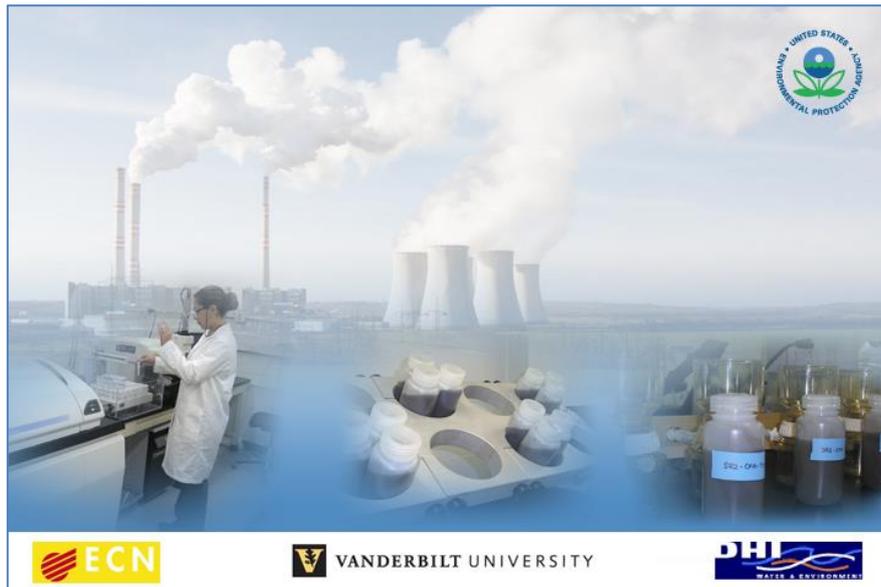


# LeachXS CBP Version 2.0

## User's Guide

User Guide (rev. 0)



### ***Authors***

*Paul Seignette*  
*Kevin G. Brown*  
*Andrew C. Garrabrants*  
*David S. Kosson*  
*Hans van der Sloot*

## Table of Contents

<b>Getting Started In LeachXS Pro</b> .....	<b>1</b>
Your license.....	1
License verification .....	1
Verification steps .....	1
Obtaining verification information .....	1
The Main Screen .....	2
Switching Databases in LeachXS .....	3
Getting Data In and Out of LeachXS.....	5
Naming Conventions in LeachXS.....	5
Global window layout .....	5
Application logo .....	6
Quick Access Toolbar .....	6
Ribbon menu with ribbon bar.....	7
Changed indicator .....	7
Current case .....	7
Database .....	7
<b>Analyze, Compare and Display Leaching Data</b> .....	<b>8</b>
Displaying the Results of Leaching Data .....	9
Selecting Data from the Database .....	10
Displaying Selected Data.....	12
Exporting Charts to Microsoft Excel®.....	15
Modifying Display and Export Figure Properties .....	18
Saving your work.....	18
Graph Appearances.....	19
More Options .....	20
General Options .....	20
Step 1 options .....	20
Step 2 options .....	21

Step 3 options .....	21
<b>Acid/Base Neutralization Capacity .....</b>	<b>23</b>
Compare Acid/Base Neutralization Capacities .....	23
Run the ANC/BNC Calculator .....	25
Calculate Acid/Base Additions .....	26
Calculate Acid/Base Additions .....	27
<b>Importing or Adding New Data.....</b>	<b>28</b>
Importing Data from a LEAF Template into a LeachXS Database .....	29
Filling a LEAF Template .....	32
<b>Classic LeachXS Modeling.....</b>	<b>33</b>
Chemical Speciation Modeling.....	33
pH Dependent Leaching Prediction .....	56
Tank Model .....	77
<b>Advanced Modeling .....</b>	<b>78</b>
Cementitious Barriers Modeling Scenarios .....	78
<b>The CBP Scenario Editor .....</b>	<b>81</b>
Scenario Editor components.....	81
Navigation pane .....	81
Components pane.....	82
Parameters pane.....	82
Ribbon bar and its elements .....	82
Application button .....	82
Organizing your work.....	83
Reporting and documenting .....	83
Navigation pane: Model Input .....	84
Navigation pane: Model Components .....	85
Navigation pane: Run.....	86
Navigation pane: Model Results .....	87
Editing your scenario .....	87
The Data Editor .....	88
The Refresh Scheme Editor.....	89

The Output Times Editor.....	90
The Model Files Editor .....	91
The Orchestra System Editor .....	92
The Species Mapping Editor.....	93
The Minerals Editor.....	95
The Species List Editor .....	97
Editing with a text editor .....	98
<b>LeachXS Cases and Case Management.....</b>	<b>100</b>
Saving a Case.....	100
Creating a New Map Store Folder.....	101
Create a Group within a Map Store .....	102
Creating a Case within a Group.....	102
Loading a Case from the Map Store.....	103
Exporting a Case.....	105
Importing a case.....	106
Using a Zip Store to Compress Files.....	107
<b>Statistical Evaluation of Data .....</b>	<b>111</b>
Statistical Calculations from the Analysis and Presentation Screen.....	111
Statistical Calculations from the Import or Add New Data Roll-up Menu.....	114
Step 1: Choosing source materials and merge options .....	116
Step 2: Interpolation .....	117
Step 3: Choosing statistical quantities .....	118
Exporting the results .....	120
<b>The Sample Selector .....</b>	<b>121</b>
Basic Operation.....	121
Manipulating the Sample List .....	122
Hiding or showing columns.....	123
More filtering .....	123
The Selected Samples panel .....	126
Saving and loading sample lists .....	126
Favorites list and often used samples.....	126

Revealing detailed sample information .....	127
<b>The Constituent Selector .....</b>	<b>128</b>
Basic Operation.....	128
Sorting, grouping and filtering constituents .....	129
Selecting by using Select by Typing.....	130
The Selected Constituents panel .....	130
Saving and loading constituent lists.....	130
Favorites list and often used constituents.....	131
<b>Graph Window .....</b>	<b>132</b>
Highlighting a series .....	132
Viewing coordinates .....	133
Translating, scaling and zooming a chart.....	133
Exporting results .....	133
General graph layouts.....	133
<b>Indicator Lines Editor .....</b>	<b>135</b>
Loading and saving indicator lines .....	136
Organizing and editing indicator lines .....	137
Sorting, grouping and filtering samples.....	138
Hiding or showing columns.....	139
Editing multiple lines.....	139
Starting from scratch .....	141
<b>The Material Line Scheme Editor .....</b>	<b>142</b>
Series Layouts Pane .....	143
Editing Layouts .....	143
Saving and Loading Layouts .....	143
<b>Directive selection dialog .....</b>	<b>144</b>
<b>Creating and Editing Lists .....</b>	<b>145</b>
Interpolation Grid Editor.....	145
Interpolation Grid Manager .....	146
List Generator .....	147
<b>Technical Topics.....</b>	<b>149</b>

File locations ..... 149

CSTR calculation ..... 150

Weights ..... 151

## Getting Started In LeachXS Pro

---

Welcome to LeachXS Pro. This manual helps you in using LeachXS. If you already have entered your license details and LeachXS has started successfully, go to “The Main Screen” on page 2. If you have trouble with your license read the section below.

### Your license

The welcome screen is displayed right after LeachXS is started and will remain visible until your license is validated. Normally, it displays the software version number and release date, and the name of the licensed user.

When started for the first time, LeachXS will prompt you to provide your license data you received along with your version of LeachXS. Supply the name of the licensed user or company and the accompanying license key. Be sure that your system has working Internet connection, because LeachXS will verify your license by querying a central license host.

Depending on the configuration of your firewall and the settings of the Internet options in the configuration panel of your system, LeachXS may ask you to supply the name of the proxy server and the proxy address. Usually, your system administrator will be able to supply this information.

### License verification

Because you have a license for a limited number of copies and a limited amount of time, LeachXS will try to verify your license every time you start it. However, this doesn't mean that you need to have an Internet connection available all the time. If you don't have an active connection when you start LeachXS, it will skip the verification stage if the last time a successful validation has been taken place is less than 15 days ago. Only if the last successful validation was more than 15 days ago and there is still no Internet connection available, LeachXS will refuse to continue.

### Verification steps

During the verification stage, LeachXS will check if your license is valid. Your license is valid if:

1. The number of installed copies of the license does not exceed the number of licenses you have.
2. The expiration date of your license has not been exceeded.

*Note that a single license will allow you to install LeachXS on at most two different systems.*

### Obtaining verification information

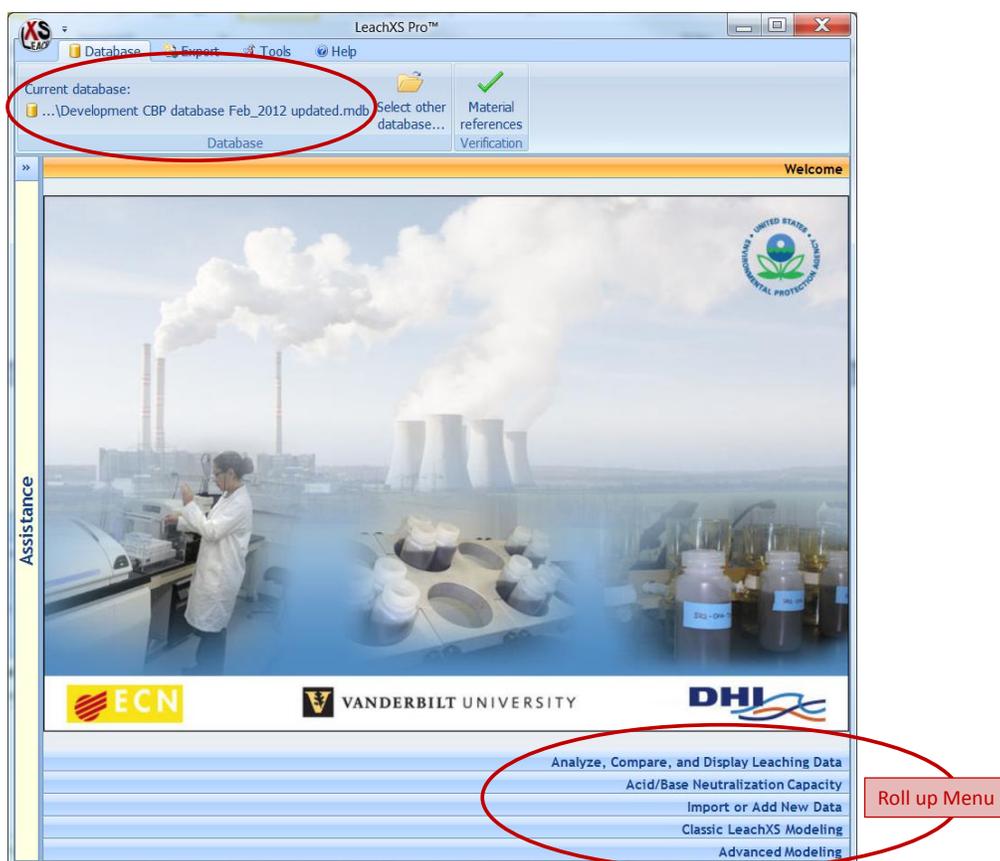
After the installation of LeachXS a separate entry is created in the LeachXS programs section in your start menu: **License Validation**. You can use this validation program to:

- Inspect details of the verification procedure. A popup window will appear with the requests to and answers from the central license host.
- Force validation. This is useful when you are about to use your computer for a while without having an Internet connection. After a successful validation procedure, it is guaranteed that you can use LeachXS for 15 days before a next validation procedure is mandatory.

*Note that this is the only way to guarantee a 15-day usage: the normal LeachXS program doesn't verify your license if the last verification has been less than 3 days ago, thus speeding up the startup process.*

## The Main Screen

The main screen (see screen capture below) is the entry point into LeachXS. This is the primary navigation screen that contains the roll-up menu for accessing the major operations in the software. The top menu bar contains tabs for database management, exporting data for reports, tools for changing the look and feel of data output and import “cases” from other LeachXS users. See the section “LeachXS Cases and Case Management” on page 100 in the guide for more details on cases.



In the screen capture above, note that the database tab is selected and the current database, **Development CBP database Sept\_2013**, is indicated in the upper left corner of the screen. This database is one of two default databases in LeachXS v2.0.0. An alternative default database is the **EPA CCRs dbase (USEPA CCR 12-2009.mdb)**.

The main screen roll-up menu comprises the primary navigation menu in LeachXS with the following possible selections:

**Welcome**

Returns the user to the main screen as shown above.

**Analyze, Compare and Display Leaching Data**

Used to compare leaching data between replicates of a single material or different materials.

**Acid/Base Neutralization Capacity**

Used to calculate acid/base titrations and project final pH based on the test data obtained from pH dependence testing.

**Import or Add New Data**

Used to import new material data (e.g., total contents, leaching test results) into an existing or user created database.

**Classic LeachXS Modeling**

Used to access chemical speciation and pH-dependent prediction modeling.

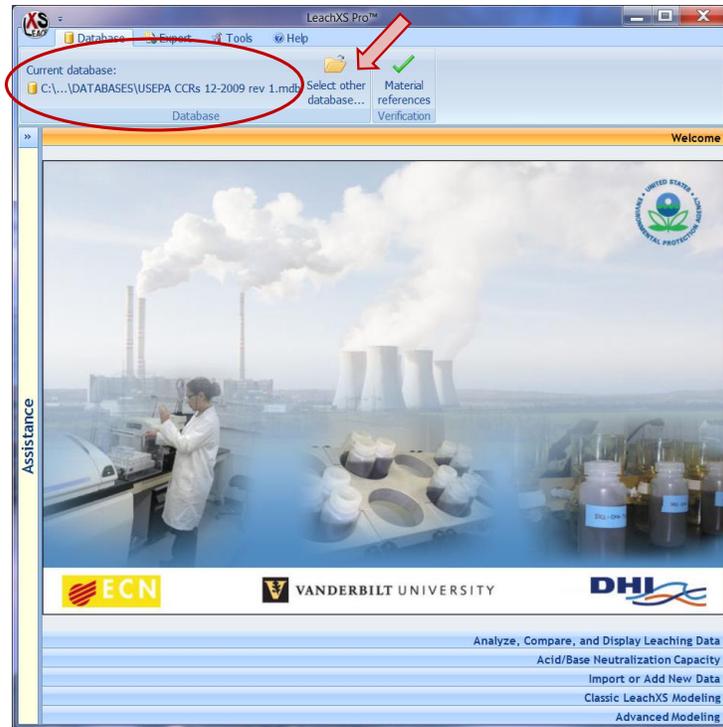
**Advanced Modeling**

Used to access more complex multi-phenomena models.

The majority of this guide will follow the main navigation roll-up menu for v2.0.0 of LeachXS Pro.

## Switching Databases in LeachXS

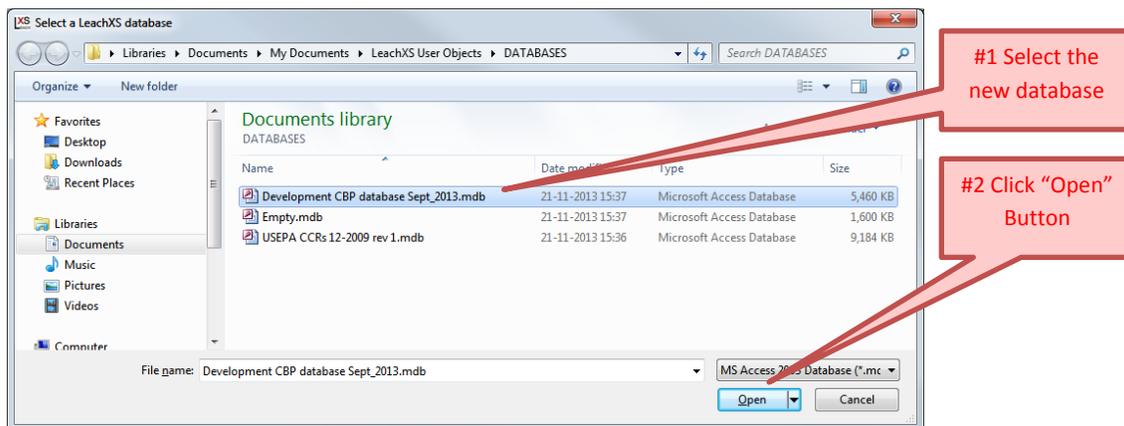
Switching databases in LeachXS can be accomplished only from the main screen by selecting the Database tab in the top menu bar. The current database is shown on the left side of the menu ribbon (e.g., see the red circle showing the **USEPA CCRs 12-2009 rev 1.mdb** database in this example). To switch to an alternative database (e.g., the **Development CBP database Sept\_2013**), click the **Select other database...** icon and navigate to the new database using the pop-up browser window.



The default LeachXS databases are stored in a DATABASES folder within the LeachXS User Object folder. User-created databases can be stored anywhere on the computer. The location of the default databases folder on the computer is:

*My Documents\LeachXS User Objects\DATABASES*

The graphical example below shows the procedure for selection of the **Development CBP database Sept\_2013** database. From the pop-up browser window, the target database is highlighted by clicking on the name of the database in the proper folder and opened by clicking the **Open** button at the bottom of the browser window.



This action will make **Development CBP database Sept\_2013** the current database in LeachXS.

LeachXS maintains a history of databases you use. You can select a previously used database by clicking on the top left LeachXS logo.

*Note that a list of objects that are previously used appears in many dialogs of LeachXS.*

## **Getting Data In and Out of LeachXS**

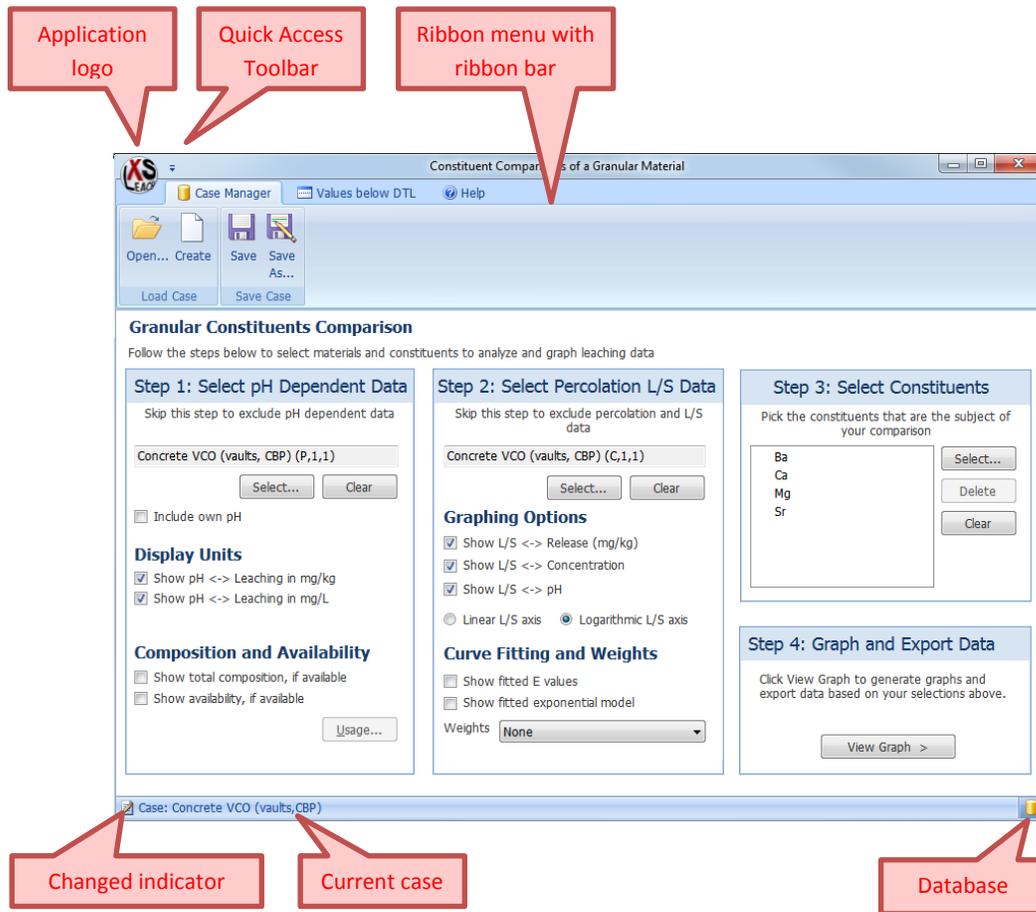
The default databases in LeachXS contain leaching test and material property data collected from a broad range of studies and projects. The user can compare their own data to selected data within these default databases by importing their data into the database. Microsoft Excel® workbooks used as the basis for uploading data into LeachXS are provided in the form of Microsoft Excel® templates for each of the leaching tests in the Leaching Environmental Assessment Framework (e.g., EPA Methods 1313 through 1316). Comparison graphs and numerical data prepared in LeachXS may be exported to Microsoft Excel® workbooks. In addition, LeachXS Pro has the capability to allow users to share “cases” with another user.

### **Naming Conventions in LeachXS**

The material name is specified in the Microsoft Excel® data template prior to loading data into LeachXS. When loaded into the software, a parenthetic extension is added to each test replicate indicating the type of data, the material replicate, and the test replicate. Replicate tests are stored as separate “materials” within the database distinguished by the test replicate identifier in the extension. The extension includes a letter (i.e., “P” for pH-dependent data, “C” for percolation column data, “B” for batch L/S dependent data, and “M” for mass transport data) followed by two numbers. The first number indicates the replication of the solid material sampling (e.g., “1” for the 1<sup>st</sup> sampling, etc.) while the second number indicates the replication of the test method (e.g., “2” for the 2<sup>nd</sup> test replicate, etc.).

### **Global window layout**

Many editors and windows in LeachXS have a common layout.



## Application logo

If you click on the **Application logo**, a small window will pop up with two panes. The left pane contains functions for copying the window or the entire screen to the clipboard or printer and for closing the window. The right pane contains the most recently used cases (see “LeachXS Cases and Case Management” on page 100 for an explanation of what a case is). If you click on a case it will be opened in the editor or window.

## Quick Access Toolbar

The **Quick Access Toolbar** is expanded if you click on it. It contains the same functions as the left pane of the **Application logo**. In addition, there are functions to manipulate the position and behavior of the ribbon bar. Many editors have two small icons to save or cancel edit operations:



Pressing the green icon will save your changes and close the editor. The red icon cancels all edit operations before closing.

*Note that you can add your own buttons to this toolbar: right-click any button on the ribbon bar and select **Add to Quick Access Toolbar**.*

### **Ribbon menu with ribbon bar**

The ribbon menu contains most functions that are available in a window or editor. Related functions are grouped together in ribbon tabs and within a tab, organized in tab groups. Many editors have a tab **Case Manager** for saving cases and loading previously saved ones.

### **Changed indicator**

This small icon shows up if you have made any changes in the data that is presented.

