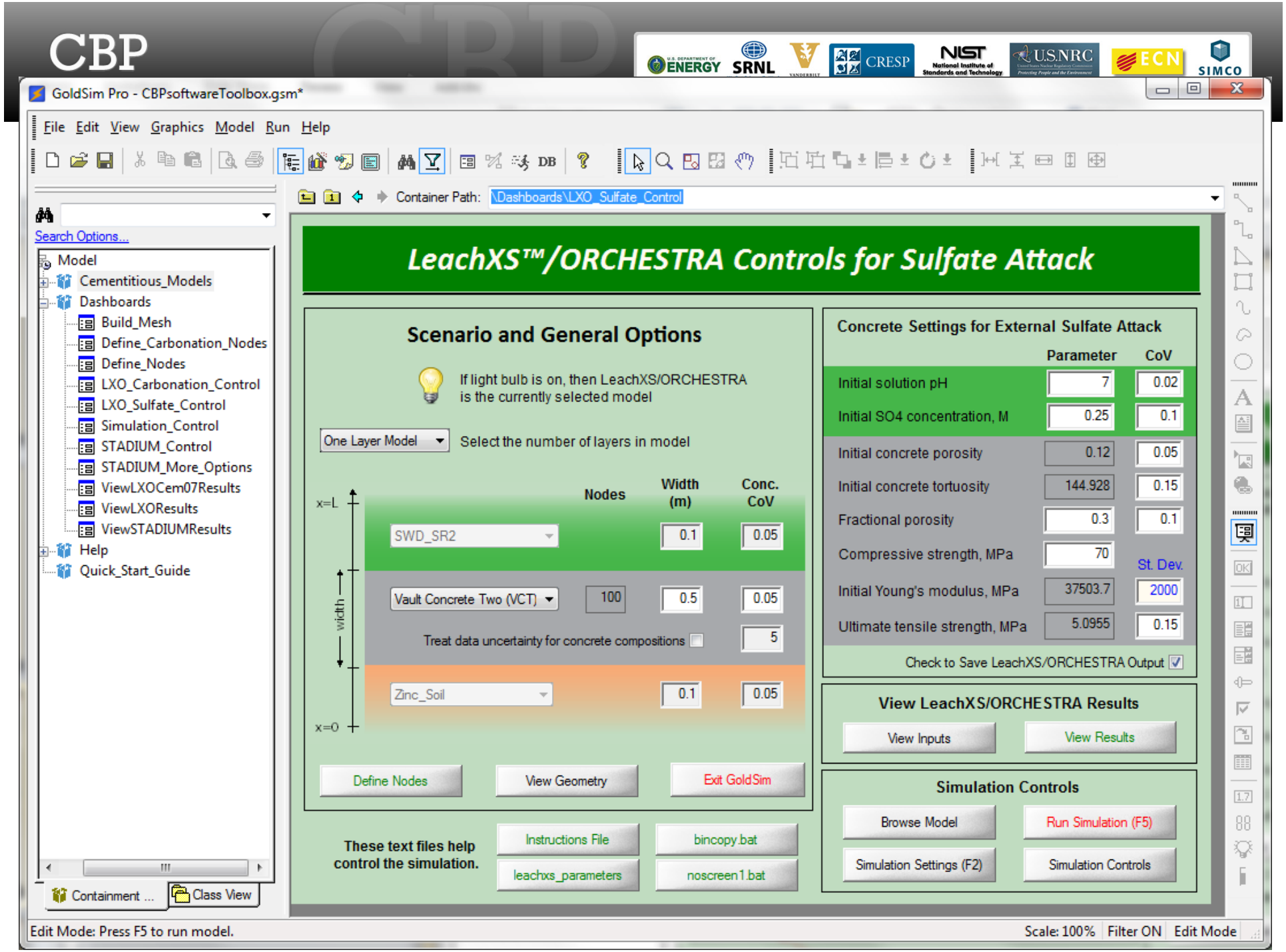
Scale: 100% | Filter ON | Edit Mode

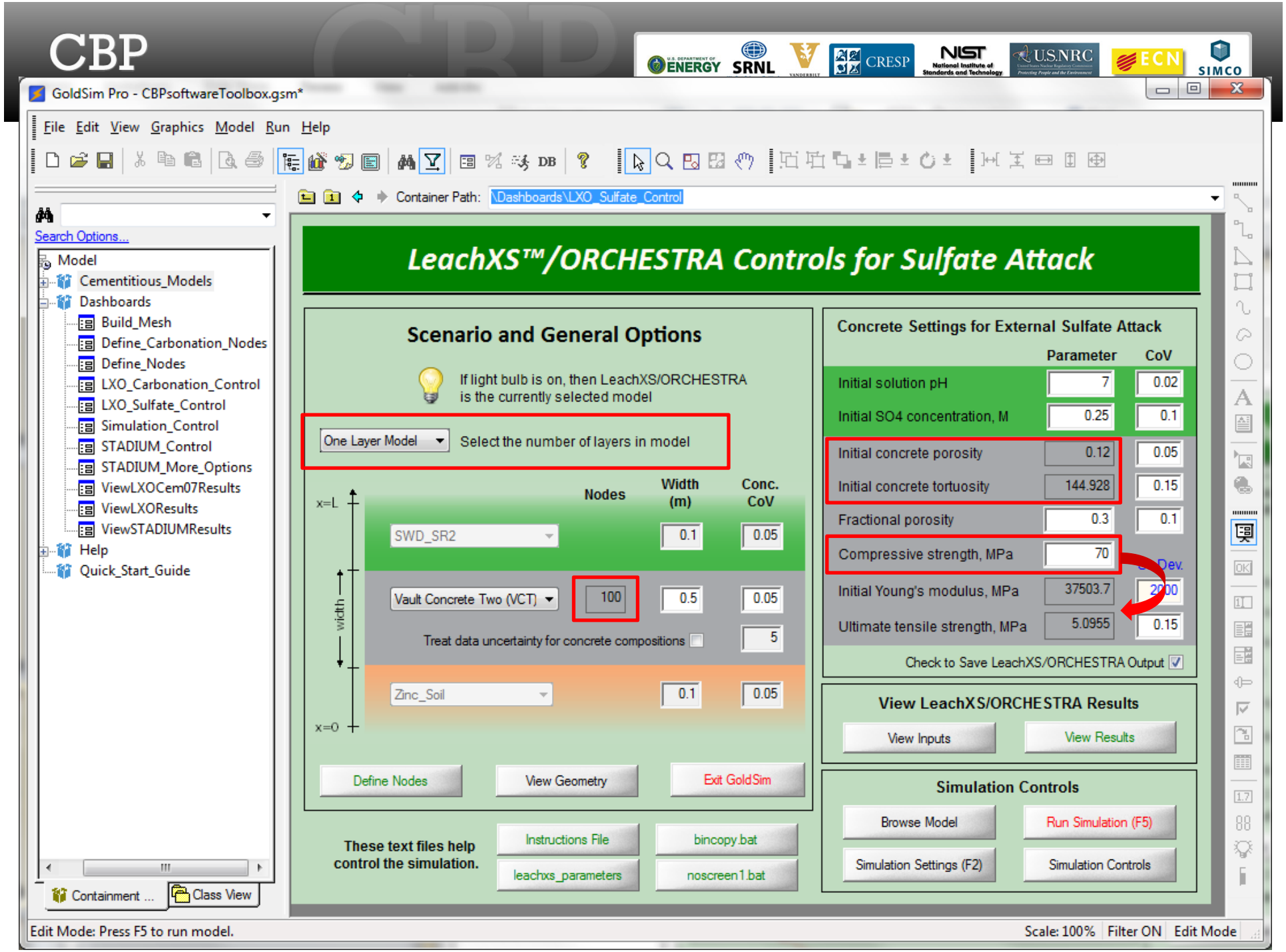
Summary of STADIUM External Linking

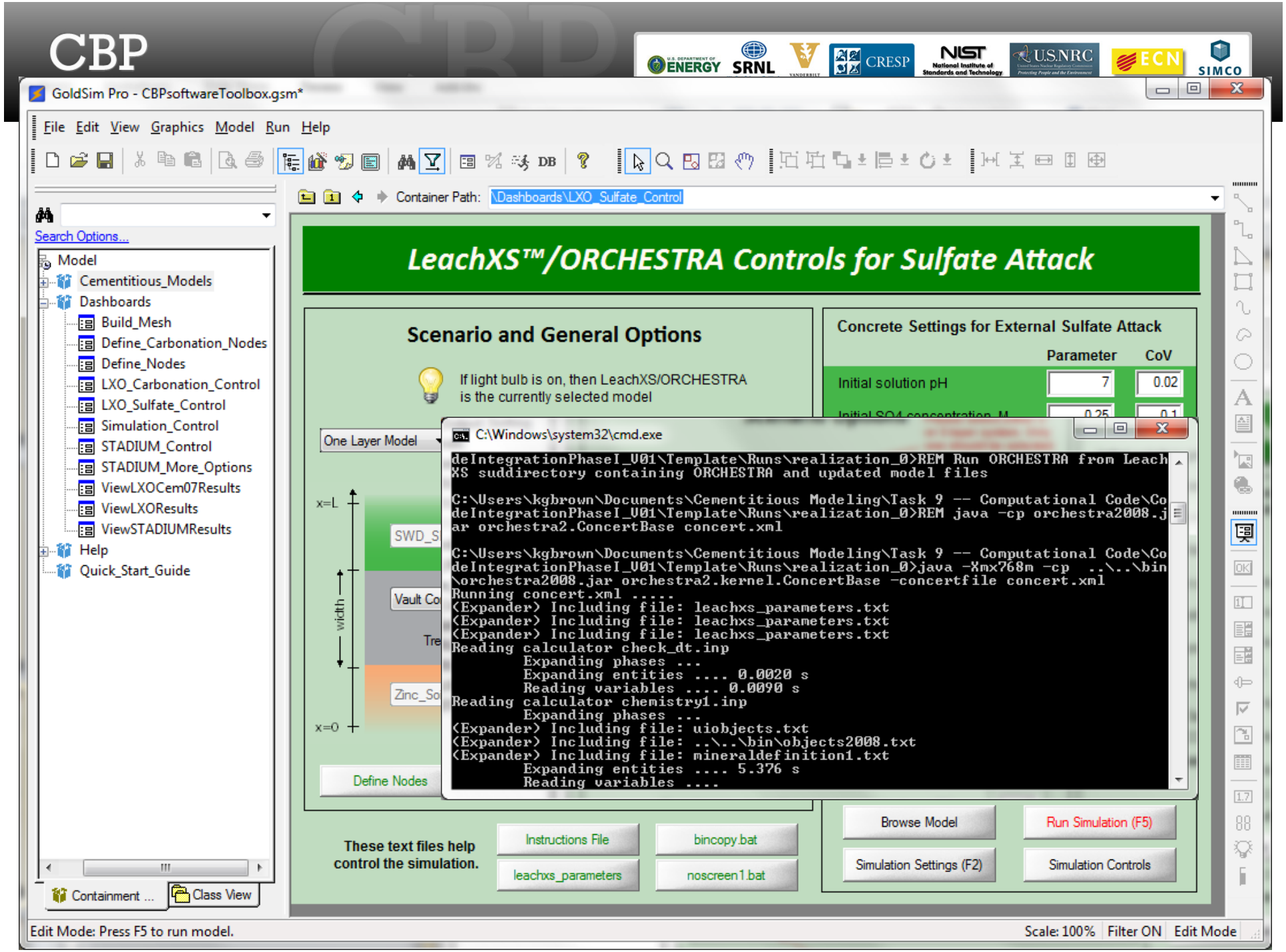