### **Current case**

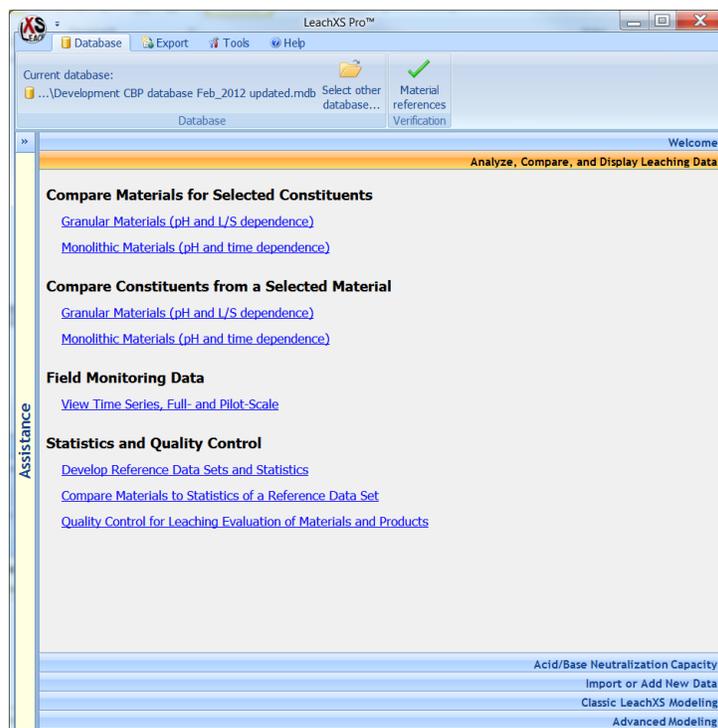
This part of the window displays the current case you are working on.

### **Database**

If you keep your mouse steady on this icon, a small window pops up with information on the database that is currently selected in LeachXS.

## Analyze, Compare and Display Leaching Data

Data visualization, comparison and reporting are conducted by selecting **Analyze, Compare and Display Leaching Data**. The following menu screen results:



The **Analyze, Compare, and Display Leaching Data** menu screen provides options for:

### Compare Materials for Selected Constituents

View and analyze the results of leaching tests for a single constituent for one or more materials or material replicates. Links provide access to **Analysis and Presentation** windows for **Granular Materials** and **Monolithic Materials**.

### Compare Constituents from a Selected Material

View and analyze the results of leaching tests for multiple constituents in a single material or material replicate. Links provide access to **Analysis and Presentation** windows for **Granular Materials** and **Monolithic Materials**.

### Field Monitoring Data

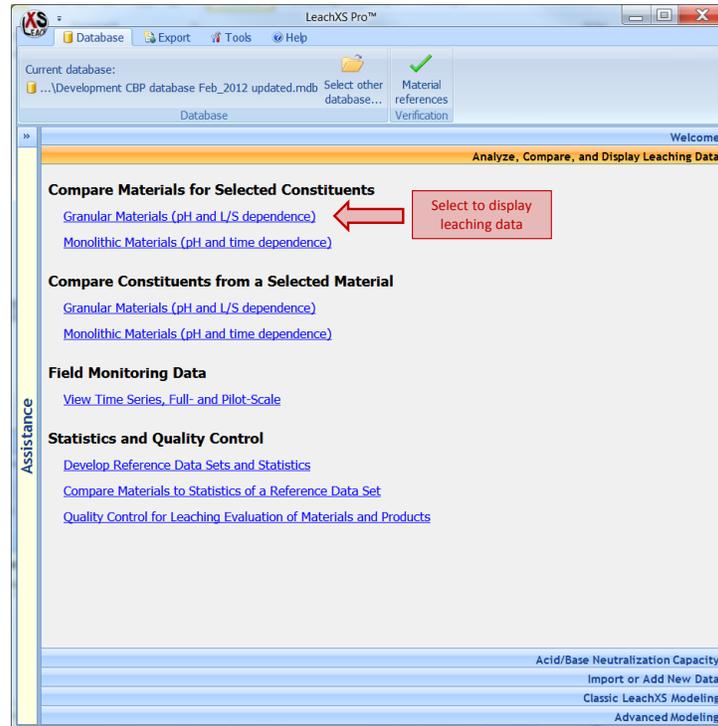
Compare field data as time series or scale-up series from field measurements.  
***This section is not described in this version of the guide.***

### Statistics and Quality Control

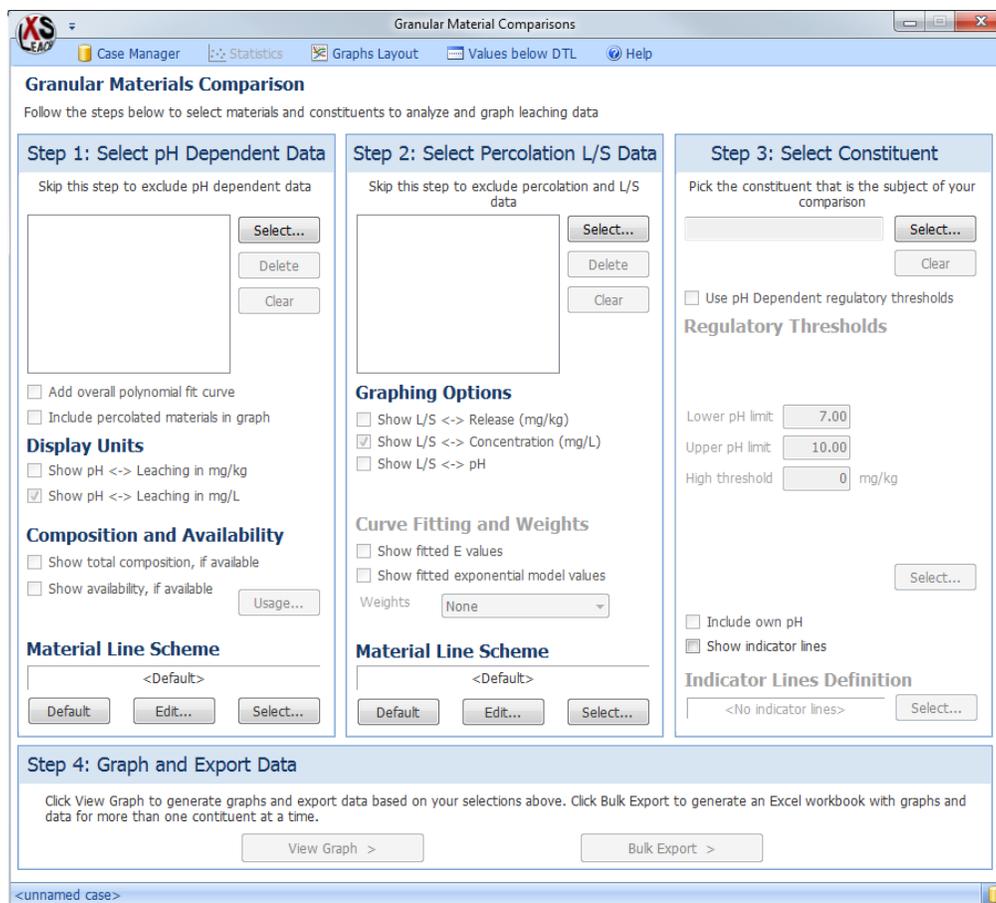
Analysis of material sets relative to statistical representations and quality control objectives.  
***This section is not described in this version of the guide.***

## Displaying the Results of Leaching Data

The operation for comparing leaching test results is similar for both granular and monolithic materials. Therefore, the procedure for displaying leaching data will be shown through an example of comparing results for granular materials. To compare leaching test results for one or more granular materials, select **Granular Materials (pH and L/S dependence)** link under the **Compare Materials for Selected Constituents** title.



The following **Granular Materials Comparison** window is displayed.

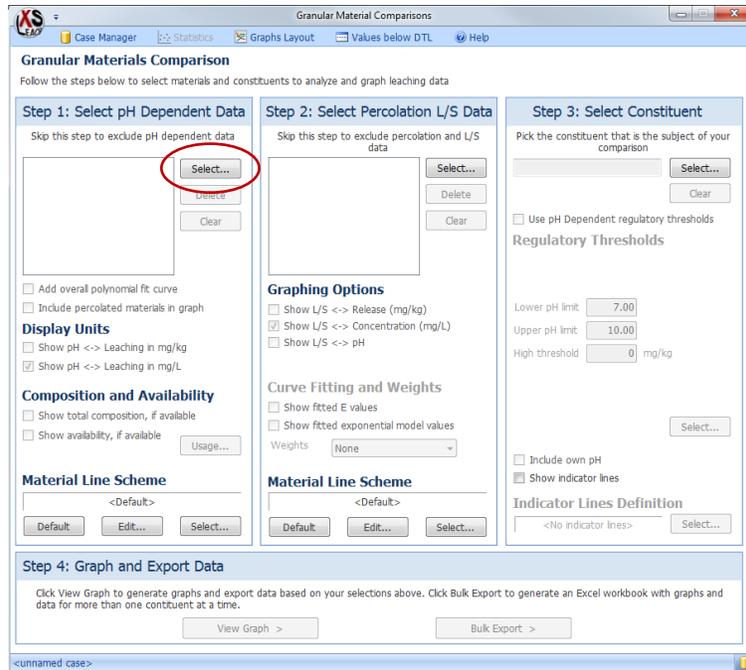


The **Analysis and Presentation** window is divided into four zones with stepwise guidance for each zone. The process for displaying data includes:

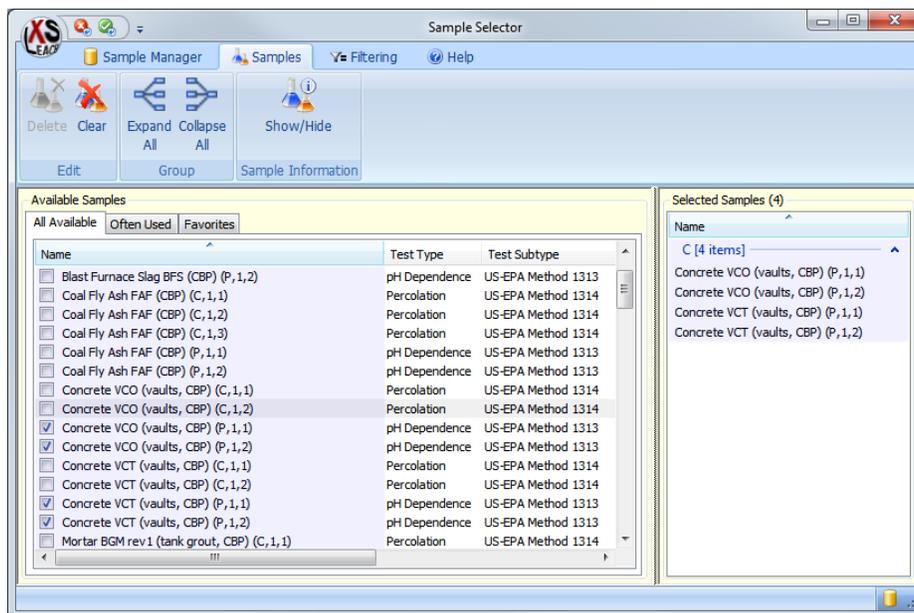
- Step 1** Select data to be displayed as a function of pH and options for displaying the data (if comparison of pH-dependence is not desired, this step may be skipped)
- Step 2** Select data to be displayed as a function of L/S and options for displaying the data (if comparison of L/S dependent data is not desired, this step may be skipped)
- Step 3** Select a constituent to be compared (mandatory)
- Step 4** View or Export the selected data.

## Selecting Data from the Database

The example below will illustrate the process of selecting datasets from the current database for comparison, although the process is the similar for selecting percolation or L/S data. Begin the process of selecting pH dependent data by clicking on the **Select...** button in the **Step 1** zone of the **Granular Materials Comparison** window.



The **Sample Selector** will show up:



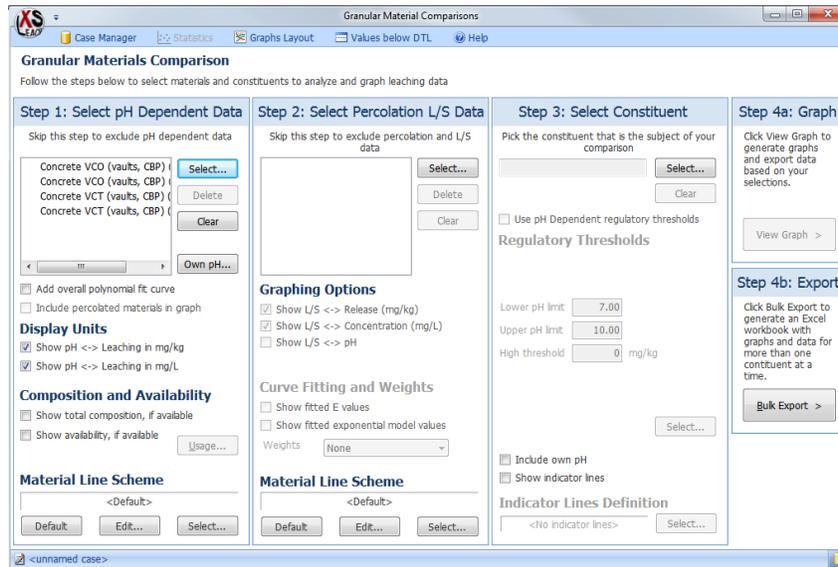
For a complete description of the **Sample Selector**, see chapter “The Sample Selector” on page 121.

Select the same samples as shown in the screenshot above:

- Cement VCO (vaults, CBP) (P, 1, 1)
- Cement VCO (vaults, CBP) (P, 1, 2)
- Cement VCT (vaults, CBP) (P, 1, 1)
- Cement VCT (vaults, CBP) (P, 1, 2)

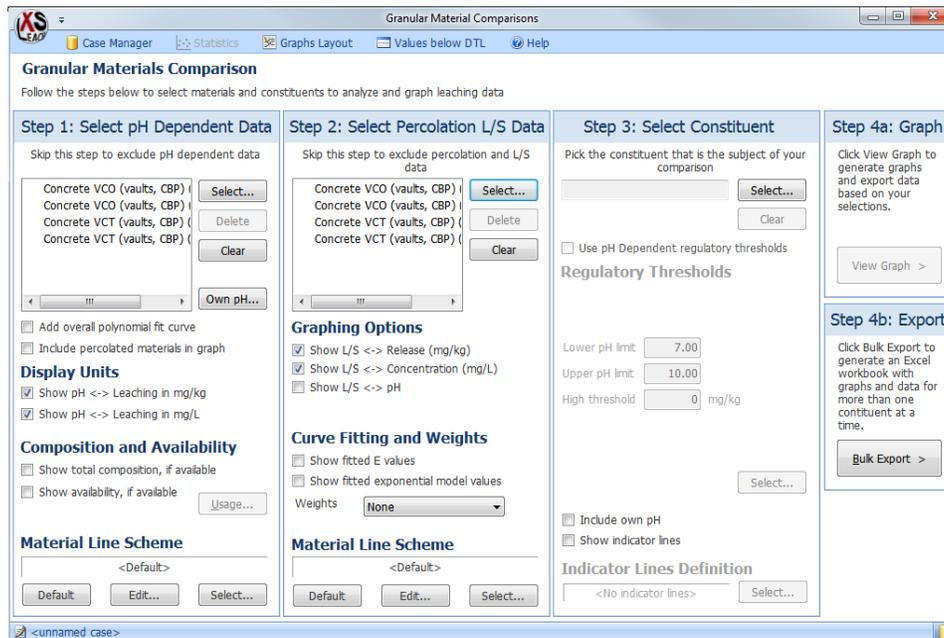
Be sure to select the pH Dependence tests of these materials.

Leave the Sample Selector by pressing the small green button in the top left corner. The samples will show up in the **pH dependent Data** list in the **Comparison Window**.



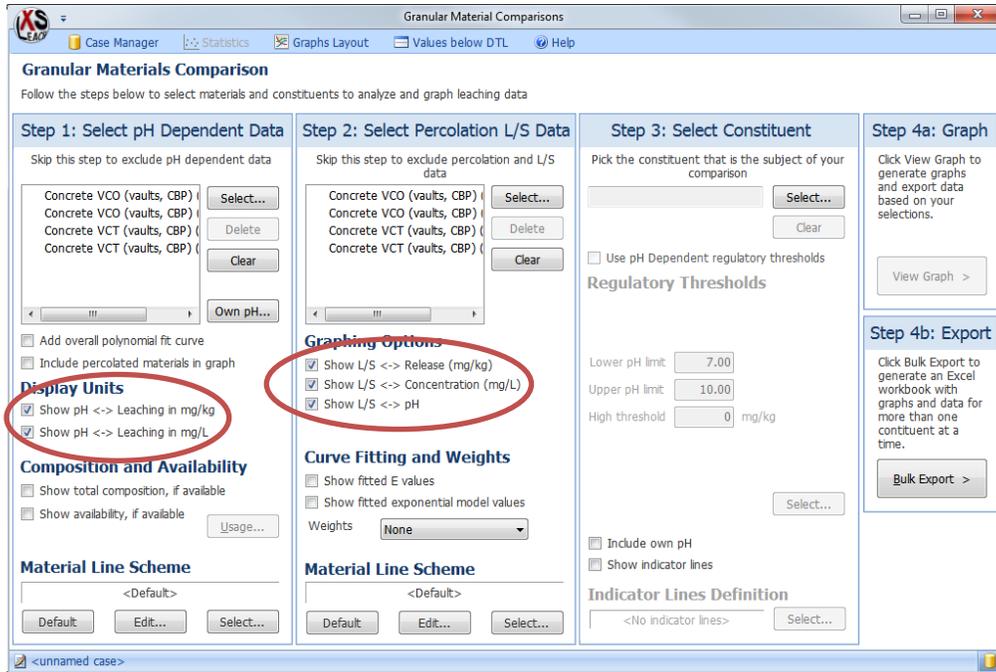
## Displaying Selected Data

After selecting the data sets for comparison, the **Granular Materials Comparison** screen will show the data sets in the appropriate windows. The example below includes selected data for both pH dependent and percolation column data (selected through a similar series of steps initiated by clicking on the **Select...** button in the **Step 2** zone).

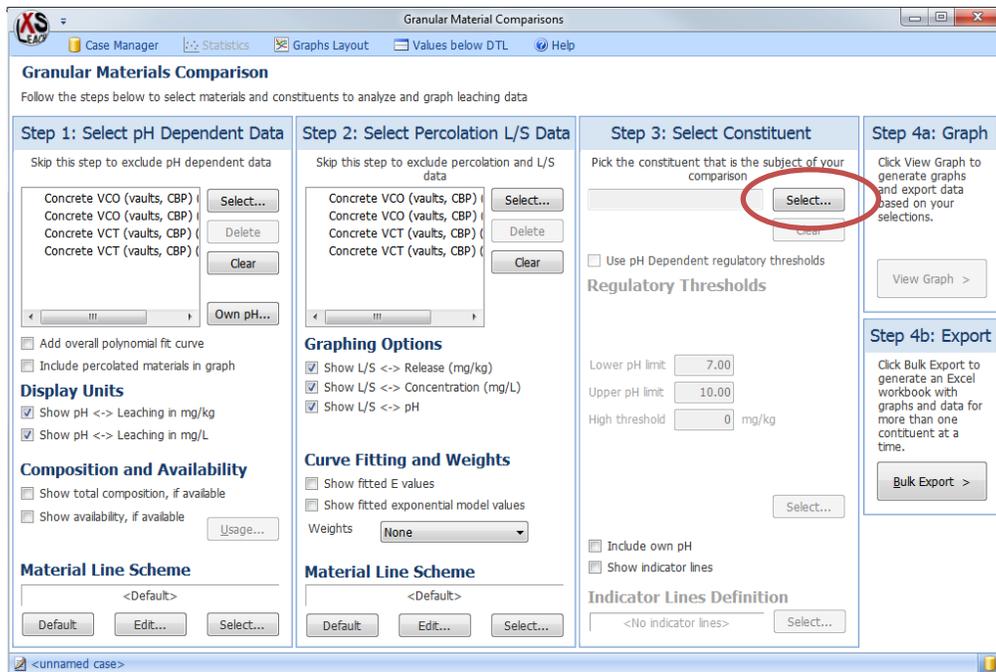


If desired, modify the graphs to be displayed by marking the check boxes on the **Display Units** under **Step 1** and the **Graphing Options** under **Step 2**. Multiple graphs may be shown at one time. Data plotted

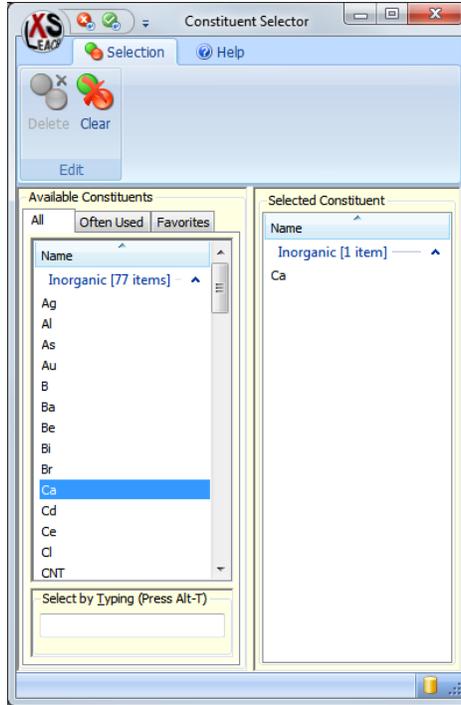
as a function of pH may be displayed as concentration in units of mg/L or as mass release in units of mg/kg. For L/S dependent data, the eluate pH, concentration, or release may be plotted as a function of L/S.



In the **Step 3: Select Constituent** zone, select a constituent to display by clicking on the **Select** button.



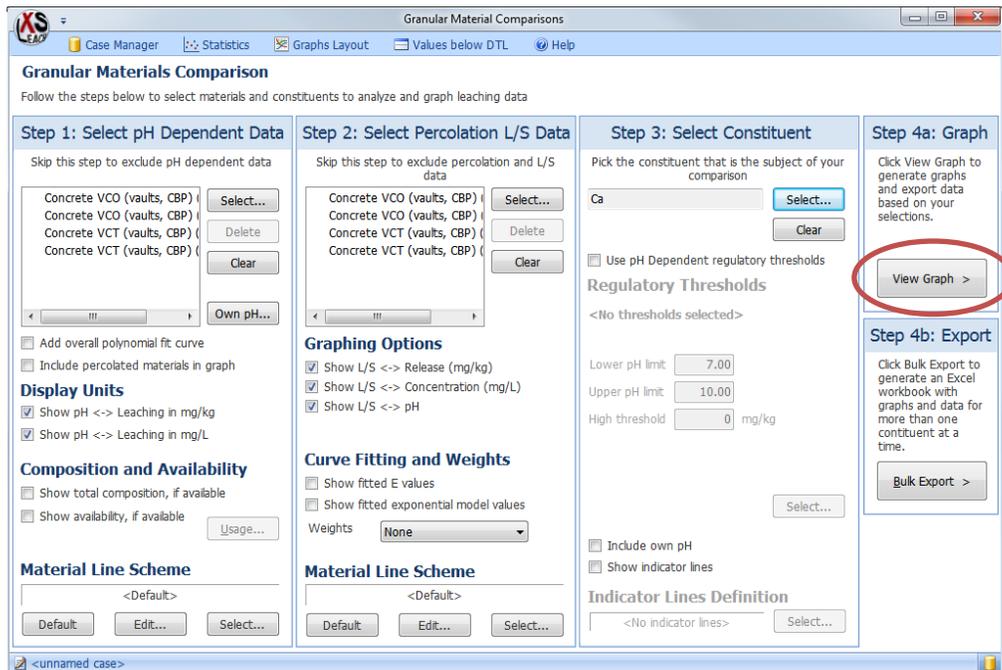
The **Constituent Selector** will show up to assist you in selecting a constituent.