CBP Custom DLL Subroutine

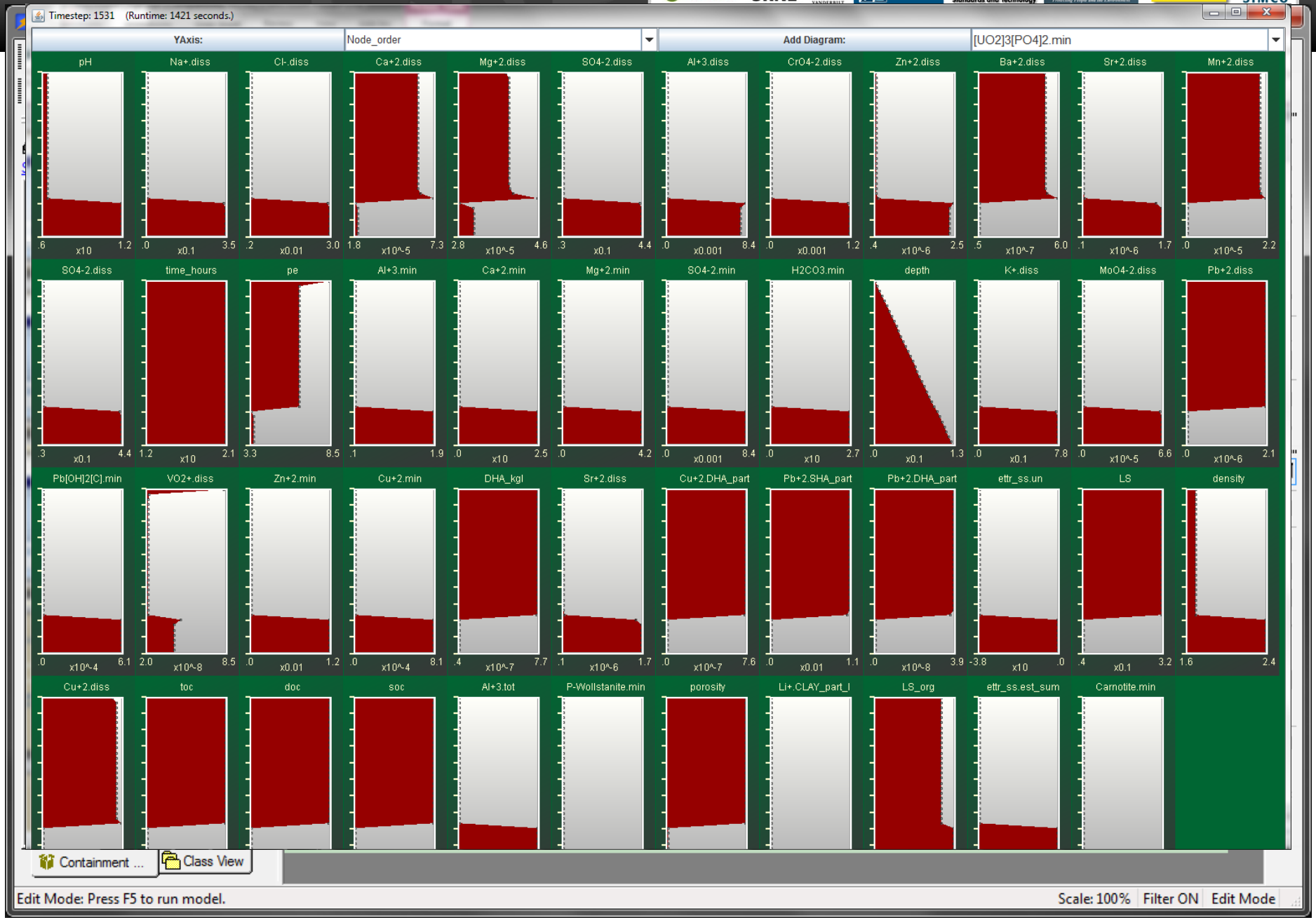
- Avoid need for low-level programming by user
  - Put generic executable content in pre-compiled subroutine (Dynamic-link Library or DLL)
  - Put application content in an "instructions file" that is interpreted at run-time
  - Primary instructions: PUT (create input), EXE (execute file), GET (retrieve 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


CBP
GoldSim Pro - CBPsoftwareToolbox.gsm*
File Edit View Graphics Model Run Help
Container Path: \Dashboards\LXO_Sulfate_Control
Search Options...
Model
Cementitious_Models
Dashboards
Build_Mesh
Define_Carbonation_Nodes
Define_Nodes
LXO_Carbonation_Control
LXO_Sulfate_Control
Simulation_Control
STADIUM_Control
STADIUM_More_Options
ViewLXOCem07Results
ViewLXOResults
ViewSTADIUMResults
Help
Quick_Start_Guide
Containment ...
Class View
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
width
x=0
Nodes
Width (m)
Conc. CoV
SWD_SR2
0.1
0.05
Vault Concrete Two (VCT)
100
0.5
0.05
Treat data uncertainty for concrete compositions
5
Zinc_Soil
0.1
0.05
Define Nodes
View Geometry
Exit GoldSim
These text files help control the simulation.
Instructions File
bincopy.bat
leachxs_parameters
noscreen1.bat
Concrete Settings for External Sulfate Attack
Parameter
CoV
Initial solution pH
7
0.02
Initial SO4 concentration, M
0.25
0.1
Initial concrete porosity
0.12
0.05
Initial concrete tortuosity
144.928
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
5.0955
0.15
Check to Save LeachXS/ORCHESTRA Output
View LeachXS/ORCHESTRA Results
View Inputs
View Results
Simulation Controls
Browse Model
Run Simulation (F5)
Simulation Settings (F2)
Simulation Controls
Edit Mode: Press F5 to run model.
Scale: 100%
Filter ON
Edit Mode


CBP
GoldSim Pro - CBPsoftwareToolbox.gsm*
File Edit View Graphics Model Run Help
Container Path: \Dashboards\LXO_Sulfate_Control
Search Options...
Model
Cementitious_Models
Dashboards
Build_Mesh
Define_Carbonation_Nodes
Define_Nodes
LXO_Carbonation_Control
LXO_Sulfate_Control
Simulation_Control
STADIUM_Control
STADIUM_More_Options
ViewLXOCem07Results
ViewLXOResults
ViewSTADIUMResults
Help
Quick_Start_Guide
Containment ...
Class View
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
width
x=0
Nodes
Width (m)
Conc. CoV
SWD_SR2
0.1
0.05
Vault Concrete Two (VCT)
100
0.5
0.05
Treat data uncertainty for concrete compositions
5
Zinc_Soil
0.1
0.05
Define Nodes
View Geometry
Exit GoldSim
These text files help control the simulation.
Instructions File
bincopy.bat
leachxs_parameters
noscreen1.bat
Concrete Settings for External Sulfate Attack
Parameter
CoV
Initial solution pH
7
0.02
Initial SO4 concentration, M
0.25
0.1
Initial concrete porosity
0.12
0.05
Initial concrete tortuosity
144.928
0.15
Fractional porosity
0.3
0.1
Compressive strength, MPa
70
Dev.
Initial Young's modulus, MPa
37503.7
2000
Ultimate tensile strength, MPa
5.0955
0.15
Check to Save LeachXS/ORCHESTRA Output
View LeachXS/ORCHESTRA Results
View Inputs
View Results
Simulation Controls
Browse Model
Run Simulation (F5)
Simulation Settings (F2)
Simulation Controls
Edit Mode: Press F5 to run model.
Scale: 100%
Filter ON
Edit Mode