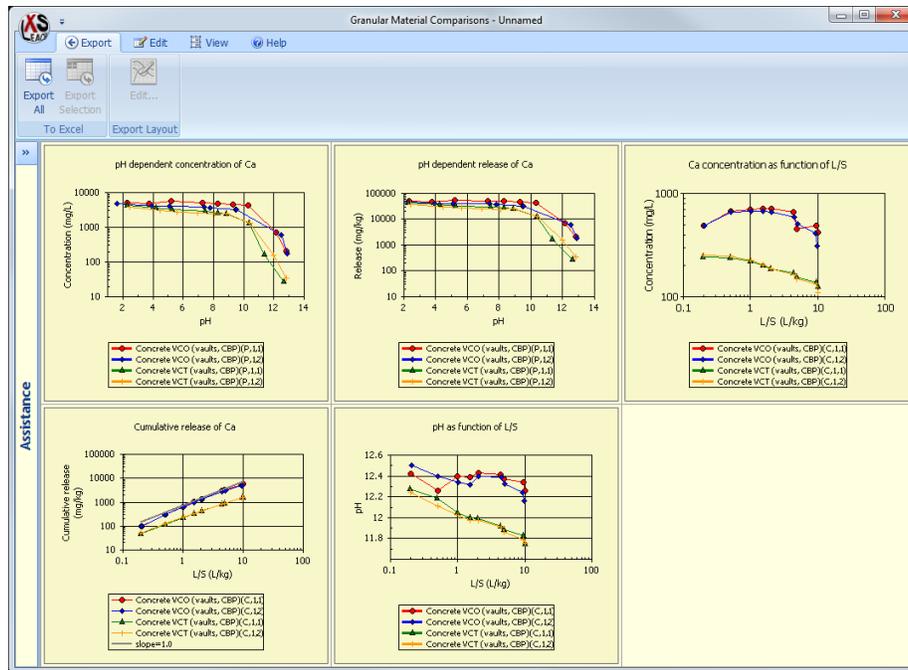
For a complete description of the **Constituent Selector**, see chapter “The Constituent Selector” on page 128.

Select constituent **Ca** as in the example and hit the small green button in the top left corner.

The last step before displaying data is to click the **View Graph** button as indicated below.



The following is an example display of selected data:

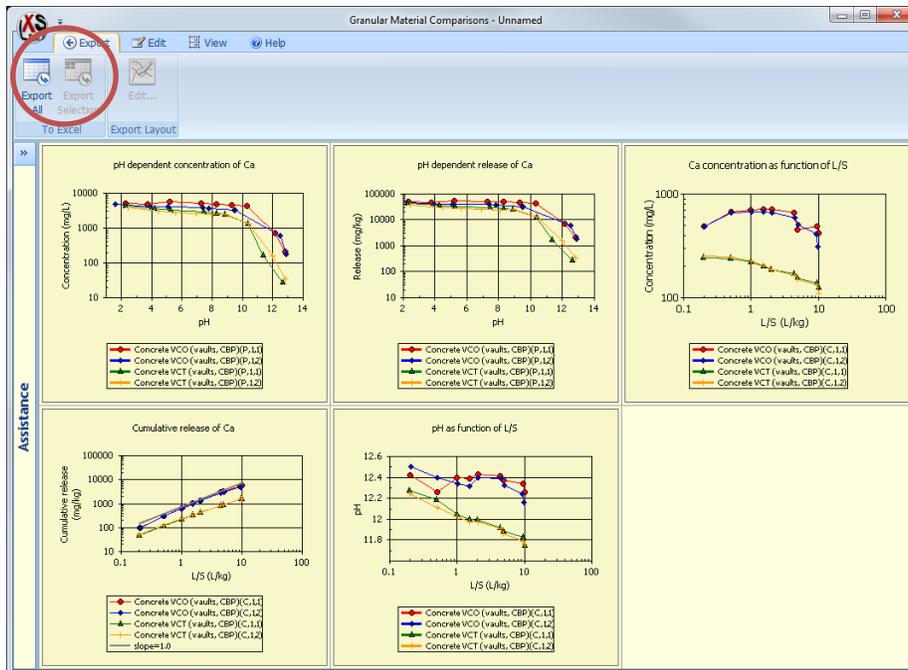


This graph window is detached from the **Granular Materials Comparison** window. This means that you can make another comparison, show its graphs and compare that window with the one above.

In order to edit the way that LeachXS formats the graphs displayed when the **View Graph** button is selected, the graph format for each type of figure can be modified using the **Graphs Layout** function on the top ribbon bar.

## Exporting Charts to Microsoft Excel®

When the charts displayed by the View Charts button have been edited as desired, the charts and associated data shown may be export to Microsoft Excel® from the **View Graph** screen using the menu ribbon under the **Export** tab on the top menu bar highlighted in the example below.

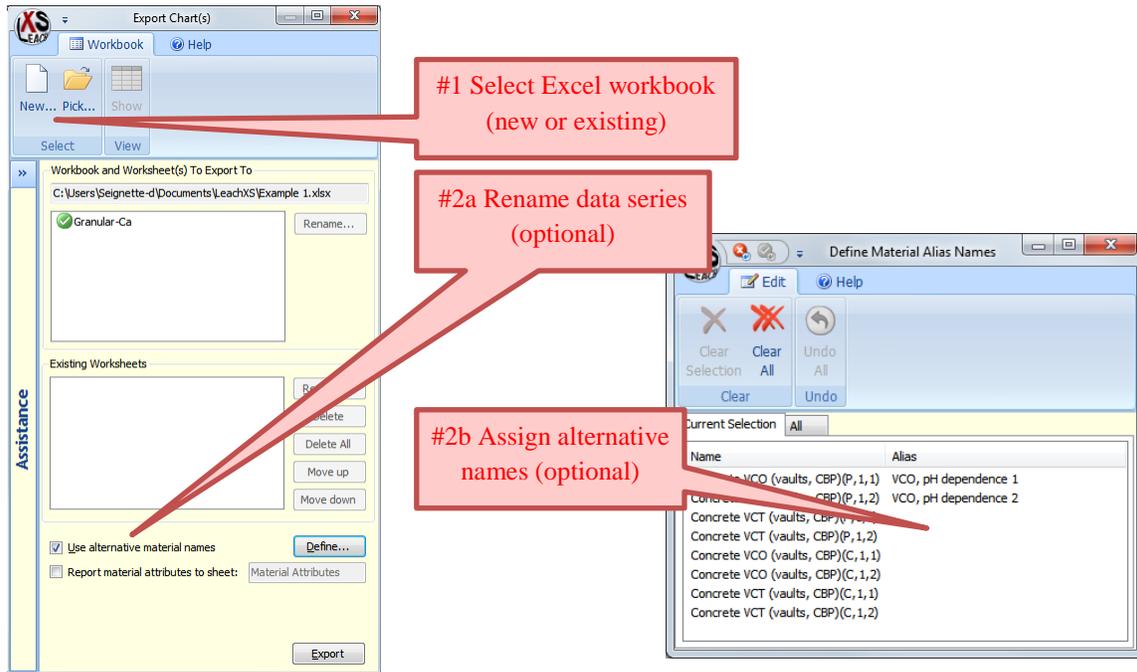


To export an individual pane in the output window, click within the white area to highlight it and then select **Export Selection**. To export the all charts, select **Export All**. Follow the instructions on the resultant **Export Charts** screen shown below.

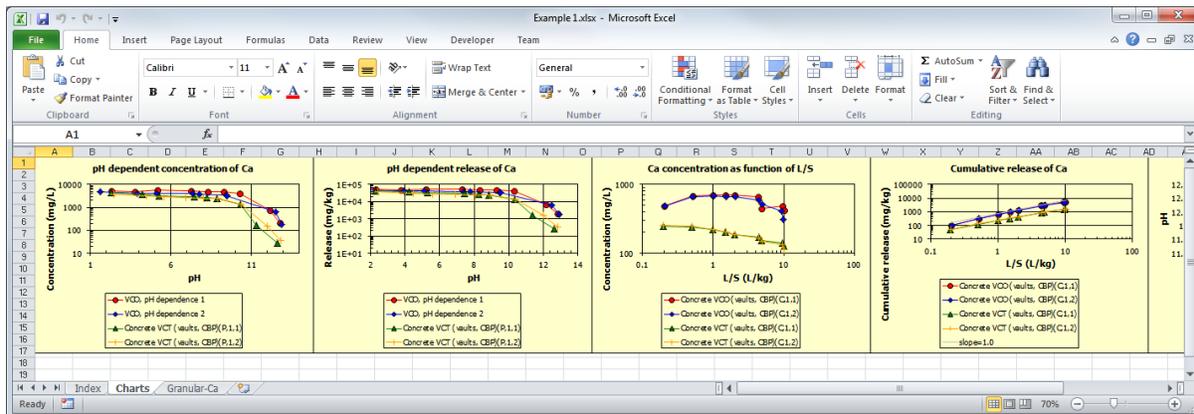


Output data may be written to a new Microsoft Excel® workbook for the output by clicking on the **New** icon and designating a filename and location. Alternatively, output data can be overwritten to an existing Microsoft Excel® workbook by clicking on the **Pick** icon and navigating to an existing workbook. An available option is the ability to rename the samples as they will appear in the Microsoft Excel® sheet by marking the check box next to **Use alternative material names** and designating new names for the data sets in the pop-up window (see example below). Sample properties for the output materials can be included in a separate worksheet in the output workbook by checking **Report material attributes** (not

checked in the example). When all desired options, click on the **Export** button to generate the output Microsoft Excel® file.



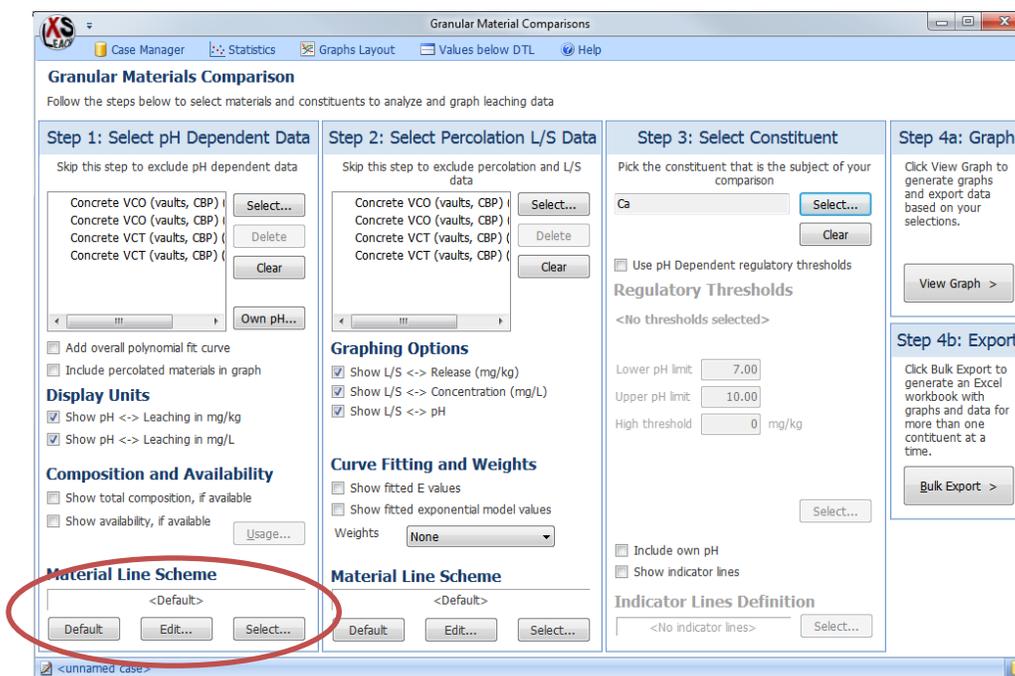
Depending on the amount of information for output, generating an output Excel file may take several minutes. A green progress bar will be shown to the left of the **Export** button. When the export is complete, click the **Show** button on the **View** group of the **Workbook** tab on the ribbon menu to open the resulting Microsoft Excel® workbook.



Data for multiple constituents may be exported to Microsoft Excel® using the **Bulk Export** button in the **Granular Materials Comparison** window in a similar manner.

## Modifying Display and Export Figure Properties

The layout of data series displayed in LeachXS or imported from LeachXS can be modified using the **Material Line Scheme** menu on the **Granular Materials Comparison** screen. The example illustrates formatting for pH dependent data; however the same process can be used to format percolation or L/S dependent data from this screen as well as monolithic data from the **Monolithic Materials Comparison** screen.



The following buttons are available from the **Material Line Scheme** menu:

- Default** Returns all display settings to their initial condition.
- Edit...** Allows for editing of established line settings.
- Select...** Allows for definition of line schemes for each data series.

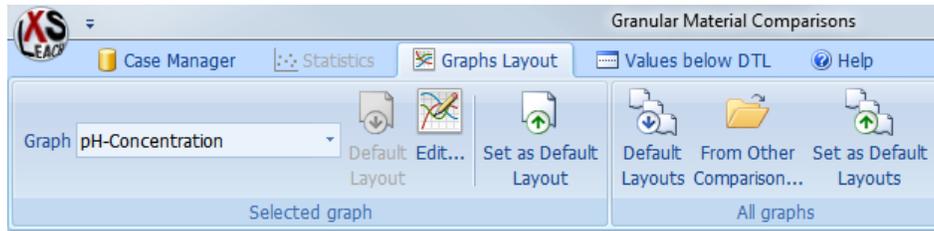
The **Material Line Scheme Editor** is displayed after clicking on the **Select...** button from the **Material Line Scheme** pane. For a complete description, see “The Material Line Scheme Editor” on page 142.

## Saving your work

You can save your selections, along with all other options you have set in a file and open or reuse it later. Such a file is called a **Case**. All case management functions can be accessed from the **Case Manager** tab on the ribbon bar. For more information about cases and the **Case Manager**, see “LeachXS Cases and Case Management” on page 100.

## Graph Appearances

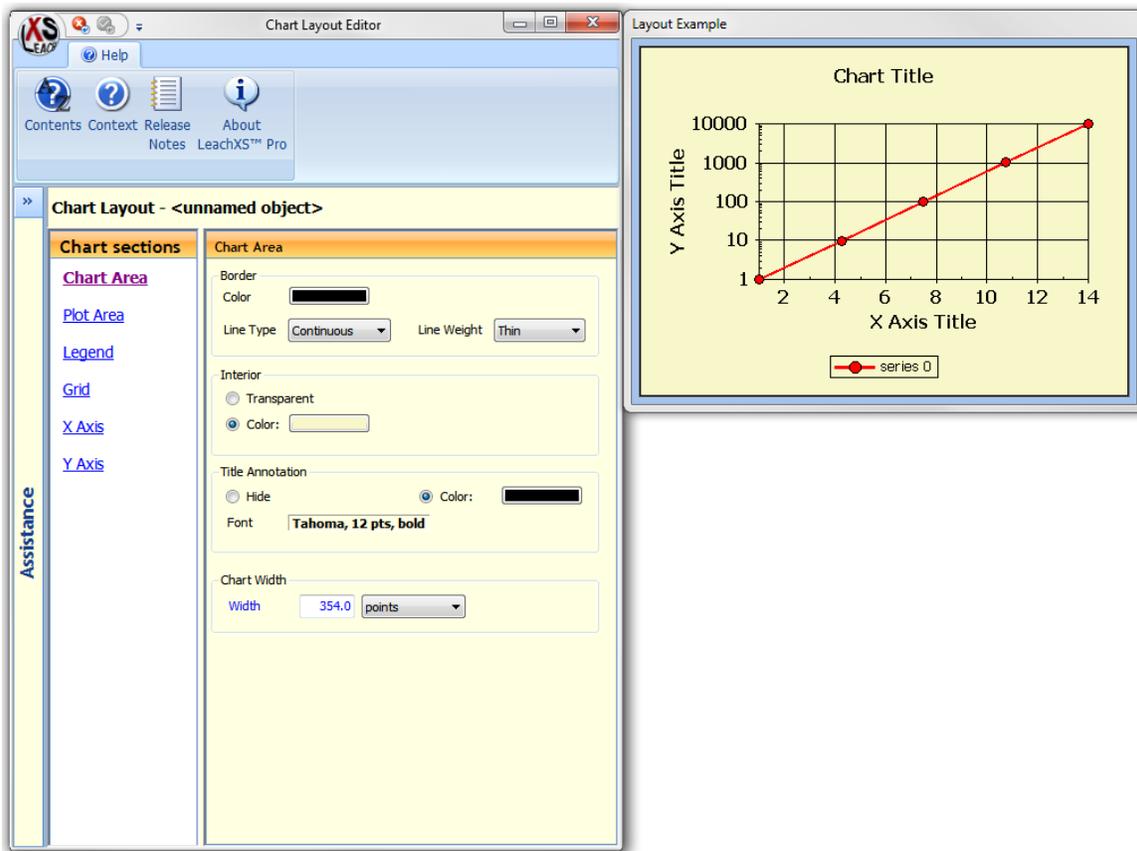
The **Graphs Layout** tab contains options to control how chart elements will appear. You can control the layout of every type of graph, save layouts for later use and change default settings for every graph type.



The left side of the tab page shows a box containing the type of graph to edit. Click on the down-pointing arrow to select the type whose layout you want to change.

Next to it there is the **Default Layout** button. Pressing this button will reset the current layout to the layout that is shipped with the installation setup of LeachXS.

Then there is the **Edit...** button. The following windows will appear:



The left pane of this window contains chart elements. Clicking on a chart element will show options to control the appearance of the element in the pane right to it. Next to the **Chart Layout Editor** you see an example of how the chart will look like, given the option values in the editor.

The rectangles to the right of a **Color** option are buttons. You can change a color by clicking on the rectangle. The fields to the right of a **Font** label are also buttons. You can change a font by clicking on the label.

Other options on the **Graphs Layout** tab are:

<b>Set as Default Layout</b>	Set the graph layout of the selected graph as default layout for new cases.
<b>Default Layouts From Other Comparison...</b>	Set layouts for all selectable graphs to their default layouts. Set all layouts of the graphs of the current case to the layouts of another case. The <b>Case Manager</b> will show up to help you selecting a case.
<b>Set as Default Layouts</b>	Make the graph layouts of all graphs in the current case the default layout for new cases.

## More Options

There are quite some options to enhance the graphs and reports with extra data or to control how they will look like.

### General Options

Some options are located in the ribbon bar. These options are described here.

The **Values below DTL** tab contains a list of options how to show values below the detection limit are treated in reports and graphs:

- **Use detection limit** will report and display concentration values below the detection limit as the detection limit value.
- **Use half of the detection limit** will report and display concentration values below the detection limit as half of the detection limit value.
- **Use the concentration** will report and display concentrations values below the detection limit not different from other concentration values: the concentration value as stored in the sample database is shown.

### Step 1 options

These options apply to the presentation of pH dependent data.

<b>Add overall polynomial fit curve</b>	A least-squares polynomial is drawn through the data points.
<b>Include percolated materials in graph</b>	If you have selected any samples in step 2 (percolation L/S data), the concentrations or

emissions of these samples are included in the pH dependence graphs.

**Show total composition, if available**

If this option is checked, total composition values are included in the pH dependence graphs. You can check if the selected samples have composition data in your database by pressing the **Usage...** button.

**Show availability, if available**

If this option is checked, availability values are included in the pH dependence graphs. You can check if the selected samples have availability data in your database by pressing the **Usage...** button.

## Step 2 options

These options apply to the presentation of percolation L/S data. You can add curves to concentrations and cumulative releases.

The **Show fitted E values** option uses the following formula:

$$E_{L/S} = \frac{C_0(1 - e^{-\kappa(L/S)})}{\kappa} \quad \text{where } L/S \text{ is in L/kg and } E_{L/S} \text{ in mg/kg.}$$

The **Show fitted exponential model values** option uses a simple CSTR model that fits the percolation data using a least squares fitting routine. The calculated concentrations are given at the sampled L/S data points. The coefficients are passed on to the Excel worksheet upon saving the data. See "File locations" on page 149 for details about how the values are obtained and for the meaning of the **Weights** that can be used.

## Step 3 options

### **Use pH Dependent regulatory thresholds**

Comparison with regulatory criteria is an important issue in relation to leaching test data. Different directives are available, which can be used for judgment of test results. The units are mg/kg. The list of directives will be expanded in the future. Besides choosing from a list of predefined directives, you can create your own directives. Check this box if you want to use and display directive criteria in your graphs.

The **Select** button will enable you to choose an appropriate directive. See "Directive selection dialog" on page 144 for details. Fill the **Lower pH limit** and the **Upper pH limit** text boxes for the appropriate pH range of the directive.

If you have chosen multiple pH dependent materials, the concentrations for the constituent may not have the same detection limit for every material. In the **Low threshold** list you can select how the lower boundary of the directive criterion is to be calculated: as minimum, maximum or average of all detection limits found.

### ***Include own pH***

If own pH (aka natural pH) values of the materials you selected are known or can be calculated from ANC/BNC data, you can check this option to make them visible in the graphs. They will appear as an asterisk in series. You can control what series will be accompanied by their own pH value. Press button **Own pH...** in the **Step 1** pane. A small dialog will pop up. Use the check buttons in front of the samples to mark which samples will have an own pH value displayed.

*Note that if the asterisk is not lying on a measured data point of the series, the own pH value is calculated. The concentration at that point only is only indicative.*

### ***Show indicator lines***

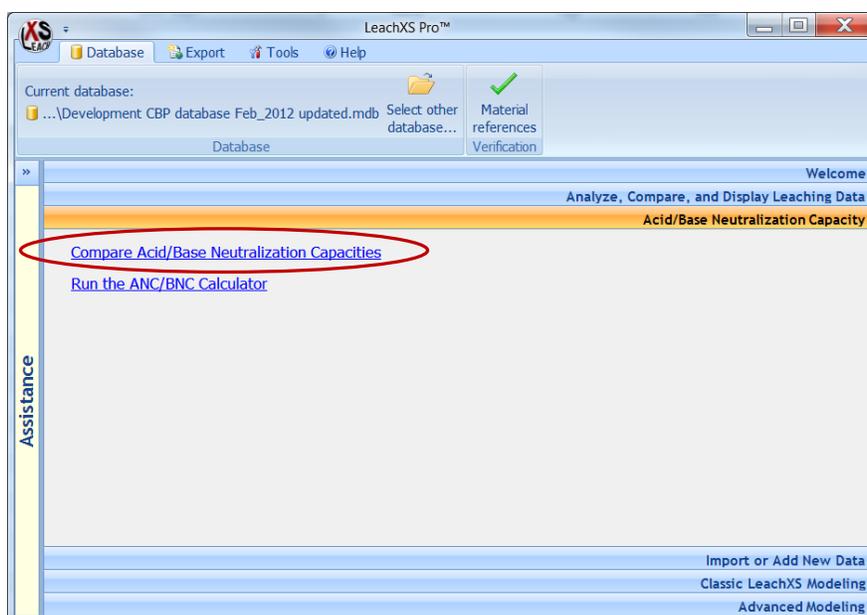
If you want to display extra guidance lines in your graphs indicating pH or concentration thresholds, you can check this option. For an explanation of indicator lines and how you can define them, see section "Indicator Lines Editor" on page 135.