CBP
GoldSim Pro - CBPsoftwareToolbox.gsm*
File Edit View Graphics Model Run Help
Container Path: \Dashboards\LXO_Sulfate_Control
Search Options...
Model
Cementitious_Models
Dashboards
Build_Mesh
Define_Carbonation_Nodes
Define_Nodes
LXO_Carbonation_Control
LXO_Sulfate_Control
Simulation_Control
STADIUM_Control
STADIUM_More_Options
ViewLXOCem07Results
ViewLXOResults
ViewSTADIUMResults
Help
Quick_Start_Guide
Containment ...
Class View
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
x=L
x=0
width
SWD_S
Vault Co
Tre
Zinc_So
Define Nodes
Concrete Settings for External Sulfate Attack
Parameter
CoV
Initial solution pH
7
0.02
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
Edit Mode: Press F5 to run model.
Scale: 100%
Filter ON
Edit Mode

CBP


Timestep: 1531 (Runtime: 1421 seconds.)
YAxis:
Node_order
Add Diagram:
[UO2]3[PO4]2.min
pH
Na+.diss
Cl-.diss
Ca+2.diss
Mg+2.diss
SO4-2.diss
Al+3.diss
CrO4-2.diss
Zn+2.diss
Ba+2.diss
Sr+2.diss
Mn+2.diss
SO4-2.diss
time_hours
pe
Al+3.min
Ca+2.min
Mg+2.min
SO4-2.min
H2CO3.min
depth
K+.diss
MoO4-2.diss
Pb+2.diss
Pb[OH]2[C].min
VO2+.diss
Zn+2.min
Cu+2.min
DHA_kgl
Sr+2.diss
Cu+2.DHA_part
Pb+2.SHA_part
Pb+2.DHA_part
ettr_ss.un
LS
density
Cu+2.diss
toc
doc
soc
Al+3.tot
P-Wollstanite.min
porosity
Li+.CLAY_part_l
LS_org
ettr_ss.est_sum
Carnotite.min
Containment ...
Class View
Edit Mode: Press F5 to run model.
Scale: 100%
Filter ON
Edit Mode

CBP

GoldSim Pro - CBPsoftwareToolbox.gsm*

File Edit View Graphics Model Run Help

Container Path: \Dashboards\LXO_Carbonation_Control

Search Options...

- Model
  - Cementitious_Models
  - Dashboards
    - Build_Mesh
    - Define_Carbonation_Nodes
    - Define_Nodes
    - LXO_Carbonation_Control
    - LXO_Sulfate_Control
    - Simulation_Control
    - STADIUM_Control
    - STADIUM_More_Options
    - ViewLXOCem07Results
    - ViewLXOResults
    - ViewSTADIUMResults
  - Help
  - Quick_Start_Guide

Containment ... | Class View

LeachXS™/ORCHESTRA Controls for Carbonation

Scenario and General Options

If light bulb is on, then LeachXS/ORCHESTRA is the currently selected model

Monolith	Nodes	Width (m)	Conc. CoV
Vault Concrete Two (VCT)	20	0.5	0.05

Treat data uncertainty for concrete compositions ☐ 5

Define Nodes | View Geometry | Exit GoldSim

These text files help control the simulation.

Instructions File | bincopy.bat | leachxs_parameters | noscreenCO3.bat

Settings for the Carbonation Model

	Parameter	CoV
CO2[g], partial pressure (atm)	0.0038	0.1
O2[g], partial pressure (atm)	0.2	0.1
Initial concrete porosity	0.12	0.05
Initial concrete tortuosity	144.928	0.15

Check to Save LeachXS/ORCHESTRA Output ☑

View LeachXS/ORCHESTRA Results

View Inputs | View Results

Simulation Controls

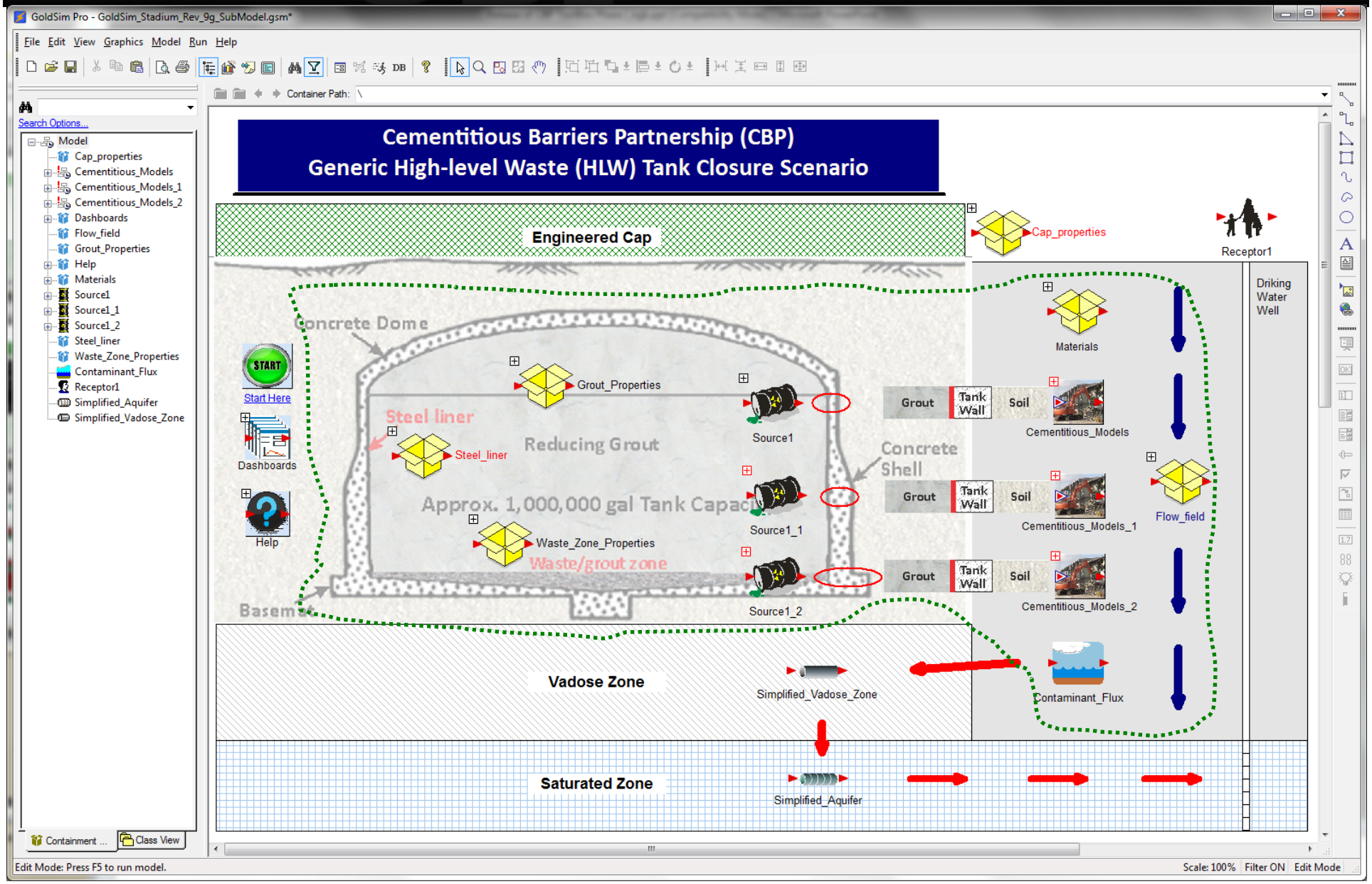
Browse Model | Run Simulation (F5)

Simulation Settings (F2) | Simulation Controls

Edit Mode: Press F5 to run model.