## Acid/Base Neutralization Capacity

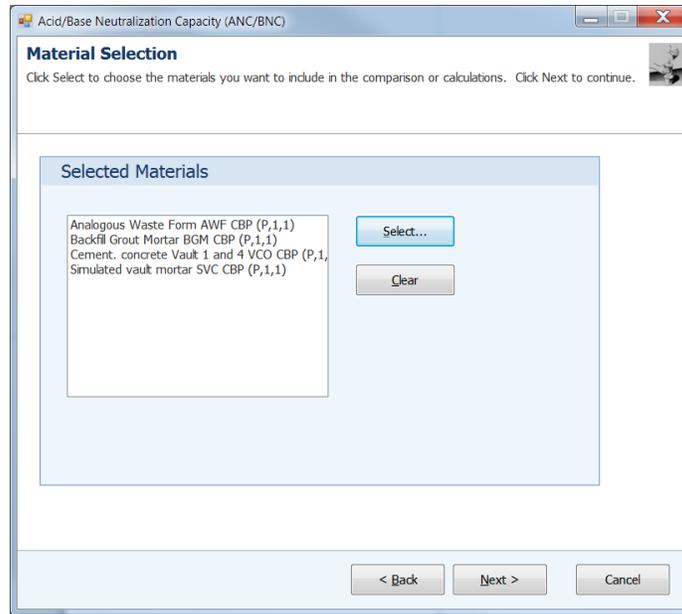
Clicking on the Acid/Base Neutralization Capacity roll-up menu item will result in the two menu options for (i) comparing the titration curve (i.e., the measured pH as a function of acid or base addition) and (ii) running the acid neutralization capacity (ANC) and base neutralization capacity (BNC) calculator.

### Compare Acid/Base Neutralization Capacities

The acid/base titration curves for one or more materials may be viewed and exported using the **Compare Acid/Base Neutralization Capacities** link in the **Acid/Base Neutralization Capacity** roll-up menu.

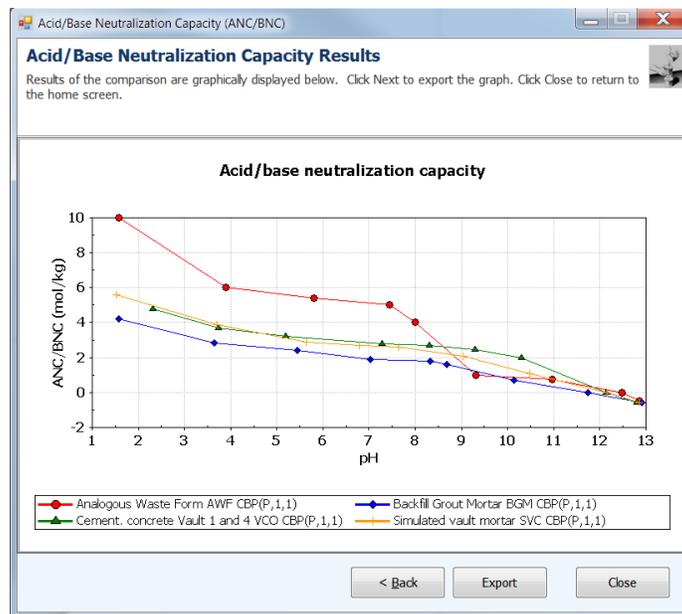


Materials to be compared may be selected using the screen below. Clicking on the **Select** button will activate the **Select Samples** window (see "The Sample Selector" on page 121 for using the **Select Samples** window).

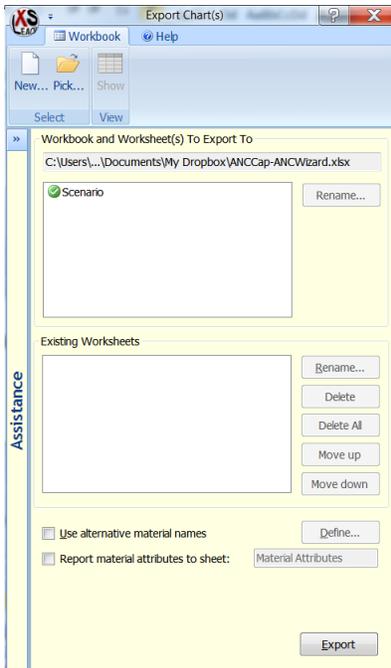


*Note that LeachXS considers test replicates of the same solid sample to be different materials distinguished by the parenthetic extension added to each data series (see "Naming Conventions in LeachXS" on page 5 for more information).*

When the material selection is complete, click the **Next** button to display the titration curves for the selected materials.

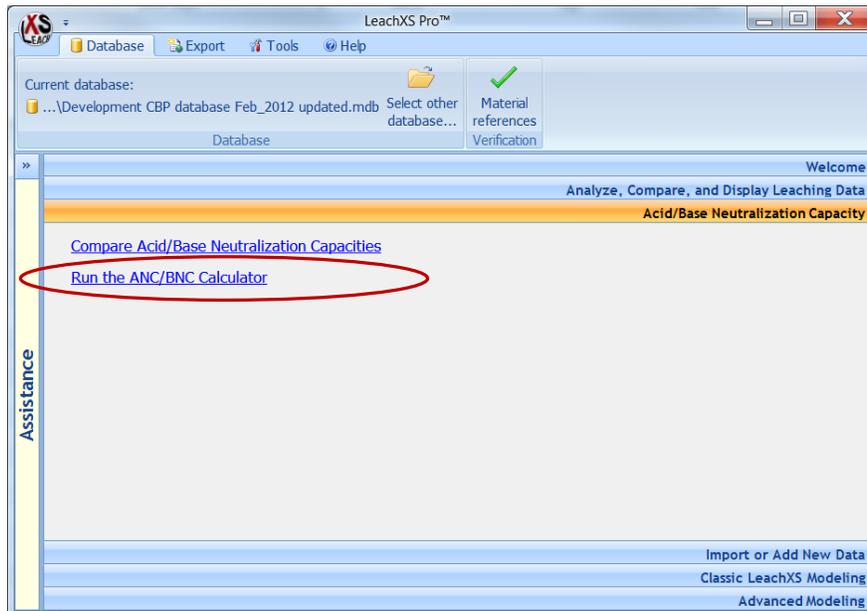


The titration curve data may be exported to an Excel workbook by clicking on the **Export** button in the **Acid/Base Neutralization Capacity Results** screen to activate the **Export Charts** window (see "Exporting Charts to Microsoft Excel®" on page 15 for more information on the **Export Charts** window).

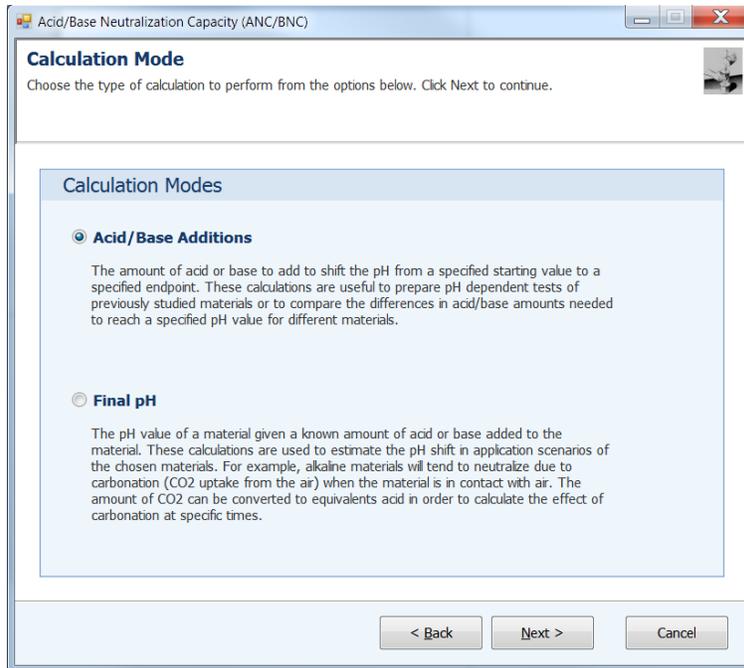


## Run the ANC/BNC Calculator

The **ANC/BNC Calculator** uses the titration curve information to predict either (i) the final pH of a material given a starting pH and an addition of acid or base or (ii) the amount of acid or base required to change the pH of a material between to pH values. The **ANC/BNC Calculator** may be accessed from the **Acid/Base Neutralization Capacity** roll-up menu.

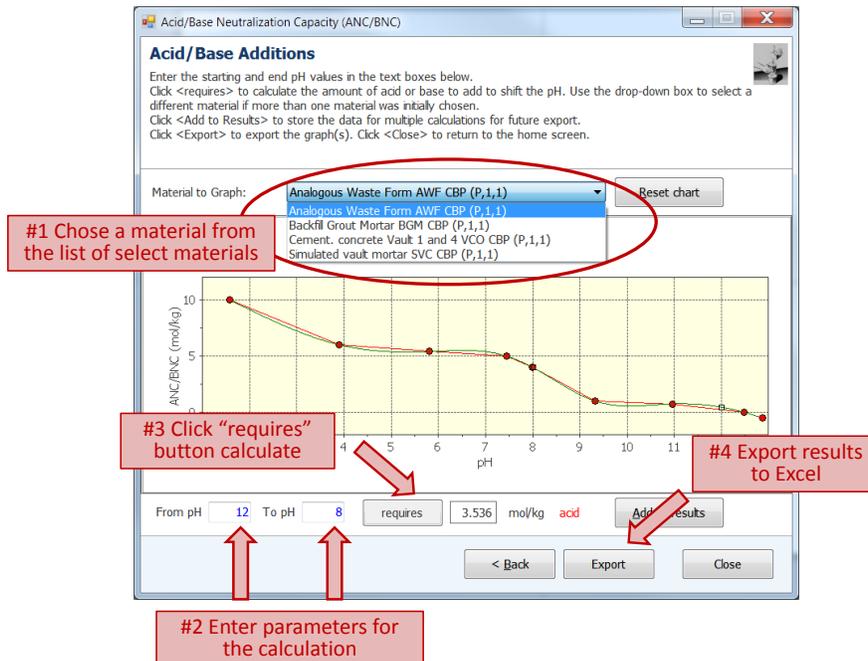


Select one of the two calculation modes for the **ANC/BNC Calculator** by clicking on the appropriate radio button. Explanations for the operator of these modes are provided.



### Calculate Acid/Base Additions

If the **Acid/Base Additions Mode** is chosen, the following window will be displayed. The calculator works on a single material at a time, so the user will need to choose a material for analysis using the drop-down menu of materials selected in the **Materials Selection** window. For a selected material, the user enters the starting and ending pH values and clicks the **requires** button to calculate the amount of acid or base needed to change the pH of the material.



The resulting titration curve and the numerical data for this calculator may be exported to a Microsoft Excel® workbook using the **Export Charts** window accessed by clicking the **Export** button.

### Calculate Acid/Base Additions

If the **Final pH Mode** is chosen, the following window will be displayed. The calculator works on a single material at a time, so the user will need to choose a material for analysis using the drop-down menu of materials selected in the **Materials Selection** window. For a selected material, the user enters an amount of acid or base to be added to the material and clicks the **yields** button to calculate the final pH of the material.

*Note: The **ANC/BNC Calculator** starts at the natural pH of the material; therefore, the amount of acid required to change the pH between two points that are not the natural pH can be determined by the difference of two calculator trials. For example, if the amount of acid required to change the pH from 8 to 6 is desired for a material with a natural pH of 12, the amount would be the difference in the amounts of acid required in two trials – one pH 12 to 6 and one pH 12 to 8).*

*In LeachXS, the “natural pH” (sometimes called the “own pH” for brevity) is defined as the pH response at a liquid-to-solid ratio of 10 L/kg when no acid or base is added.*

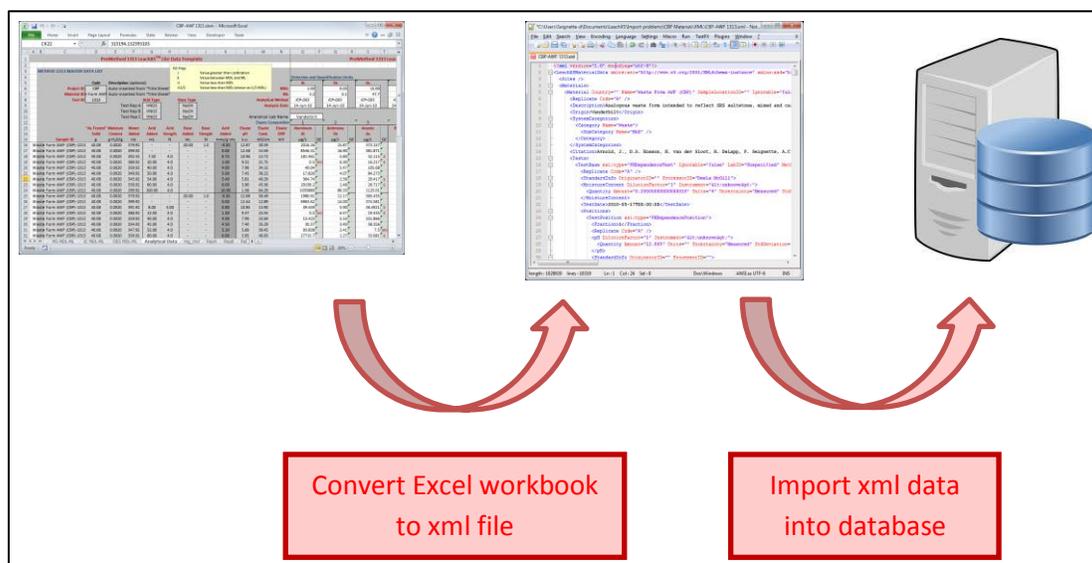
The screenshot shows the 'Acid/Base Neutralization Capacity (ANC/BNC)' window. At the top, it says 'Final pH' and provides instructions. Below that is a 'Material to Graph' dropdown menu with a list of materials: Analogous Waste Form AWF CBP (P,1,1), Backfill Grout Mortar BGM CBP (P,1,1), Cement concrete Vault 1 and 4 VCO CBP (P,1,1), and Simulated vault mortar SVC CBP (P,1,1). A red circle highlights this list with the callout '#1 Chose a material from the list of select materials'. Below the dropdown is a graph showing ANC/BNC (mol/kg) on the y-axis (0 to 10) and pH on the x-axis (6 to 11). A red arrow points to the 'yields' button with the callout '#3 Click “yields” button calculate'. Below the graph are input fields: 'Adding 5 mol/kg acid to pH 12 yields pH 6.88'. A red arrow points to these fields with the callout '#2 Enter parameters for the calculation'. To the right of the graph, a red arrow points to the 'Export results' button with the callout '#4 Export results to Excel'. At the bottom, there are '< Back', 'Export', and 'Close' buttons.

The resulting titration curve and the numerical data for this calculator may be exported to a Microsoft Excel® workbook using the **Export Charts** window accessed by clicking the **Export** button.

## Importing or Adding New Data

If you want to work with leaching test results of your own, you'll need to import them into a LeachXS database. LeachXS has quite a number of Excel templates that you can use to supply your data. All data import functions are collected in pane **Import or Add New Data** from the main window.

A two-step process is involved in importing leaching data:



First, all data in a Microsoft Excel® workbook is read and converted to an intermediate xml file structure. Then, the data in the xml file is imported into a database. You can choose to save the intermediate xml file. This is particularly useful if you want to distribute your data to other LeachXS users.

The following options are available for importing data:

### From Existing Workbook

Import new leaching data from Microsoft Excel® data templates.

### From Existing XML File

Import new leaching data from a saved XML file.

### New Data (Using Data Template)

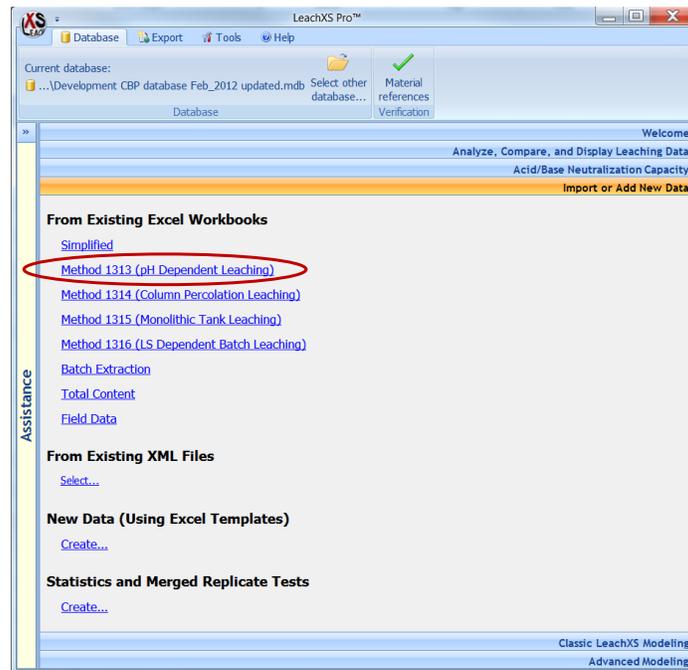
Accesses blank Microsoft Excel® data templates for data entry from within the LeachXS program.

***This section is not described in this version of the guide.***

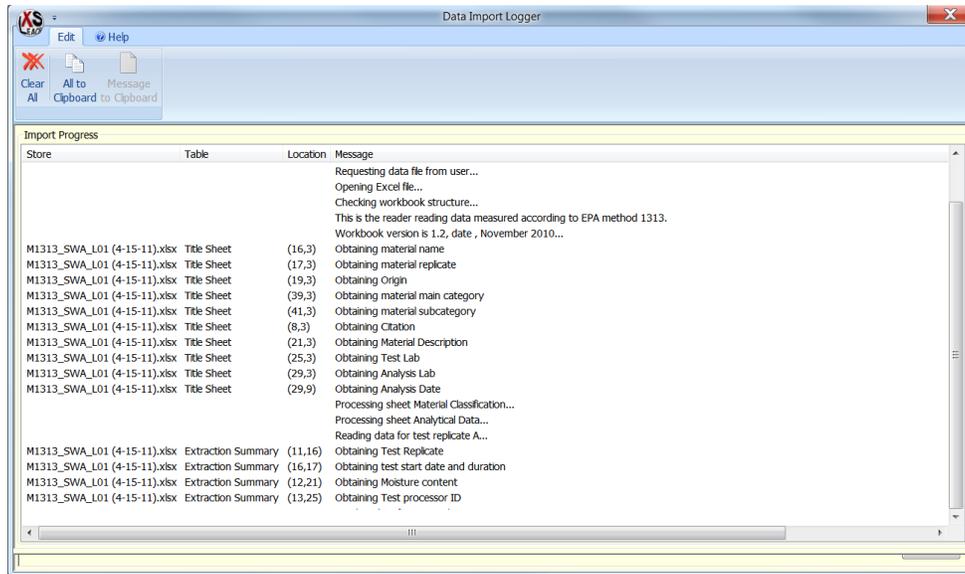
## Importing Data from a LEAF Template into a LeachXS Database

Leaching data may be imported from Microsoft Excel® data templates provided LeachXS for archiving and importing laboratory and analytical data. Importing of data in LeachXS is initiated from the Import or **Add New Data** roll-up menu in the LeachXS main window (see example below). In the following example, import process will be demonstrated using data from EPA Method 1313 (Liquid-Solid Partitioning as a Function of Eluate pH); however, the same process is identical for each data template.

To begin the procedure for importing data, select a link for the test type corresponding to data to be imported, for example, **Method 1313 (pH Dependent Leaching)**.

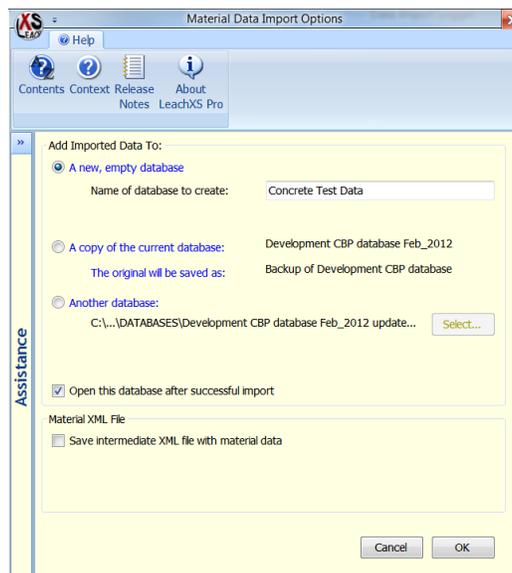


This action will activate a pop-up browser window. Using the browser, navigate the desired data template and select the **Open** button to start the import tool. A **Data Import Logger** window will pop up and the import tool will read the data template looking for the correct formatting of a set of test data. Any errors will be displayed as red text.

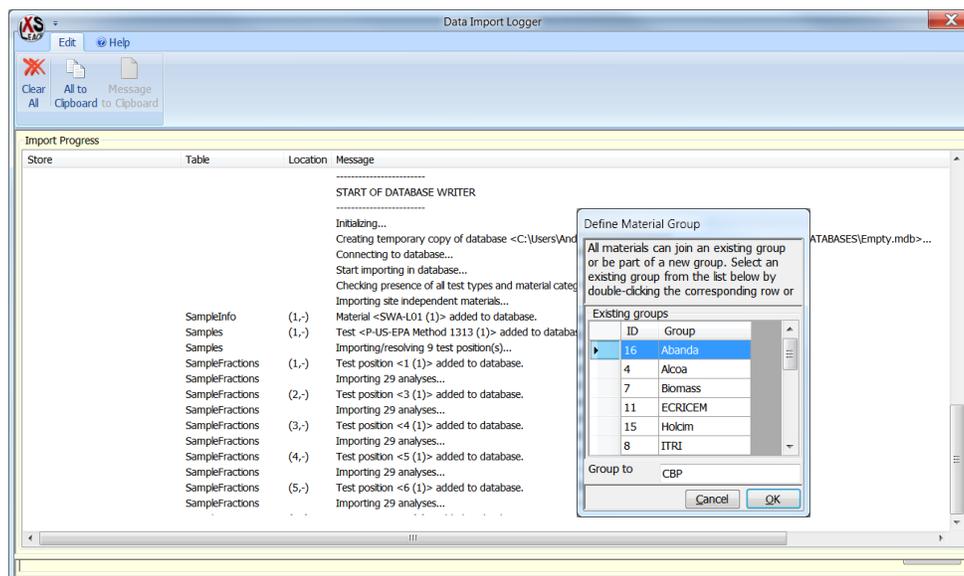


Upon a successful reading of the data template, LeachXS will display a **Material Data Import Options** dialog box used to assign the data to a database. The options on this dialog box include:

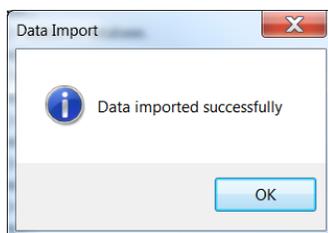
- A new, empty database**  
Creates a new database and activates a dialog box for naming the database to be created
- A copy of the current database**  
Saves a backup of the current database (e.g., the database displayed) and adds the new data to the current database.
- Another database**  
Activates a browser window to locate an existing database, saves a backup of the selected database and adds the new data to the selected database.



At the bottom of the **Material Data Import Options** screen are options for opening the database after a successful import (i.e., make the new database the current database in LeachXS) and for saving the data in an XML file format. Checking the “Save intermediate XML file with material data” box will activate a browser window for the user to locate and name the XML file. When all desired options are complete, click the **OK** button to close the **Material Data Import Options** screen and initiate the Database Writer in the **Data Import Logger** window.

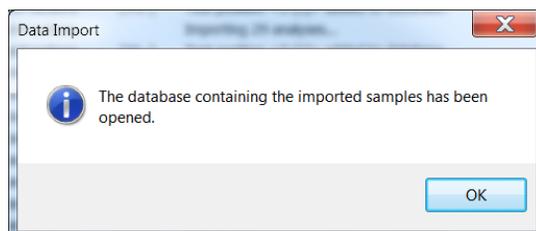


If fields (e.g., laboratory names, material source groups, etc.) in the data template do not match the categories native to LeachXS, a pop-up window (e.g., see the **Define Material Group** window above) will allow the user to “map” the field to an accepted LeachXS category). Upon a successful import, the following box will be displayed.



Click on **OK**, to clear the box.

If the **Open this database after a successful import** check box was checked in the **Material Data Import Options** screen, the following pop-up box will be displayed.



Click on **OK**, to clear the box.

The import process is complete and LeachXS returns to the **Import or Add New Data** roll-up menu.

## Filling a LEAF Template

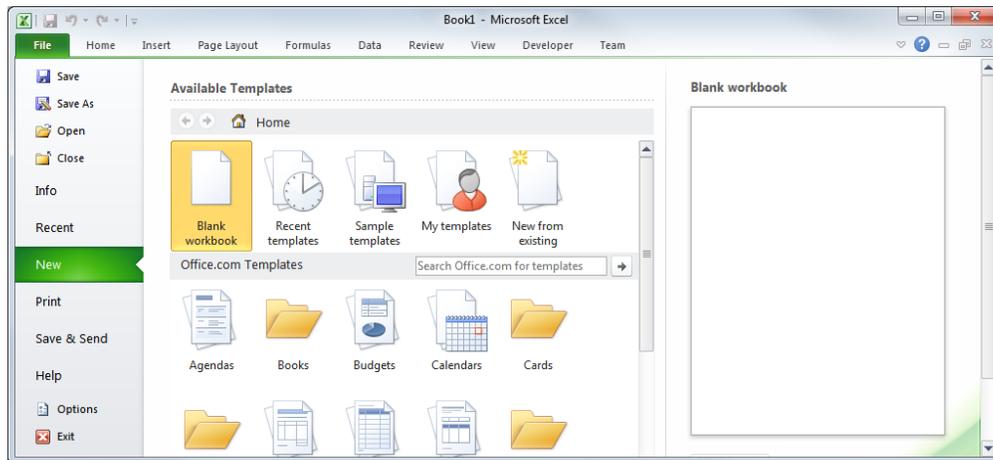
LeachXS provides templates for quite a number of leaching tests. The templates are installed along with the installation of LeachXS and are put in the location where Microsoft Excel® expects user templates. This is usually:

```
C:\Users\\AppData\Roaming\Microsoft\Templates
```

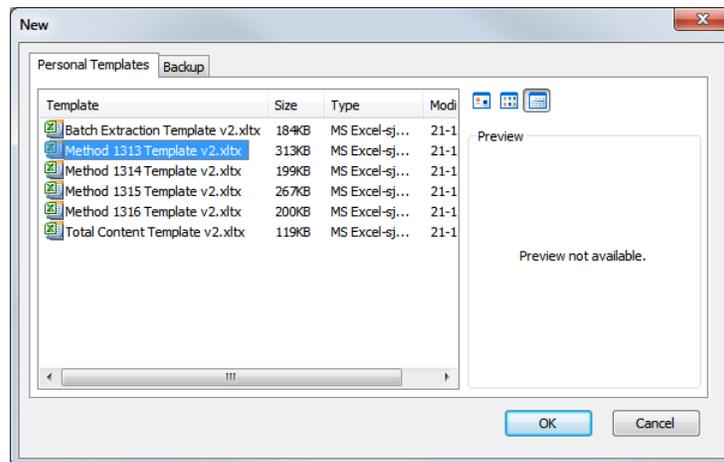
Where <username> is the name you use to log on to your computer.

You can create a new workbook from a template by starting Microsoft Excel®:

- Navigate to File->New



- Select **My templates**



- Select the desired template and hit the **OK** button.

## Classic LeachXS Modeling

The tradition modeling efforts in LeachXS included the ability to identify likely solid phases that explain the pH dependence leaching data of a material through precipitation/dissolution reactions and the ability to incorporation solid phase dissolution with sorption phenomena to model the pH dependence behavior over a range of pH values. Therefore, the Classic LeachXS Modeling roll-up menu contains the following options:

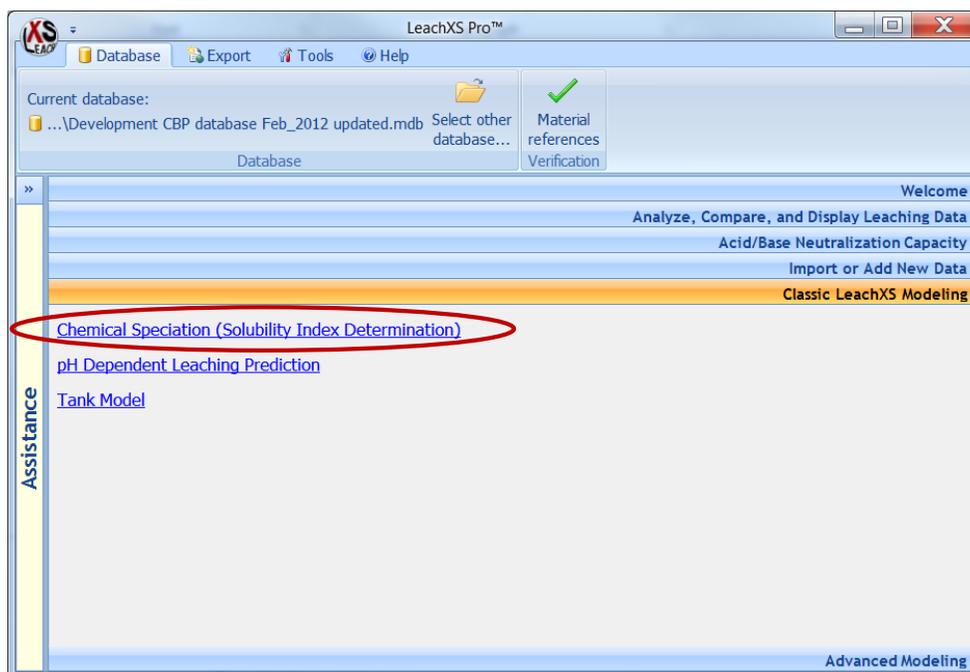
- Chemical Speciation Modeling
- pH Dependence Prediction Modeling

### Chemical Speciation Modeling

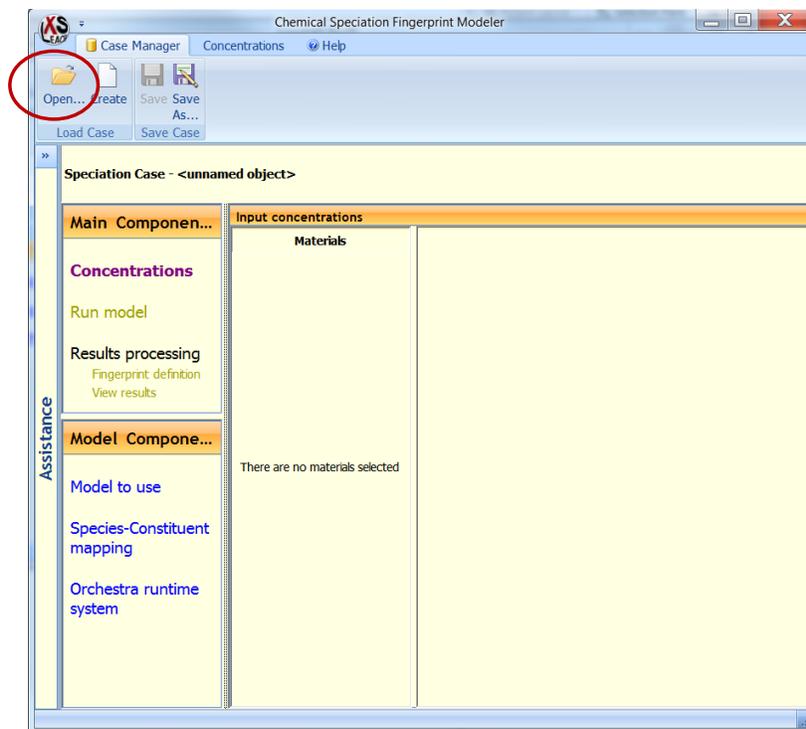
The **Chemical Speciation Model** is used to identify potentially relevant minerals for a material through calculation of Saturation Indices (SI). The result is a list of mineral phases that provide a preliminary description of the concentrations in the aqueous phase as a function of pH.

*Note: The calculation of saturation indices is based on total measured concentrations in solution and, therefore, does not take into account interactions between multiple phases, sorption to clay surfaces, or sorption to hydrated oxides.*

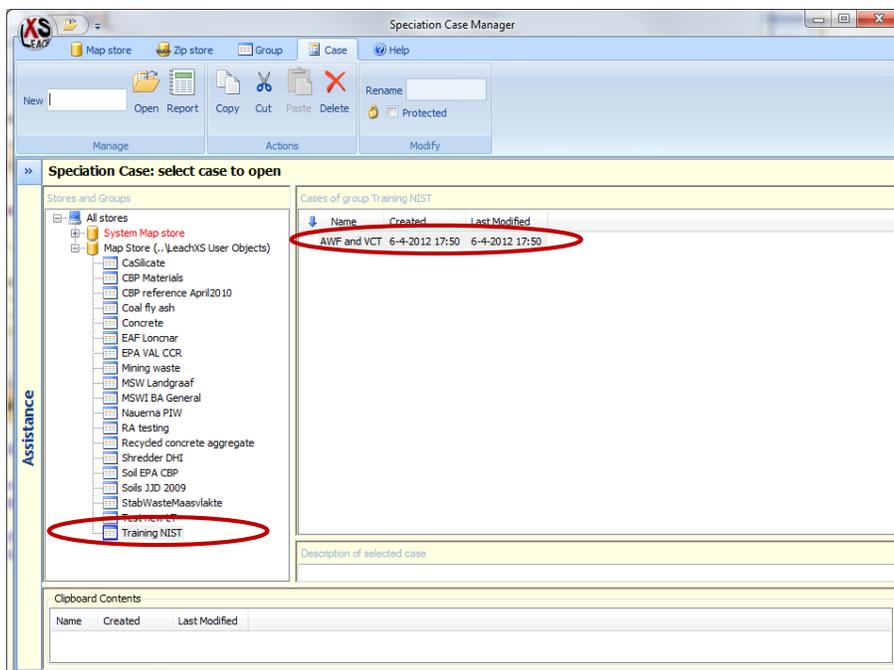
In order to start the **Chemical Speciation Model**, click on the **Chemical Speciation (Solubility Index Determination)** link in the Classic LeachXS Modeling roll-up menu.



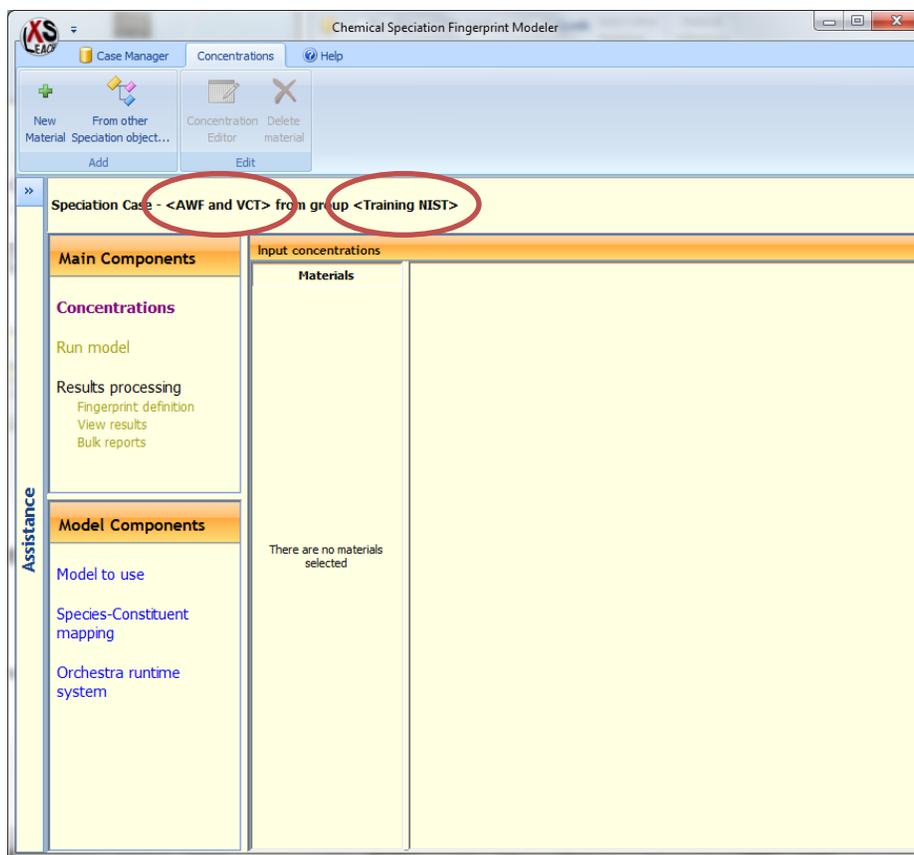
Select the **Open** icon from ribbon menu of the **Case Manager** tab on the top bar menu.



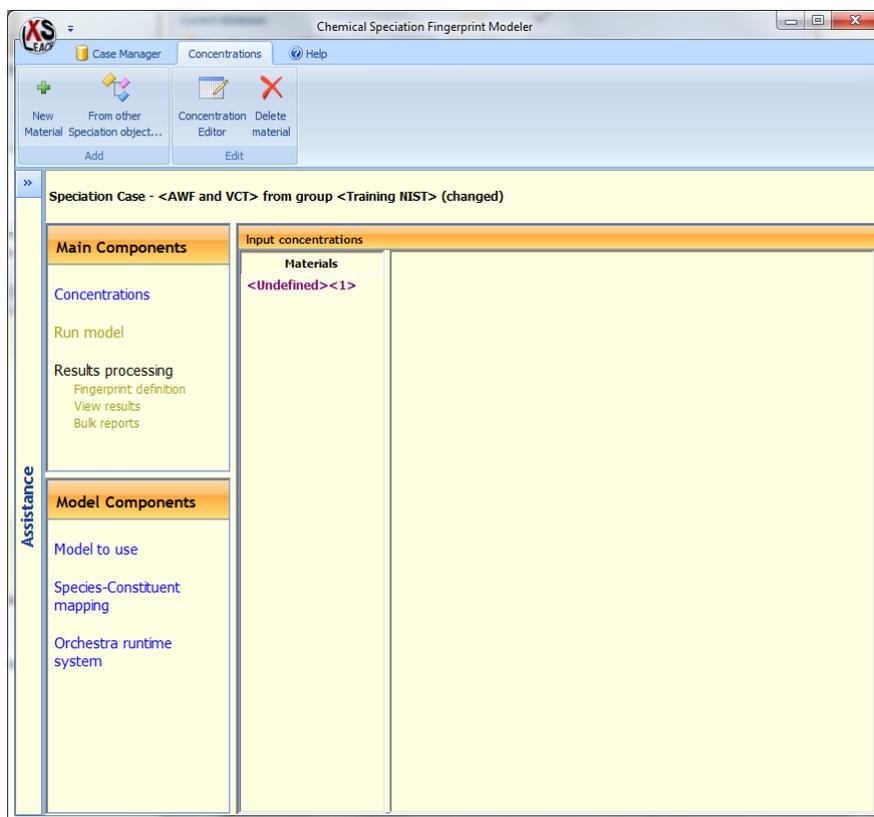
Create a **Group** and a **Case** (see “LeachXS Cases and Case Management” on page 100 for details on creating groups and cases). In this example, the group is named **Training NIST** and the case is named **AWF and VCT**).



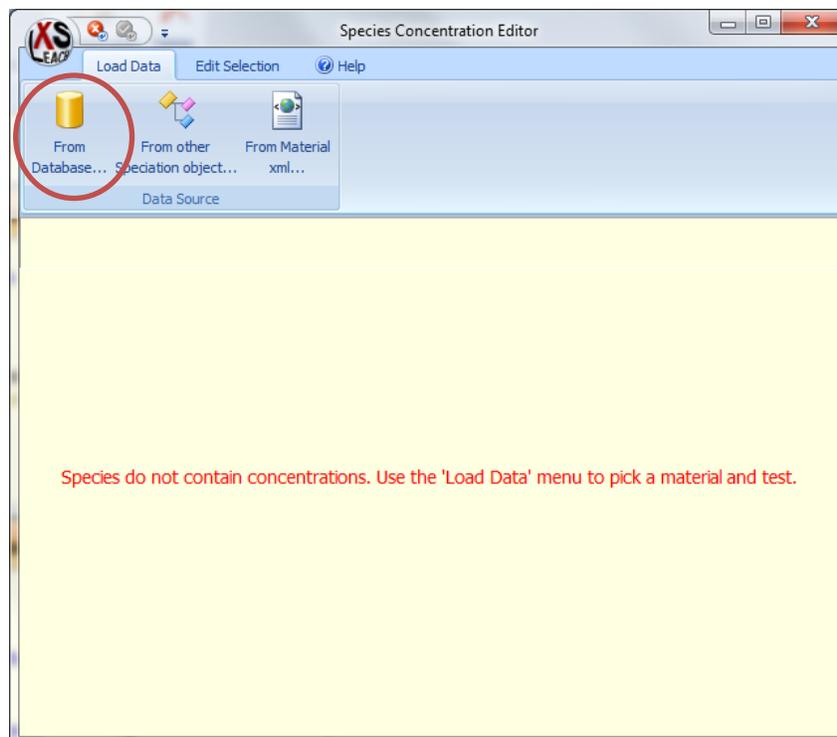
Double click on newly created case name (**AWF and VCT**) to start the **Chemical Speciation Fingerprint Modeler** window.



As a first step the information on which the model runs are based need to be loaded. Click on **Select new material**. This creates an **<Undefined > <1>** material in the panel **Materials**. Click on **<Undefined > <1>** and then click on the **Concentrations Editor**.



This opens a new window with choices where to obtain the info from.

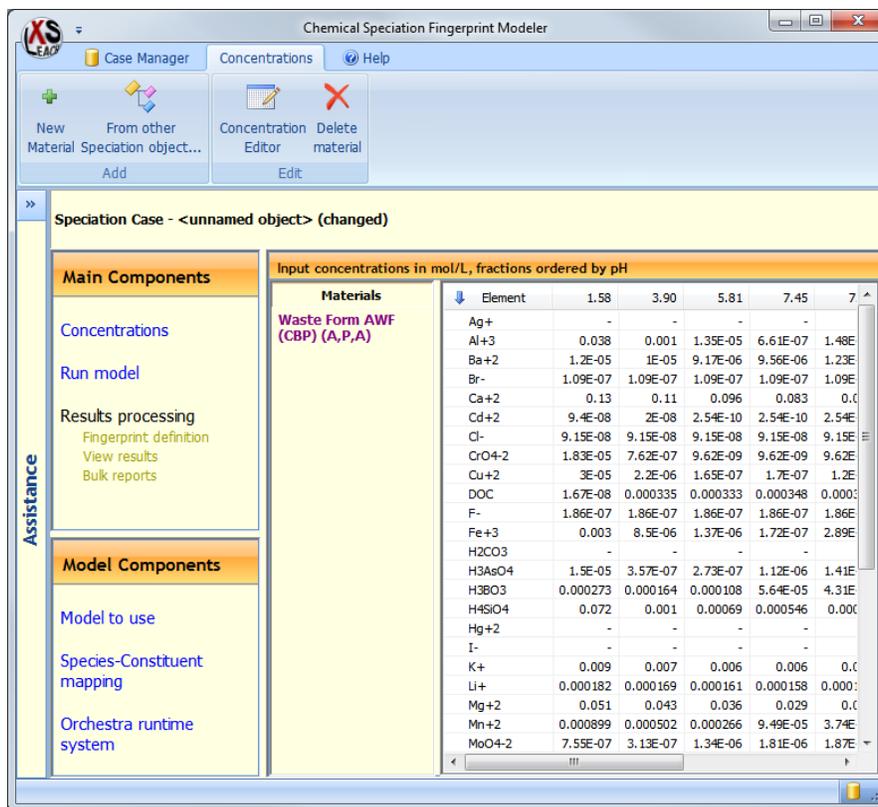


The chemical speciation model mainly uses pH dependence test data, but can be used also for any other type of data. Here we select pH dependence test data. We choose **Waste Form AWF (CBP) (P,1,1)** with the aid of "The Sample Selector" on page 121. After you have selected the sample and closed the **Sample Selector**, the concentrations are loaded into the editor.