Scale: 100% | Filter ON | Edit Mode

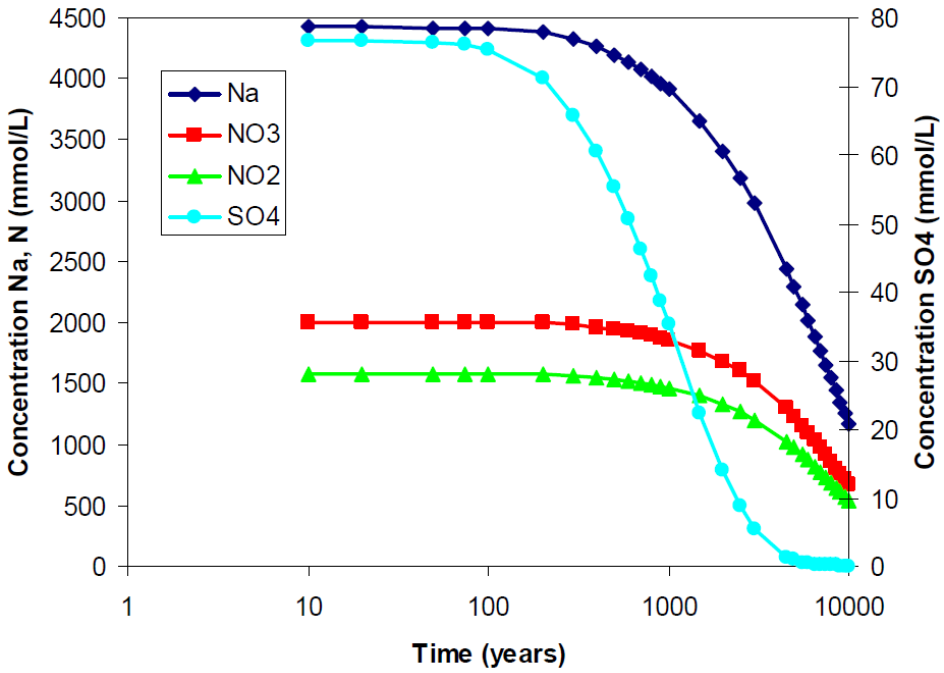
CBP
Cementitious Barriers Partnership



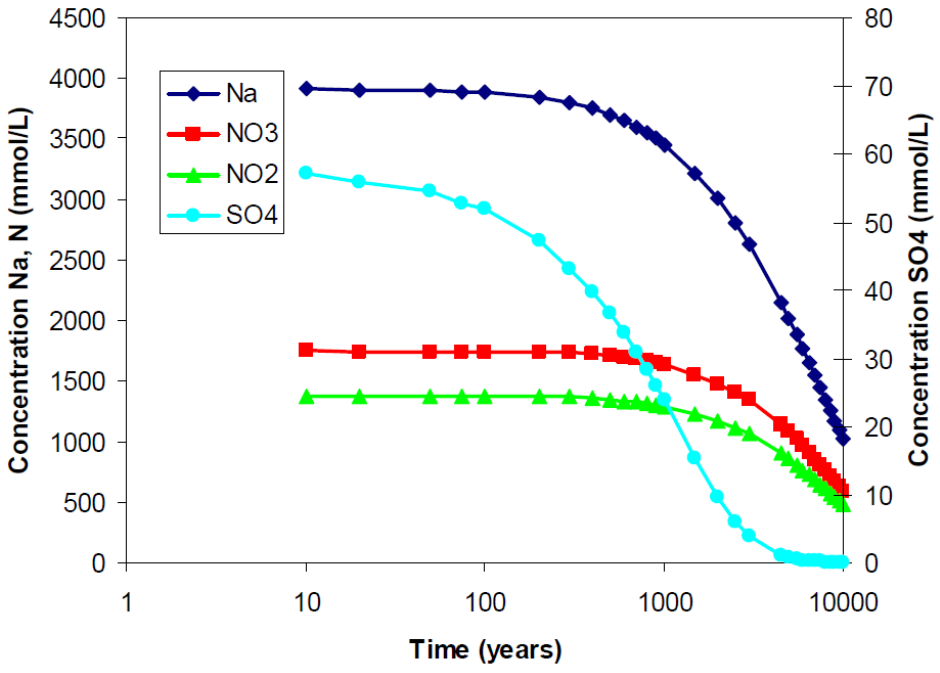
Uncertainty Analysis

- 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

STADIUM Ion Concentrations

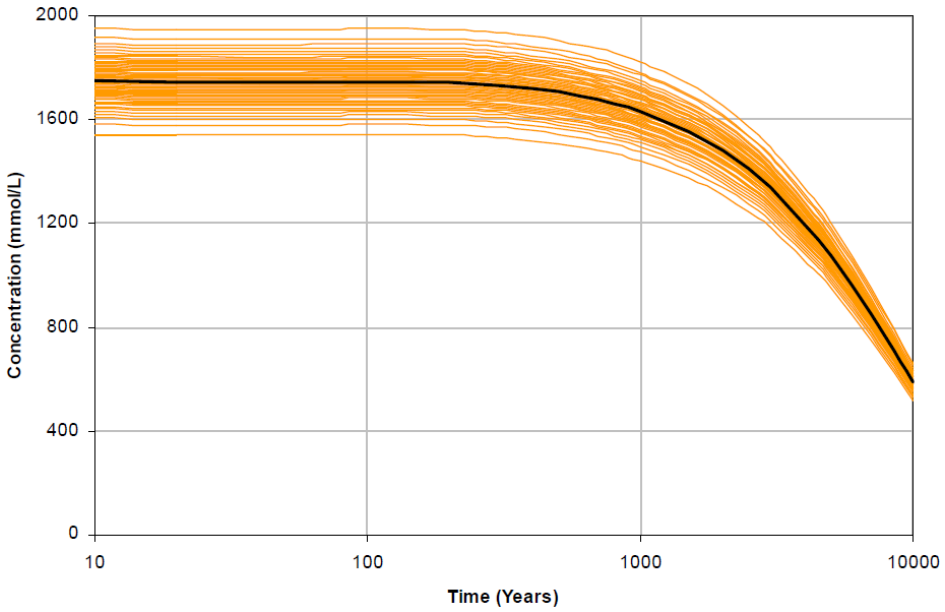


End of Saltstone Domain

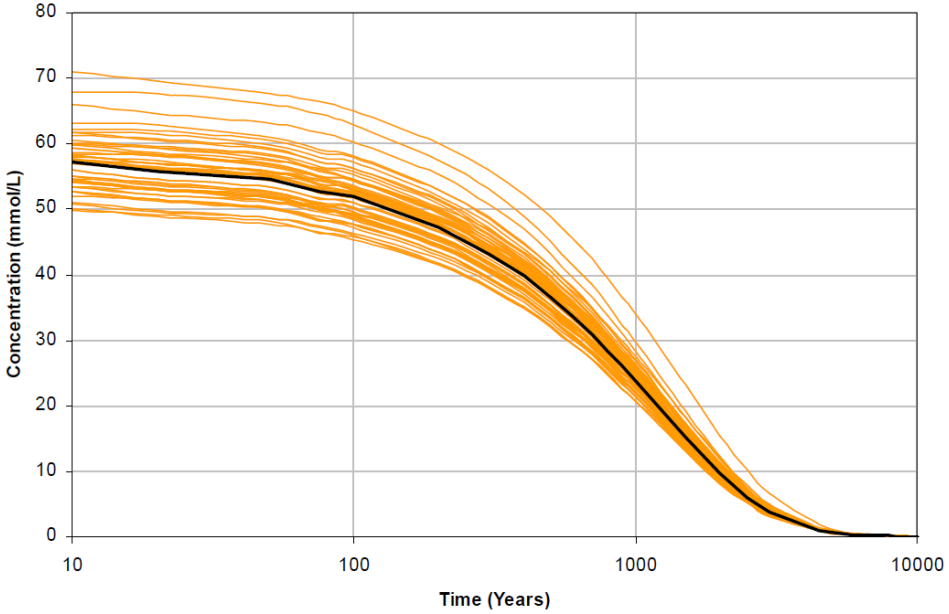


Saltstone-Concrete Interface

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



Nitrate



Sulfate