The screenshot shows the 'Species Concentration Editor' window. At the top, there are buttons for 'Load Data', 'Edit Selection', and 'Help'. Below these are icons for 'Reset to Measured', 'Undo Edits', 'Set as Not Measured', 'Copy', and 'Paste'. A 'Concentration selection' section is also visible. The main area contains a table with the following data:

Fractions are ordered by pH									
Constituent	1.58	3.90	5.81	7.45	7.99	9.32	10.96	12.48	12.87
Ag+									
Al+3	0.0384	0.00108	1.35E-05	6.61E-07	1.48E-06	1.85E-08	6.73E-06	0.000317	7.47E-05
Ba+2	1.2E-05	1E-05	9.17E-06	9.56E-06	1.23E-05	7.45E-06	1.05E-06	5.41E-08	3.64E-05
Br-	1.09E-07								
Ca+2	0.128	0.111	0.0955	0.0831	0.0777	0.0388	0.00516	8.53E-05	2.85E-06
Cd+2	9.4E-08	2E-08	2.54E-10						
Cl-	3.66E-05	0.0036	0.00737	0.00803	0.0083	0.00778	0.00871	0.00909	0.00906
CrO4-2	1.83E-05	7.62E-07	9.62E-09	9.62E-09	9.62E-09	6.48E-08	3.75E-07	5.29E-07	1.23E-07
Cu+2	3E-05	2.2E-06	1.65E-07	1.7E-07	1.2E-07	3.23E-08	3.23E-08	3.23E-08	3.23E-08
DOC	1.67E-08	0.000335	0.000333	0.000348	0.000355	0.000369	0.000439	0.00104	0.00117
F-	1.86E-07								
Fe+3	0.00252	8.5E-06	1.37E-06	1.72E-07	2.89E-07	6.66E-08	6.72E-08	8.89E-07	3.72E-07
H2CO3									
H3AsO4	1.5E-05	3.57E-07	2.73E-07	1.12E-06	1.41E-06	2.16E-07	4.29E-07	5.1E-06	4.98E-06
H3BO3	0.000273	0.000164	0.000108	5.64E-05	4.31E-05	1.28E-05	2.05E-05	6.03E-05	6.18E-05
H4SiO4	0.0718	0.00112	0.00069	0.000546	0.00059	0.00041	0.00103	0.00343	0.00344

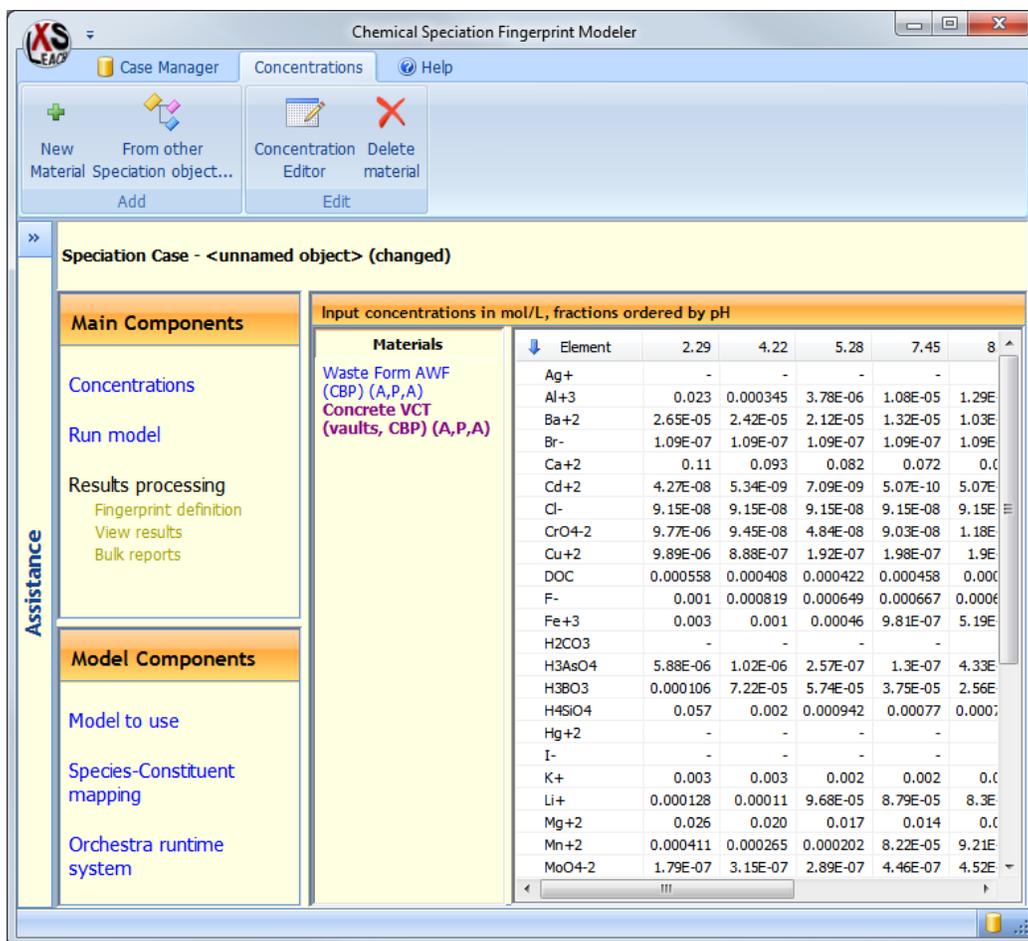
Hit the green button in the top left of the panel to accept the data.



Add an extra material by hitting **New Material** on the top left. This creates an **<Undefined > <1>** material in the panel **Materials**.

Click on **<Undefined > <1>** and then click on the **Concentrations Editor** to select the additional material. Then click on **From database** and select the sample of interest. We pick **Concrete VCT (vaults,CBP) (P,1,1)**.

Next hit the green button on the top left of the pane to accept the selected material.

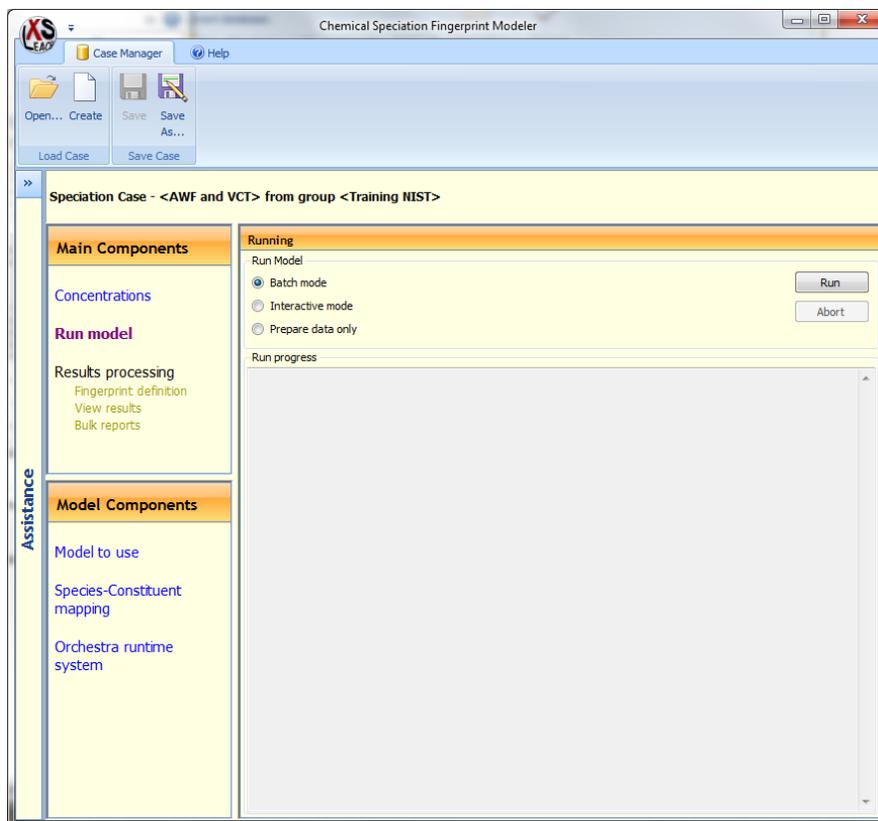


There are choices to be made, when the model components need to be changed, such as adding substances to the list of modeled elements. This will require a new **Mapping of the species** for the model (This aspect will be dealt with later). The model itself will normally not change.

With the concentration editor modifications to the information obtained from the database can be made, if needed. Or additions can be made for substances not measured or substances not yet entered in the database. For this the concentration editor is opened by clicking **Concentrations Editor**. Any change will result in the green button, which is greyed out to turn green.

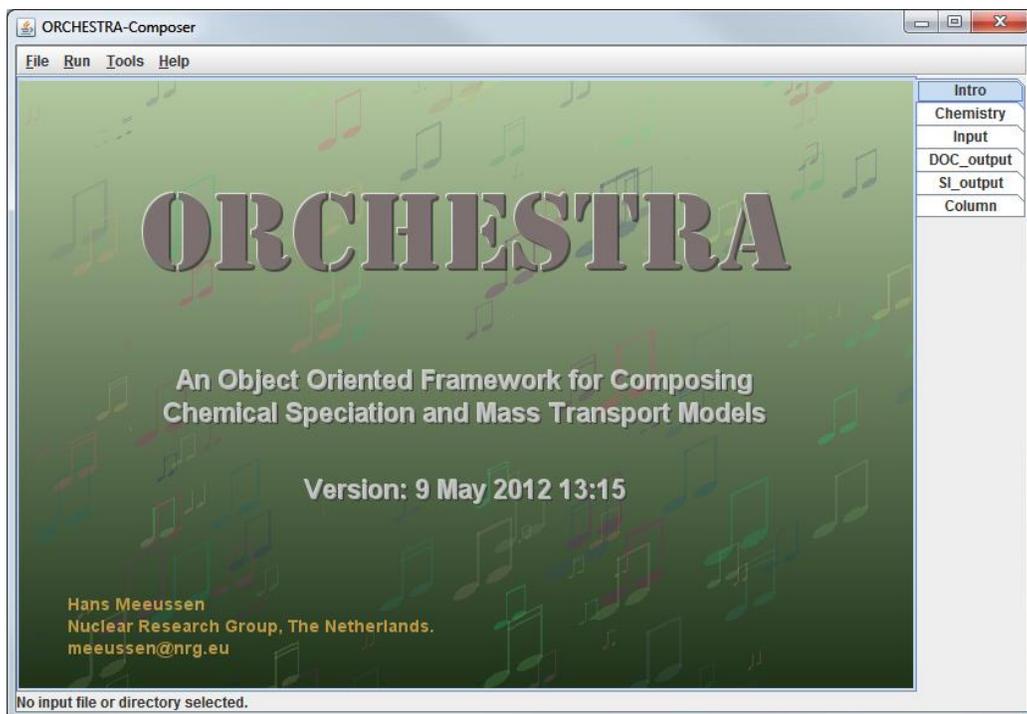
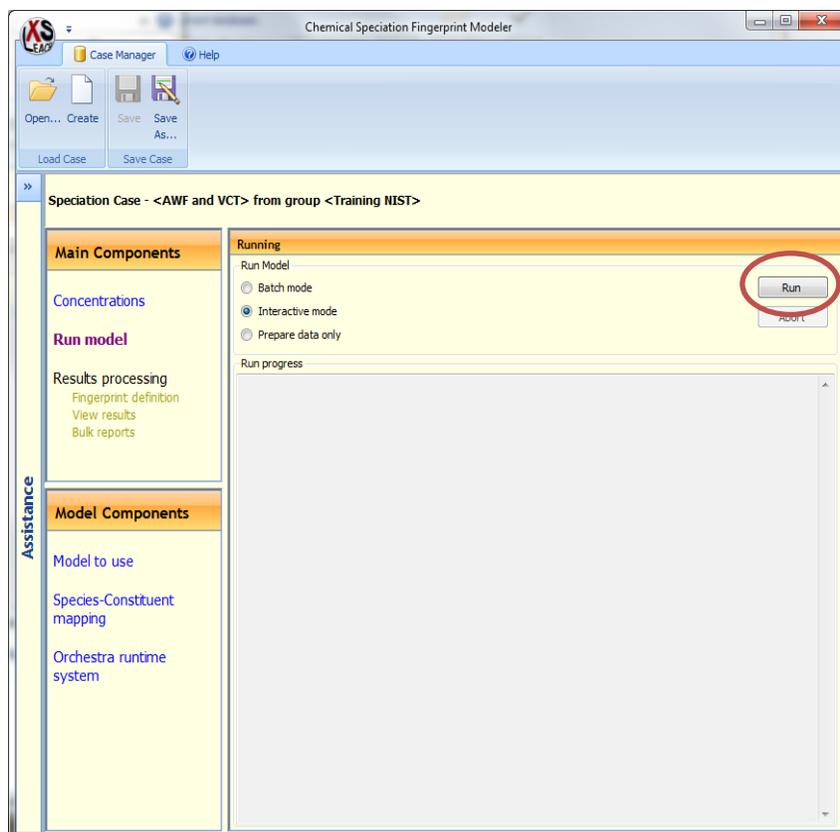
Hit **Run model** to start the model run.

Hit **Save** to save the choices made for this model run.

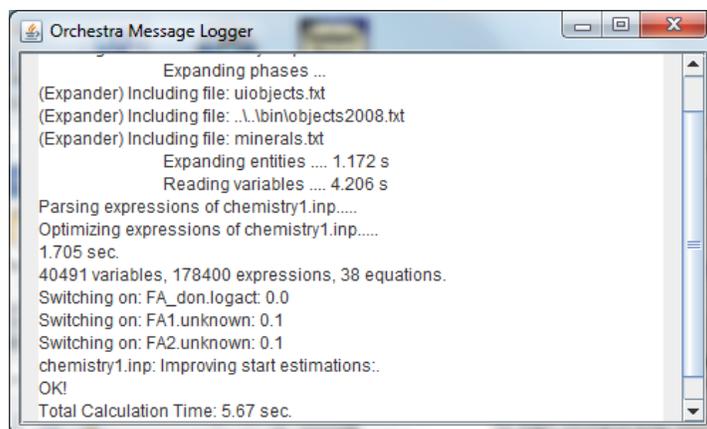


The model can be run either in **Batch mode** or **Interactive mode**. For this model **Prepare data only** is not so functional, unless the process of importing data and modifying the model run needs to be continued at a later time.

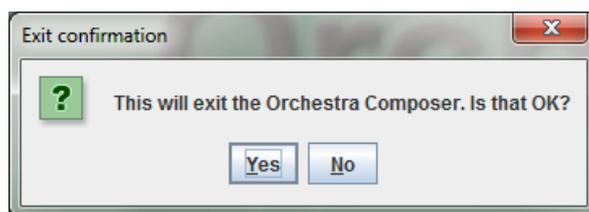
To understand what is happening in the background it is useful to run Orchestra interactively. Hit **Run** to start the model.



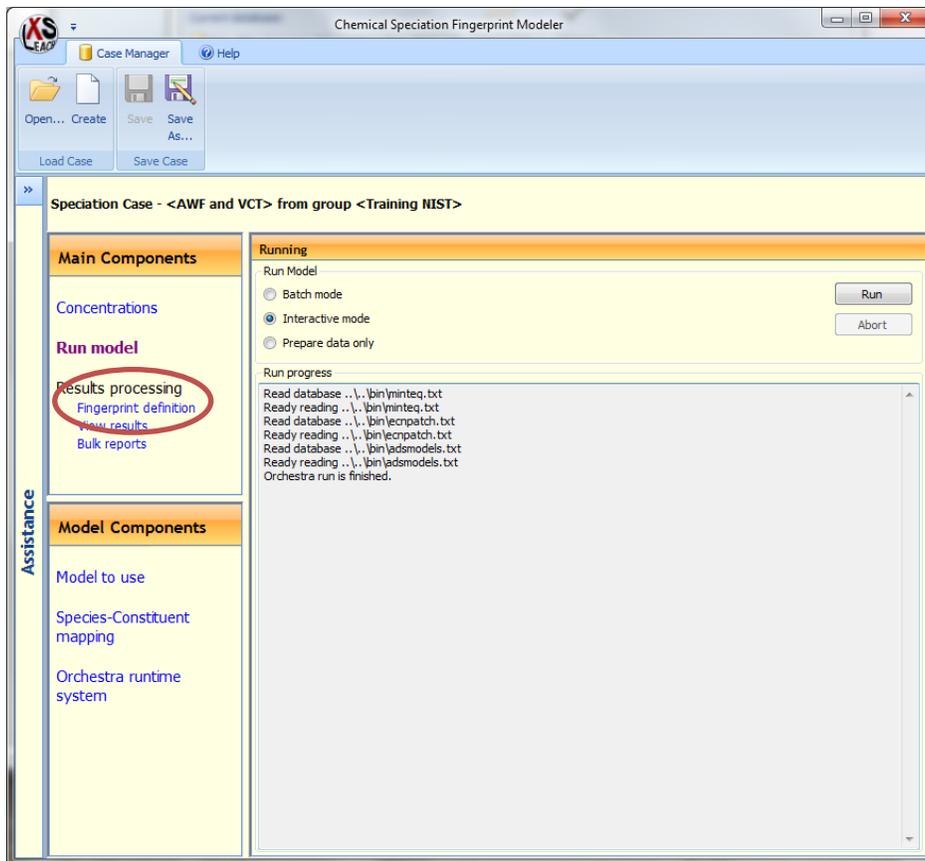
To start Orchestra by hitting **Run** (top left) twice (safety to avoid accidental starting of the model)



This screen shows the progress and the time needed for calculation. A time to go bar is shown during the run. To close Orchestra and return to LeachXS, hit the cross on the top right hand corner of the main screen.

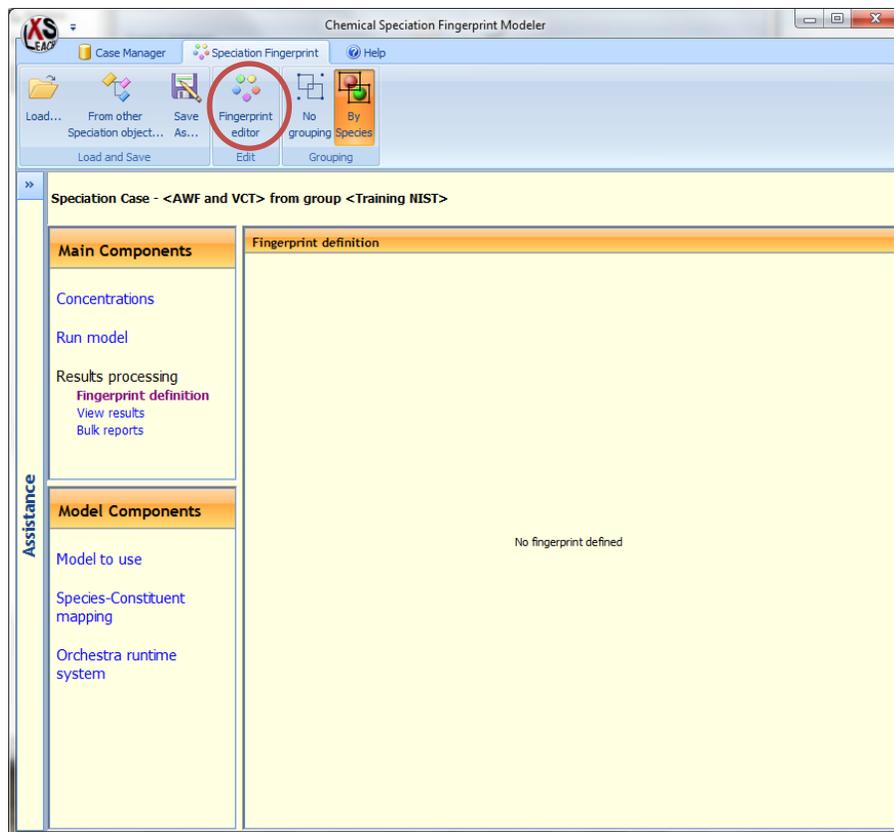


Hit **Yes** in the confirmation screen that pops up to close Orchestra and transfer the model output data to LeachXS.



Next the first estimate of the mineral part of the chemical speciation **Fingerprint** can be defined.

Hit **Fingerprint definition** then select the **Fingerprint editor**.



In opening the **Fingerprint editor** switch to **AI+3**.

Mineral Selector by Saturation Indexes

Minerals View Help

Delete Clear No grouping By Species

Selection Grouping

Available species

Species

Ag+  
Al+3  
Ba+2  
Br-  
Ca+2  
Cd+2  
Cl-  
Co+2  
CrO+2  
Cu+2  
F-  
Fe+3  
H2CO3  
H3AsO4  
H3BO3  
H4SiO4  
Hg+2  
I-  
K+  
Li+  
Mg+2  
Mn+2  
MoO4-2

Selected minerals

Mineral

Analogous Waste Form AWF CBP (A,P,A) Cement. concrete Vault 2 VCT CBP (A,P,A)

Fractions or positions are ordered by pH

Mineral	Combined	Hit rate	Fit rate	1.58	3.90	5.81	7.45
AA_2CaO_Al2O3_8H2O[s]	000	000	000	-9.96	-5.01	-2.99	-2.67
AA_2CaO_Al2O3_5iO2_8H2O[s]	038	022	055	-6.40	-2.80	-1.23	-0.99
AA_3CaO_Al2O3[Ca(OH)2]0_5_[CaCO3]0_5_11_5H2O[s]	000	000	000	-11.05	-6.59	-4.17	-3.04
AA_3CaO_Al2O3_6H2O[s]	000	000	000	-11.69	-6.81	-4.43	-3.53
AA_3CaO_Al2O3_CaCO3_11H2O[s]	000	000	000	-10.32	-6.18	-3.94	-2.94
AA_3CaO_Al2O3_CaSO4_12H2O[s]	053	022	084	-7.50	-3.98	-2.29	-1.66
AA_4CaO_Al2O3_13H2O[s]	006	011	000	-12.31	-7.48	-4.85	-3.56
AA_Al(OH)3[am]	000	000	000	-3.94	1.36	1.50	-1.02
AA_CO3-hydroxalcite	010	011	009	-7.98	-3.86	-1.67	-0.70
AA_CaO_Al2O3_10H2O[s]	025	022	028	-6.14	-1.07	0.35	-0.31
AA_Ettringite	006	011	000	-2.33	-0.05	1.00	1.40
AA_Gibbsite	006	011	000	-2.46	2.84	3.06	0.46
AA_OH-hydroxalcite[cr]	000	000	000	-7.79	-2.97	-0.41	0.84
AA_Tricarboaluminate	000	000	000	-8.82	-5.35	-3.23	-2.15
Al2O3	000	000	000	-7.69	-2.39	-2.17	-4.77
Al4(OH)10SO4	000	000	000	-2.05	1.32	0.70	-2.03
AlAsO4·2H2O	000	000	000	-2.71	-1.71	-2.66	-4.95
AlOH5O4	006	011	000	-0.12	0.35	-1.51	-4.44
AlPO4	000	000	000	-5.31	-3.08	-4.01	-6.65
AlSb	000	000	000	-108.61	-107.63	-108.35	-110.36
Al(OH)3[a]	006	011	000	-5.08	0.22	0.44	-2.16
Albite[low]	000	000	000	-1.63	-1.19	-0.89	-1.15
AlumK	000	000	000	1.34	1.03	-0.42	-2.30
Alunite	006	011	000	0.03	1.59	0.69	-1.43
Analbite	000	000	000	-1.82	-1.37	-1.07	-1.33
Analcime	000	000	000	-2.04	-1.03	-0.61	-0.90
Annite	000	000	000	-5.69	-5.23	-8.64	-11.57
Anorthite	000	000	000	-4.32	-2.01	-1.24	-1.67
Boehmite	000	000	000	-4.27	1.03	1.24	-1.36
C2AH8_ECN	000	000	000	-17.02	-12.07	-10.05	-9.73
Ca-Nontronite	000	000	000	2.67	2.18	-0.94	-3.45
CaAH10_ECN	000	000	000	-20.63	-15.56	-14.14	-14.80
Ca-Ettringite	034	022	045	-4.38	-1.89	-0.94	-0.49

Change the range of SI values in **View**.

Mineral Selector by Saturation Indexes

Minerals View Help

Undersaturation value: -1.0 Over/undersaturation Fit weight: 1  
 Oversaturation value: 1.00 Within limits Hit weight: 1

Saturation Indexes Saturation Coloring Figure of Merit weights

Available species Analogous Waste Form AWF CBP (A,P,A) Cement, concrete Vault 2 VCT CBP (A,P,A)

Species

Ag+ Al+3 Ba+2 Br- Ca+2 Cd+2 Cl- Co+2 CrO+2 Cu+2 F- Fe+3 H2CO3 H3AsO4 H3BO3 H4SiO4 Hg+2 I- K+ Li+ Mg+2 Mn+2 MoO+2

Selected minerals

Mineral

Fractions or positions are ordered by pH

Mineral	Combined	Hit rate	Fit rate	1.58	3.90	5.81	7.45	7.99	9.32	10.96	12.48	12.87
<input type="checkbox"/> AA_2CaO_Al2O3_8H2O[s]	021	022	020	-9.96	-5.01	-2.99	-2.67	-2.22	-2.63	-0.95	-0.61	-1.71
<input type="checkbox"/> AA_2CaO_Al2O3_5H2O[s]	066	044	087	-6.40	-2.80	-1.23	-0.99	-0.62	-1.01	0.18	0.06	-1.02
<input type="checkbox"/> AA_3CaO_Al2O3[Ca(OH)2]0_5_[CaCO3]0_5_11_5H2O[s]	039	022	056	-11.05	-6.59	-4.17	-3.04	-2.47	-2.09	-0.51	-0.35	-1.53
<input type="checkbox"/> AA_3CaO_Al2O3_6H2O[s]	021	022	020	-11.69	-6.81	-4.43	-3.53	-2.95	-2.79	-0.97	-0.59	-1.78
<input type="checkbox"/> AA_3CaO_Al2O3_CaCO3_11H2O[s]	014	022	006	-10.32	-6.18	-3.94	-2.94	-2.44	-2.21	-0.91	-0.97	-2.12
<input type="checkbox"/> AA_3CaO_Al2O3_Ca5O4_12H2O[s]	058	022	095	-7.50	-3.96	-2.29	-1.66	-1.24	-1.15	0.07	-0.02	-1.17
<input type="checkbox"/> AA_4CaO_Al2O3_13H2O[s]	045	022	068	-12.31	-7.48	-4.85	-3.56	-2.90	-2.37	-0.44	-0.04	-1.25
<input type="checkbox"/> AA_Al(OH)3[am]	000	000	000	-3.94	1.36	1.58	-1.02	-1.19	-4.44	-3.48	-3.33	-4.34
<input type="checkbox"/> AA_CO3-hydroxalcalite	050	044	057	-7.98	-3.86	-1.67	-0.70	-0.22	-0.32	-0.34	-1.12	-1.51
<input type="checkbox"/> AA_CaO_Al2O3_10H2O[s]	058	067	050	-6.14	-1.07	0.35	-0.31	-0.06	-1.42	0.02	0.30	-0.81
<input type="checkbox"/> AA_Ettringite	026	022	029	-2.33	-0.05	1.00	1.40	1.66	1.70	2.36	1.86	0.74
<input type="checkbox"/> AA_Gibbsite	042	022	061	-2.46	2.84	3.06	0.46	0.29	-2.95	-2.00	-1.85	-2.86
<input type="checkbox"/> AA_OH-hydroxalcalite[cr]	028	022	034	-7.79	-2.97	-0.41	0.84	1.49	1.64	2.03	1.58	1.26
<input type="checkbox"/> AA_Tricarboaluminate	012	011	014	-8.82	-5.35	-3.23	-2.15	-1.73	-1.42	-0.61	-1.06	-2.17
<input type="checkbox"/> Al2O3	000	000	000	-7.69	-2.39	-2.17	-4.77	-4.94	-8.18	-7.23	-7.08	-8.09
<input type="checkbox"/> Al(OH)10SO4	006	011	000	-2.05	1.32	0.70	-2.03	-2.38	-5.49	-5.33	-5.81	-6.78
<input type="checkbox"/> Al(OH)2H2O	000	000	000	-2.71	-1.71	-2.66	-4.95	-5.52	-8.87	-10.62	-11.51	-12.63
<input type="checkbox"/> Al(OH)SO4	048	022	074	-0.12	0.35	-1.51	-4.44	-5.07	-7.97	-9.01	-10.44	-11.34
<input type="checkbox"/> AlPO4	000	000	000	-5.31	-3.08	-4.01	-6.65	-7.29	-10.40	-11.87	-12.93	-13.82
<input type="checkbox"/> AlSb	000	000	000	-108.61	-107.63	-108.35	-110.36	-110.66	-112.91	-113.27	-113.72	-114.44
<input type="checkbox"/> Al(OH)3[a]	044	022	065	-5.08	0.22	0.44	-2.16	-2.33	-5.97	-4.62	-4.47	-5.48
<input type="checkbox"/> Albite[low]	006	011	000	-1.63	-1.19	-0.89	-1.15	-1.05	-1.60	-1.55	-2.41	-2.98
<input type="checkbox"/> AlumiK	016	011	021	1.34	1.03	-0.42	-2.30	-2.75	-4.50	-5.37	-6.47	-7.02
<input type="checkbox"/> Alunite	011	022	000	0.03	1.59	0.69	-1.43	-1.79	-4.04	-4.30	-4.98	-5.68
<input type="checkbox"/> Analbite	000	000	000	-1.82	-1.37	-1.07	-1.33	-1.23	-1.78	-1.73	-2.12	-3.18
<input type="checkbox"/> Analcime	028	033	023	-2.04	-1.03	-0.61	-0.90	-0.79	-1.40	-1.15	-1.72	-2.25
<input type="checkbox"/> Annite	000	000	000	-5.69	-5.23	-8.64	-11.57	-11.19	-12.98	-12.79	-11.45	-12.63
<input type="checkbox"/> Anorthite	000	000	000	-4.32	-2.01	-1.24	-1.67	-1.51	-2.44	-1.89	-2.51	-3.46
<input type="checkbox"/> Boehmite	000	000	000	-4.27	1.03	1.24	-1.36	-1.52	-4.77	-3.82	-3.66	-4.68
<input type="checkbox"/> C2AH8_ECN	000	000	000	-17.02	-12.07	-10.05	-9.73	-9.28	-9.69	-8.01	-7.67	-8.83
<input type="checkbox"/> Ca-Nontronite	006	011	000	2.67	2.18	-0.94	-3.45	-3.13	-4.66	-4.87	-4.40	-5.65
<input type="checkbox"/> CaAH10_ECN	000	000	000	-20.63	-15.56	-14.14	-14.80	-14.55	-15.91	-14.47	-14.19	-15.30
<input type="checkbox"/> Cr-Ettringite	056	078	035	-4.38	-1.89	-0.94	-0.49	-0.23	0.05	0.96	0.52	-0.76

Based on the SI units selections of minerals can be made by going through all elements and all possible mineral phases. This does require some knowledge of possible mineral phases, as some phases are kinetically very slow and thus do not take part in the equilibrium based modeling. Other phases are only formed under extreme conditions unlikely for atmosphere exposed materials. See also the note at the beginning of this guide.

Selections are made by hitting the tick boxes in front of a mineral. As ettringite is described as a solid solution in chemical speciation modeling ettringites of Cr and other trace substances are not selected.

LeachXS CBP Version 2.0 User's Guide (rev. 0)

Mineral Selector by Saturation Indexes

Minerals View Help

Undersaturation value: -1.0 Over/undersaturation Fit weight: 1  
 Oversaturation value: 1.00 Within limits Hit weight: 1

Saturation Indexes Saturation Coloring Figure of Merit weights

Available species Analogous Waste Form AWF CBP (A,P,A) Cement, concrete Vault 2 VCT CBP (A,P,A)

Species

Ag+ Al+3 Ba+2 Br- Ca+2 Cd+2 Cl- Co+2 CrO+2 Cu+2 F- Fe+3 H2CO3 H3AsO4 H3BO3 H3SiO4 Hg+2 I- K+ Li+ Mg+2 Mn+2 MoO+2

Selected minerals

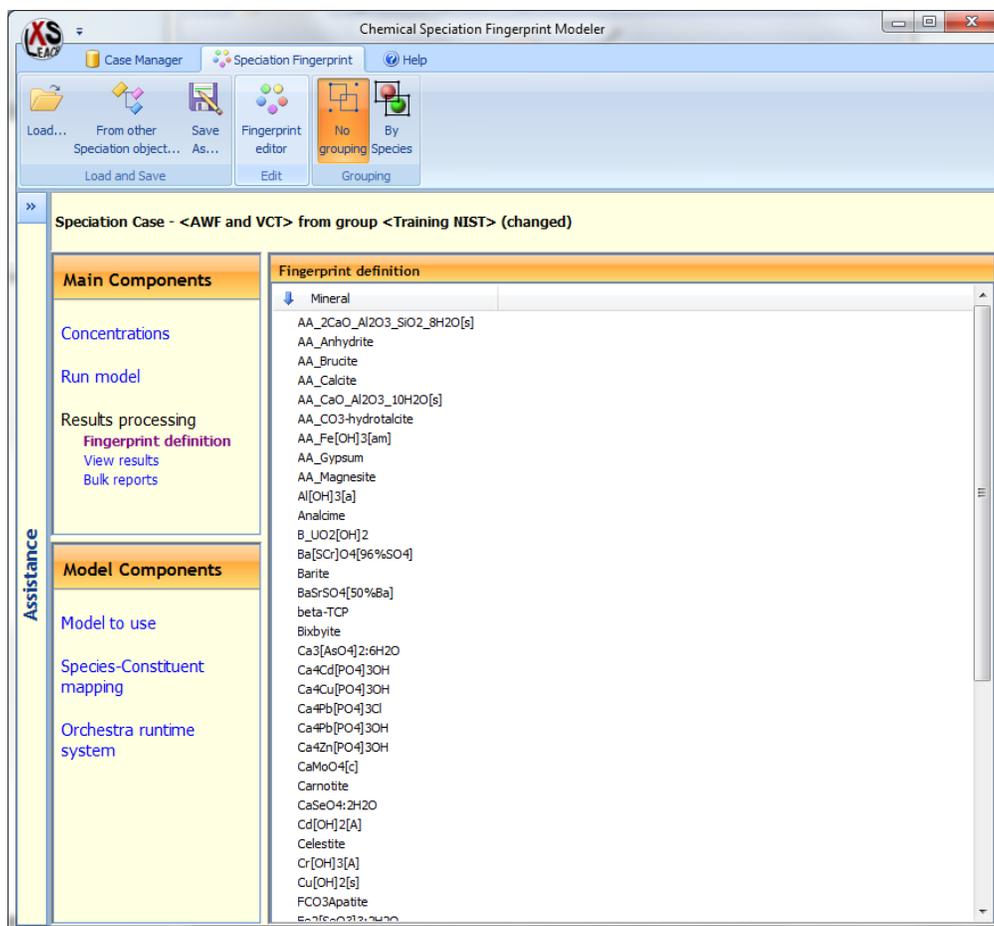
Mineral

AA\_2CaO\_Al2O3  
 AA\_CaO\_Al2O3  
 AA\_CO3-hydro  
 Al[OH]3[a]  
 Analcime  
 Laumontite

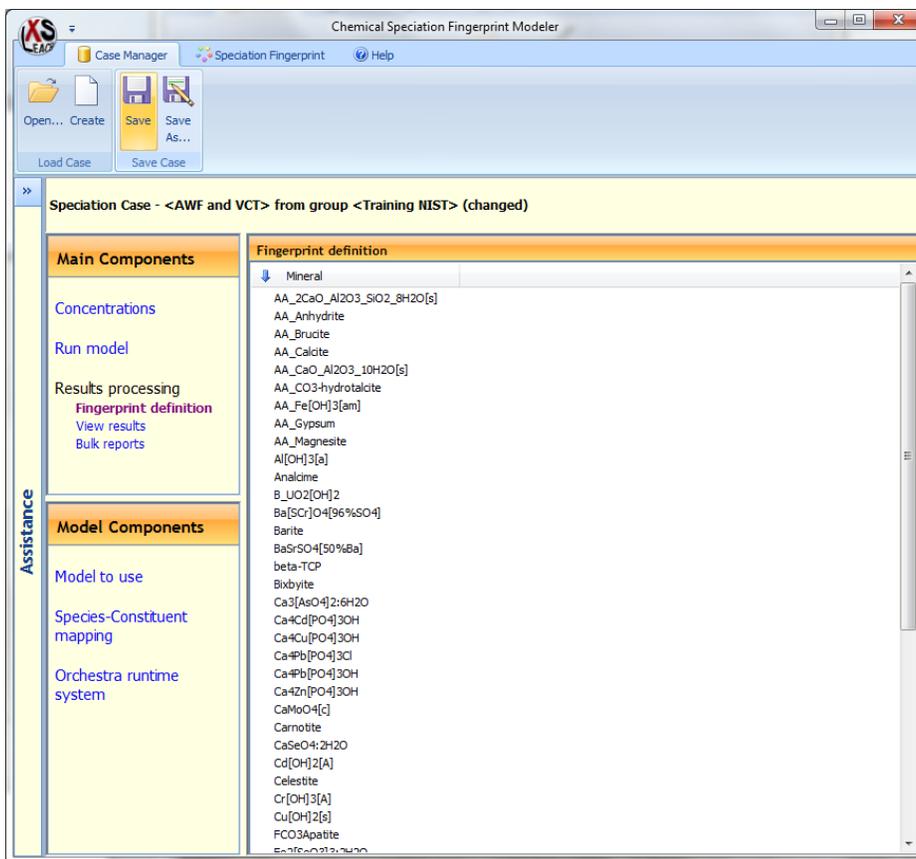
Mineral Combined Hit rate Fit rate 1.58 3.90 5.81 7.45 7.99 9.32 10.96 12.48 12.87

Mineral	Combined	Hit rate	Fit rate	1.58	3.90	5.81	7.45	7.99	9.32	10.96	12.48	12.87
AA_2CaO_Al2O3_8H2O[s]	021	022	020	-9.96	-5.01	-2.99	-1.67	-1.22	-2.63	-0.95	-0.61	-1.71
<input checked="" type="checkbox"/> AA_2CaO_Al2O3_5iO2_8H2O[s]	066	044	087	-6.40	-2.80	-1.23	-0.99	-0.62	-1.01	0.18	0.06	-1.02
AA_3CaO_Al2O3[Ca(OH)2]0_5_[CaCO3]0_5_11_5H2O[s]	039	022	056	-11.05	-6.59	-4.17	-3.04	-2.47	-2.09	-0.51	-0.35	-1.53
AA_3CaO_Al2O3_6H2O[s]	021	022	020	-11.69	-6.81	-4.43	-3.53	-2.95	-2.79	-0.97	-0.59	-1.78
AA_3CaO_Al2O3_CaCO3_11H2O[s]	014	022	006	-10.32	-6.18	-3.94	-2.94	-2.44	-2.21	-0.91	-0.97	-2.12
AA_3CaO_Al2O3_Ca5O4_12H2O[s]	058	022	095	-7.50	-3.96	-2.29	-1.66	-1.24	-1.15	0.07	-0.02	-1.17
AA_4CaO_Al2O3_13H2O[s]	045	022	068	-12.31	-7.48	-4.85	-3.56	-2.90	-2.37	-0.44	-0.04	-1.25
AA_Al[OH]3[am]	000	000	000	-3.94	1.36	1.58	-1.02	-1.19	-4.44	-3.48	-3.33	-4.34
<input checked="" type="checkbox"/> AA_CO3-hydratalcite	050	044	057	-7.98	-3.86	-1.67	-0.70	-0.22	-0.32	-0.34	-1.12	-1.51
<input checked="" type="checkbox"/> AA_CaO_Al2O3_10H2O[s]	058	067	050	-6.14	-1.07	0.35	-0.31	-0.06	-1.42	0.02	0.30	-0.81
AA_Ettringite	026	022	029	-2.33	-0.05	1.00	1.40	1.66	1.70	2.36	1.86	0.74
AA_Gibbsite	042	022	061	-2.46	2.84	3.06	0.46	0.29	-2.95	-2.00	-1.85	-2.86
AA_OH-hydratalcite[cr]	028	022	034	-7.79	-2.97	-0.41	0.84	1.49	1.64	2.03	1.58	1.26
AA_Tricarboaluminate	012	011	014	-8.82	-5.35	-3.23	-2.15	-1.73	-1.42	-0.61	-1.06	-2.17
Al2O3	000	000	000	-7.69	-2.39	-2.17	-4.77	-4.94	-8.18	-7.23	-7.08	-8.09
Al[OH]1.05O4	006	011	000	-2.05	1.32	0.70	-2.03	-2.38	-5.49	-5.33	-5.81	-6.78
Al(OH)2H2O	000	000	000	-2.71	-1.71	-2.66	-4.95	-5.52	-8.87	-10.02	-11.51	-12.63
Al(OH)O4	048	022	074	-0.12	0.35	-1.51	-4.44	-5.07	-7.97	-9.01	-10.44	-11.34
AlPO4	000	000	000	-5.31	-3.08	-4.01	-6.65	-7.29	-10.40	-11.87	-12.93	-13.82
Asb	000	000	000	-108.61	-107.63	-108.35	-110.36	-110.66	-112.91	-113.27	-113.72	-114.44
<input checked="" type="checkbox"/> Al[OH]3[a]	044	022	065	-5.08	0.22	0.44	-2.16	-2.33	-5.97	-4.62	-4.47	-5.40
Albite[low]	006	011	000	-1.63	-1.19	-0.89	-1.15	-1.05	-1.60	-1.55	-2.41	-2.98
AlumK	016	011	021	1.34	1.03	-0.42	-2.30	-2.75	-4.50	-5.37	-6.47	-7.02
Alunite	011	022	000	0.03	1.59	0.69	-1.43	-1.79	-4.04	-4.30	-4.98	-5.68
Analcime	000	000	000	-1.82	-1.37	-1.07	-1.33	-1.23	-1.78	-1.73	-2.59	-3.15
<input checked="" type="checkbox"/> Analcime	028	033	023	-2.04	-1.03	-0.61	-0.90	-0.79	-1.40	-1.15	-1.72	-2.25
Annite	000	000	000	-5.69	-5.23	-8.64	-11.57	-11.19	-12.98	-12.79	-11.45	-12.63
Anorthite	000	000	000	-4.32	-2.01	-1.24	-1.67	-1.51	-2.44	-1.89	-2.51	-3.46
Boehmite	000	000	000	-4.27	1.03	1.24	-1.36	-1.52	-4.77	-3.82	-3.66	-4.68
C2AH8_ECN	000	000	000	-17.02	-12.07	-10.05	-9.73	-9.28	-9.69	-8.01	-7.67	-8.83
Ca-Nontronite	006	011	000	2.67	2.18	-0.94	-3.45	-3.13	-4.66	-4.87	-4.40	-5.65
CaAH10_ECN	000	000	000	-20.63	-15.56	-14.14	-14.80	-14.55	-15.91	-14.47	-14.19	-15.30
Cr-Ettringite	056	078	035	-4.38	-1.89	-0.94	-0.49	-0.23	0.05	0.96	0.52	-0.76

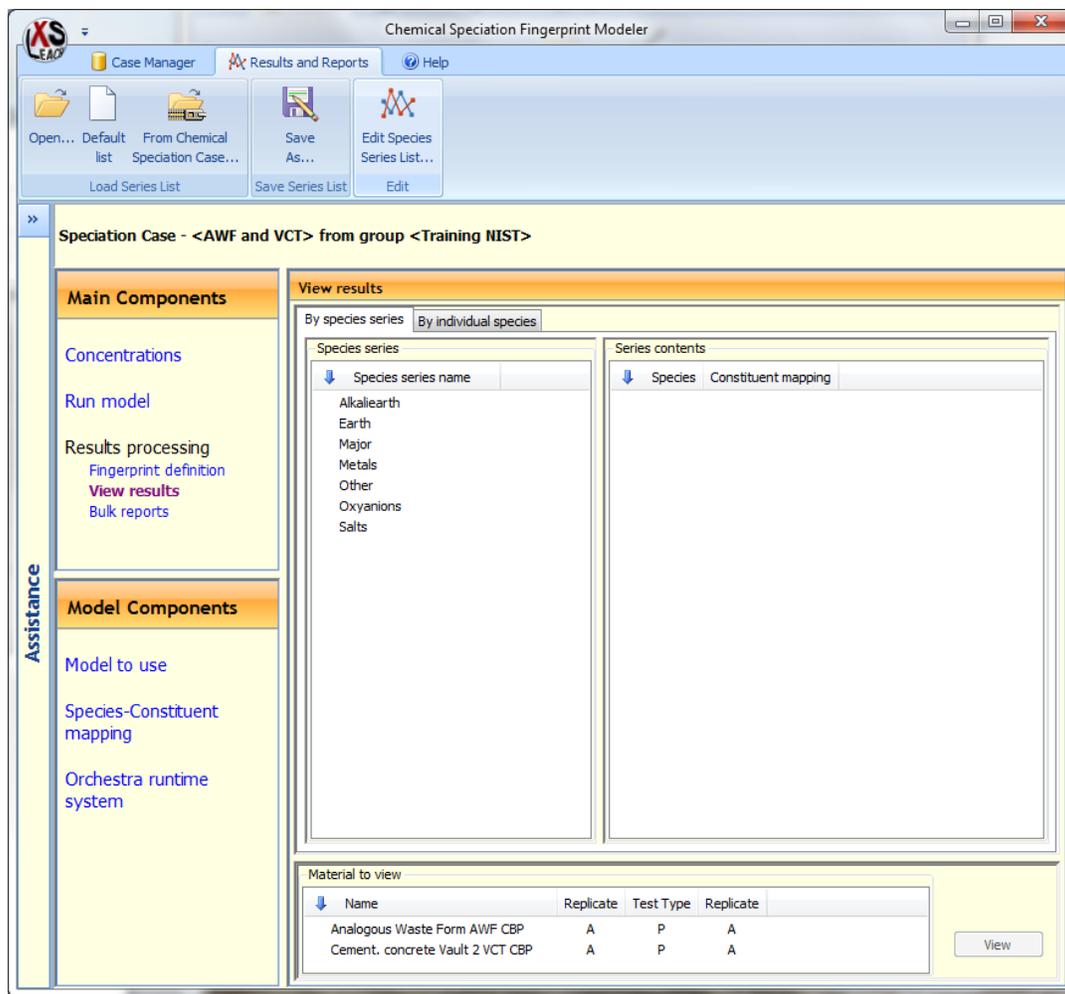
Confirm selections by hitting the green button in the top left of the pane.