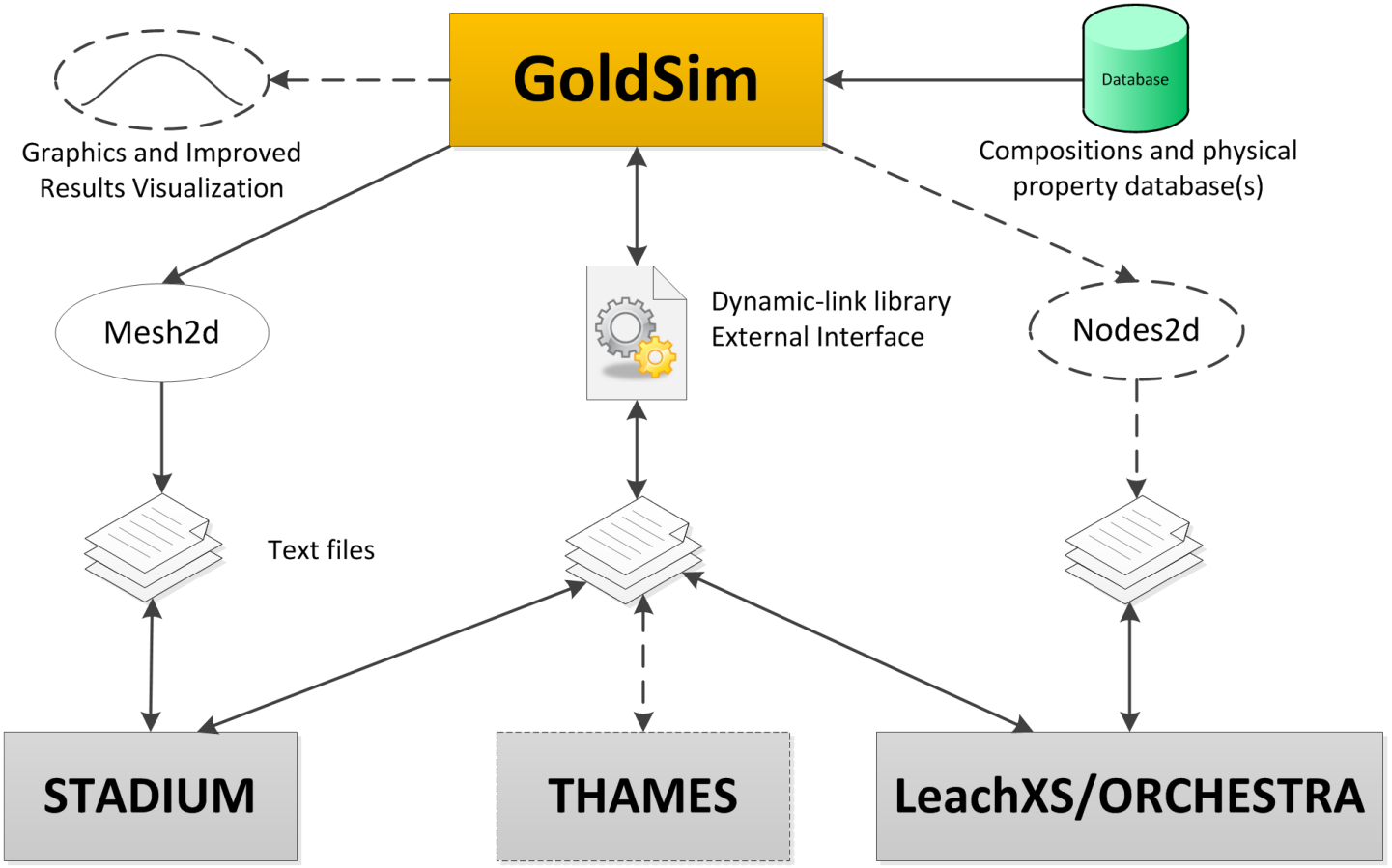
Summary of Uncertainty Analysis

- 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



CBP
Cementitious Barriers Partnership

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

Being Completed

- Mechanistic / Phenomenological Basis
- Parameter Estimation and Measurement
- Boundary Conditions (physical, chemical interfaces)
- Uncertainty Characterization

Basic Elements of the Performance Evaluation

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