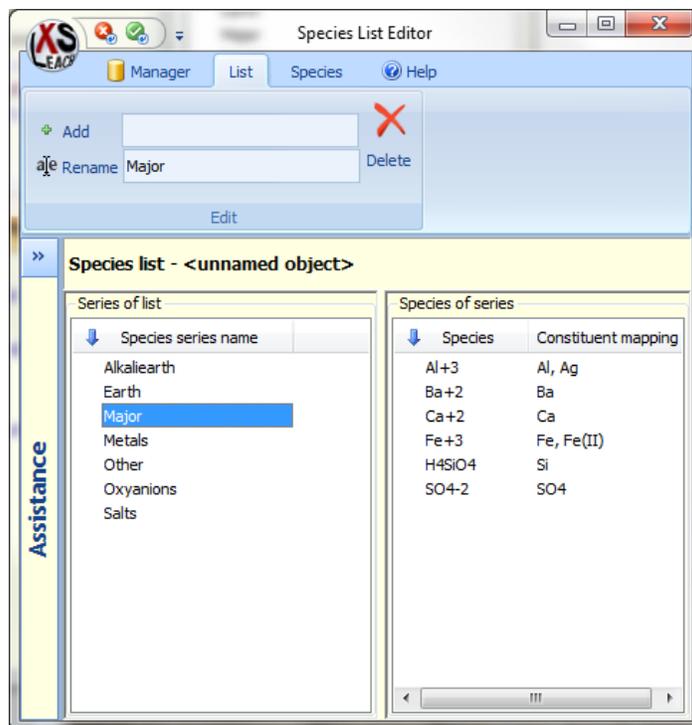
This forms the **Fingerprint definition** for the subsequent modeling of pH dependence test data. In the top button bar, hit **Case manager** and then hit **Save** to retain the selection.



The results of the SI unit calculation can be viewed by hitting **View results**.



Under **Species series** element selections can be made with the **Edit Species list editor**.



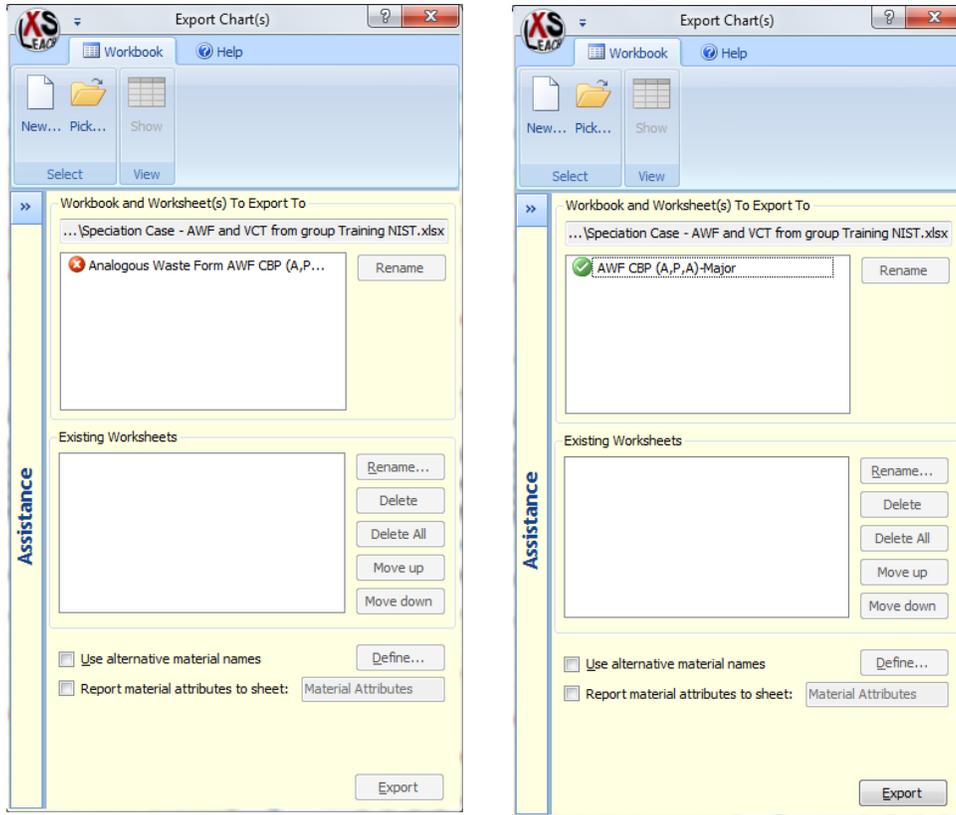
With **Add** one can add a new Substances list. It is only possible to view substances that have been mapped in the model. To view additional substances, the list of substances must be expanded first in the model.

Select a species list to **View results** and select a **Material to view** (bottom of the pane).

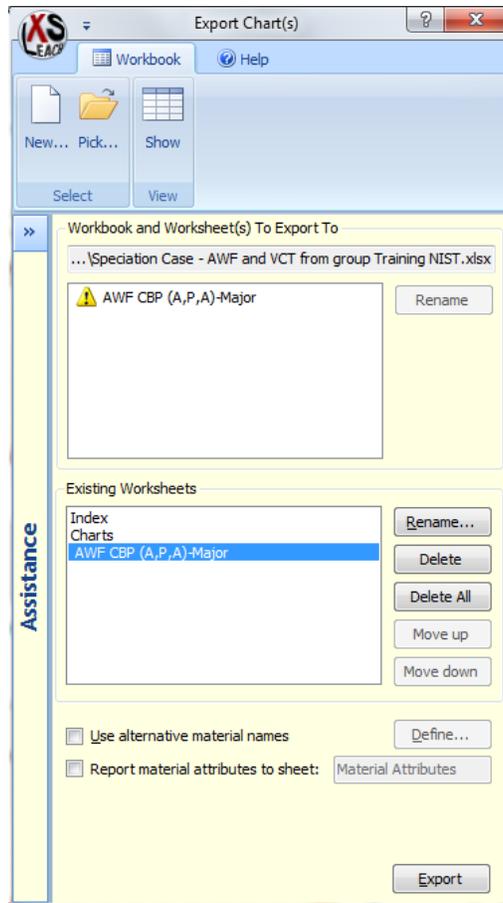


The results can be exported to Microsoft Excel® for separate data handling.

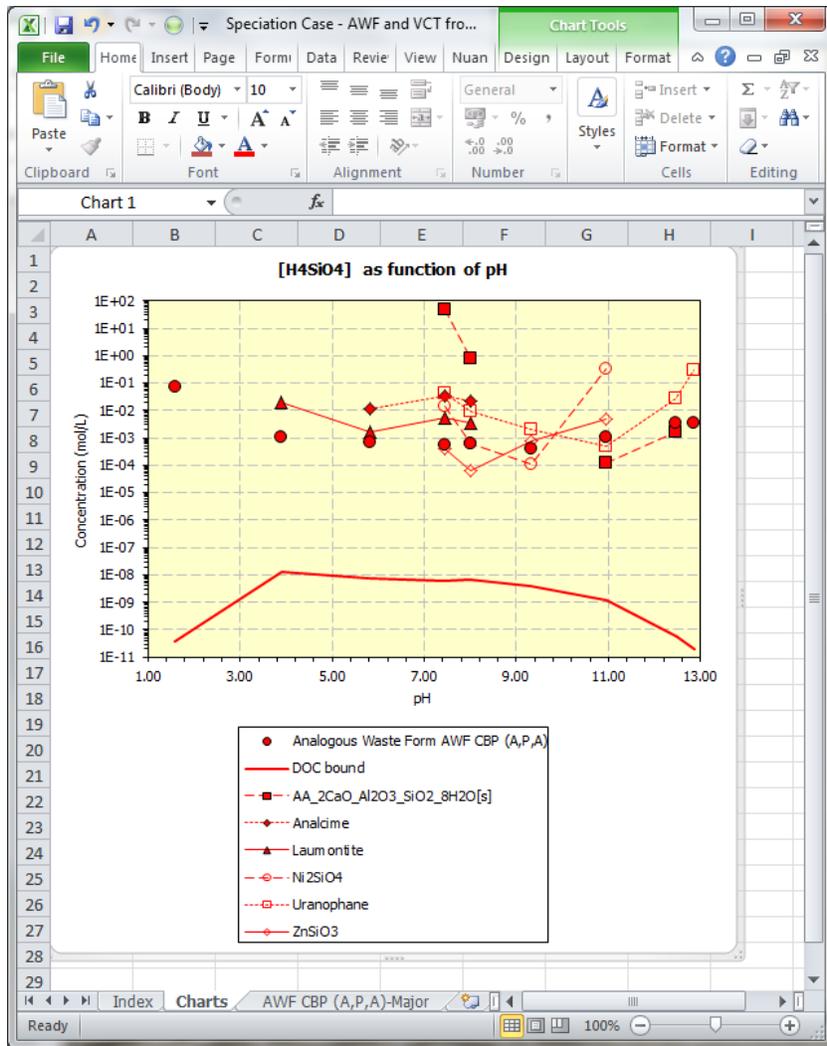
Hit **Export selection** of **Export all**. The first will export a selection of graphs. The latter will export all species in the list.



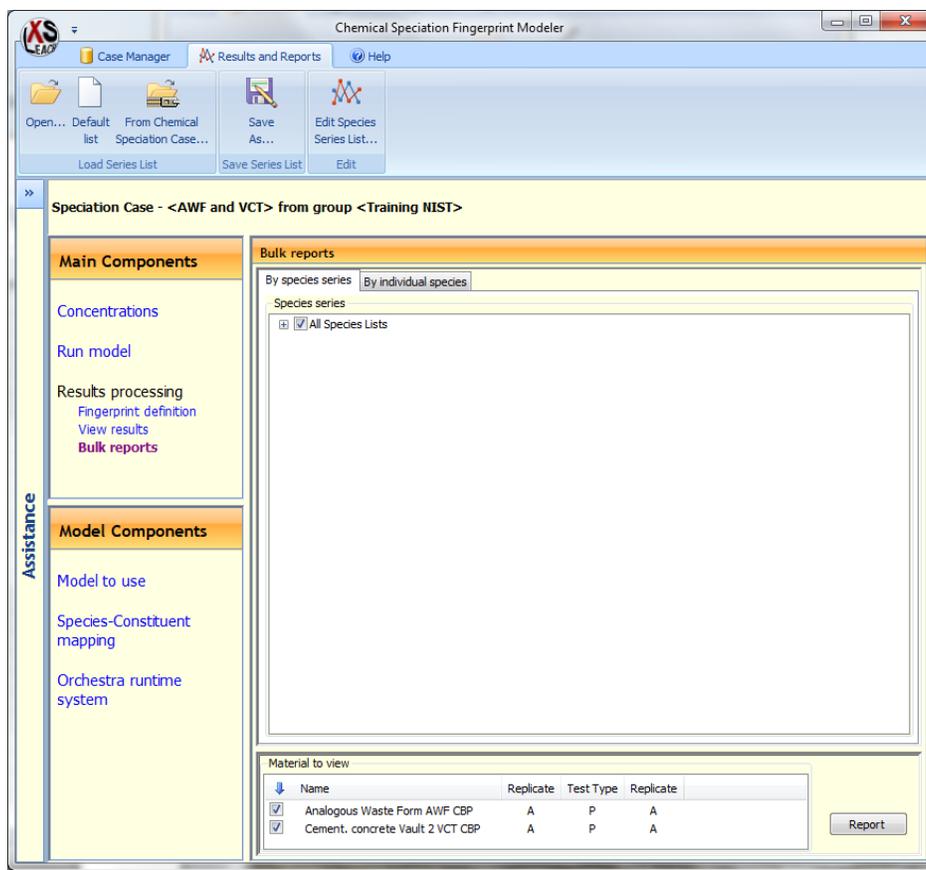
The default name for the worksheet that is to be created is too long, so we need to change the name.



Hit **Show** to see the Microsoft Excel® workbook.



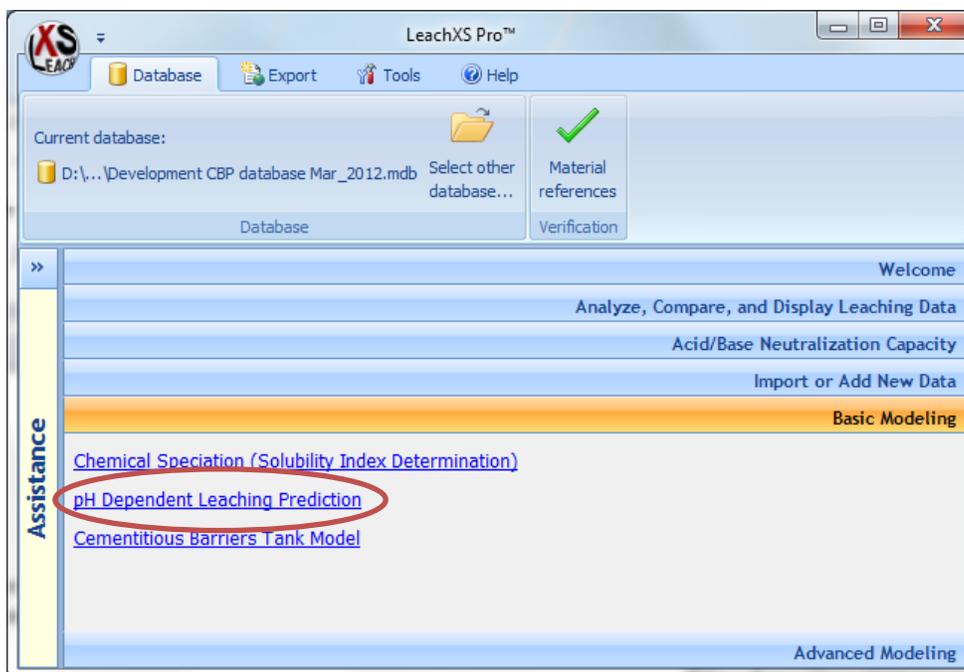
Under **Bulk export** , all selected species lists can be exported to Microsoft Excel® in one go.



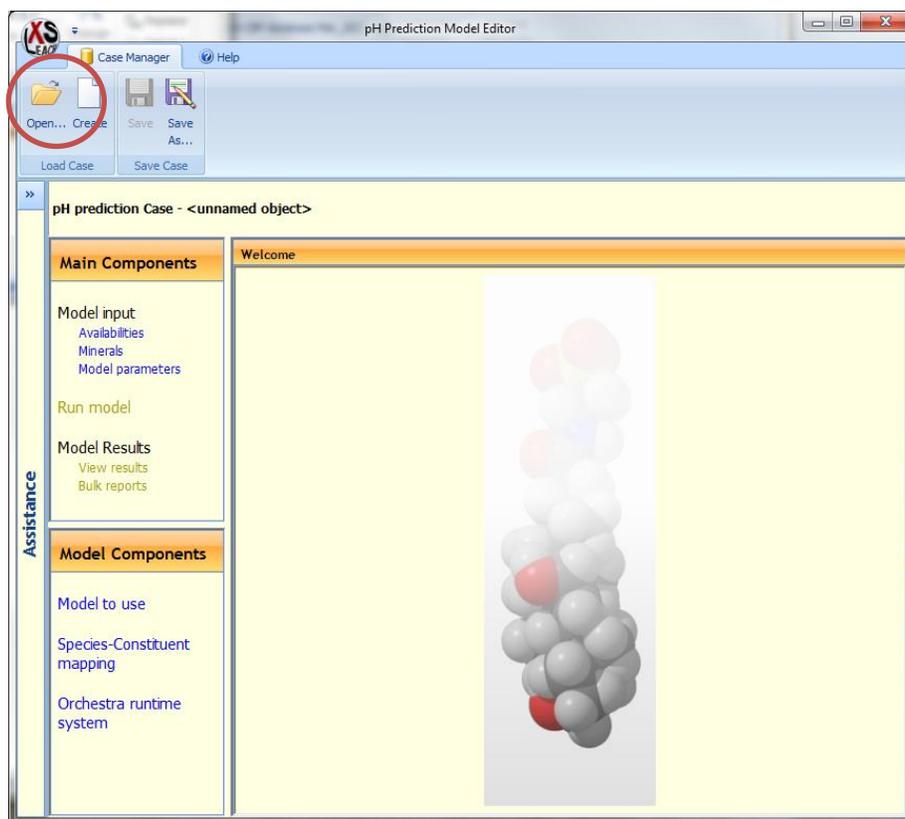
The speciation fingerprint is used in the subsequent pH dependence test modeling.

## pH Dependent Leaching Prediction

The pH Dependent Leaching Prediction model describes the measured leaching behavior in the pH dependent method 1313. The output from “Chemical Speciation Modeling” on page 33 is used to describe the leaching behavior as a function of pH.

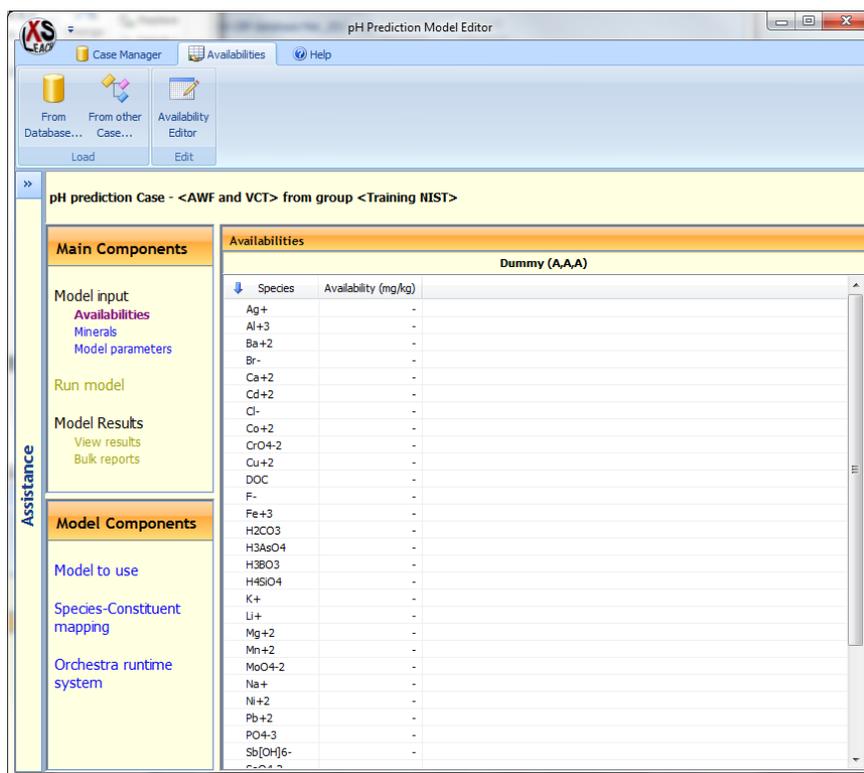


Click on **pH Dependent Leaching Prediction** to start the Model run.



Click **Open** to create a **Group** (here **Training NIST**) and a **Case** (**AWF and VCT**). See “LeachXS Cases and Case Management” on page 100 for details on how to do this.

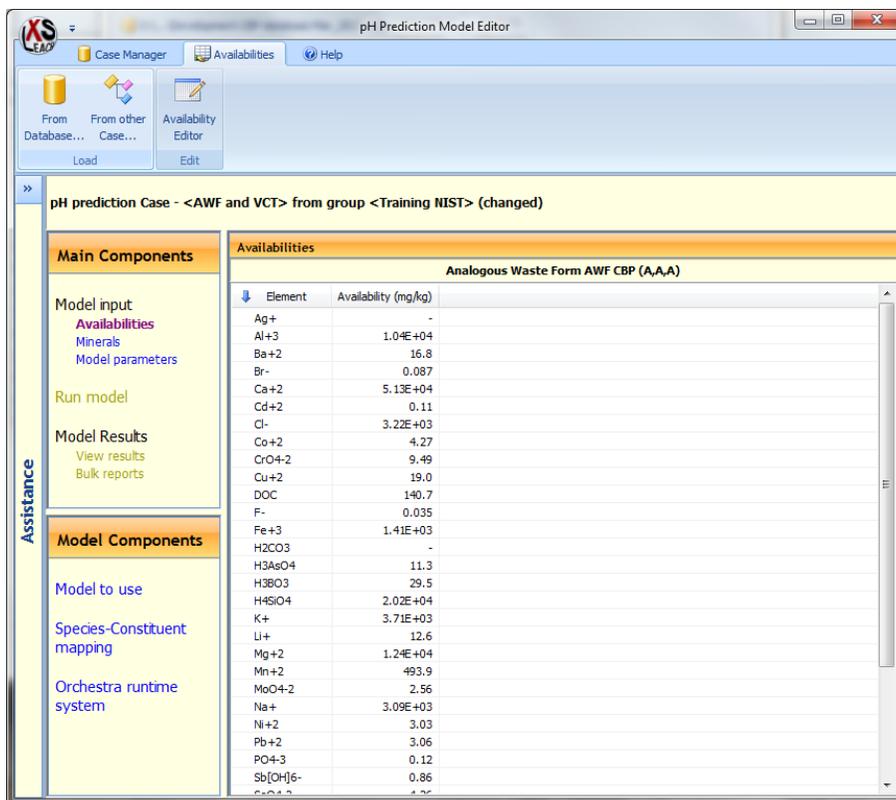
Double click on the created case (**AWF and VCT**) to start the model preparation.



As a first step the information on which the model run is based needs to be loaded. This relates for this model to element **Availabilities**, **Minerals** and **Model parameters**.

To fill the availabilities table either select **From other case** or **From Database...**. Click on **From Database...** to select the material to be modeled (here **Analogous Waste form**).

The **Sample Selector** appears. Select sample **Analogous Waste Form AWF**. For details on how to use the **Sample Selector**, see “The Sample Selector” on page 121.



The composition taken from the database can be adjusted, if needed with the **Availability editor**.

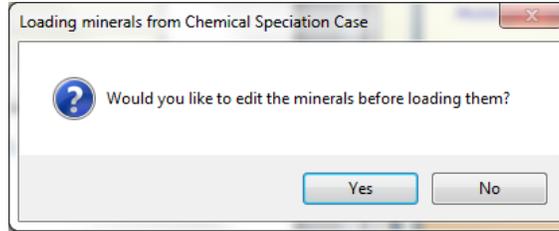
The next step is to include a mineral selection by clicking on **Minerals**. The minerals can be selected from a few different locations:

- By **Load....** The **Case Manager** is shown with groups of mineral sets. If you have saved mineral sets, they will show up here.
- **From a Speciation Object**, such as the one described in “Chemical Speciation Modeling” on page 33.
- **From Other Case...** The **Case Manager** is shown with groups of pH Prediction cases. If you have saved pH Prediction case, they will show up here. The mineral set in the selected case is extracted and put in the current case.

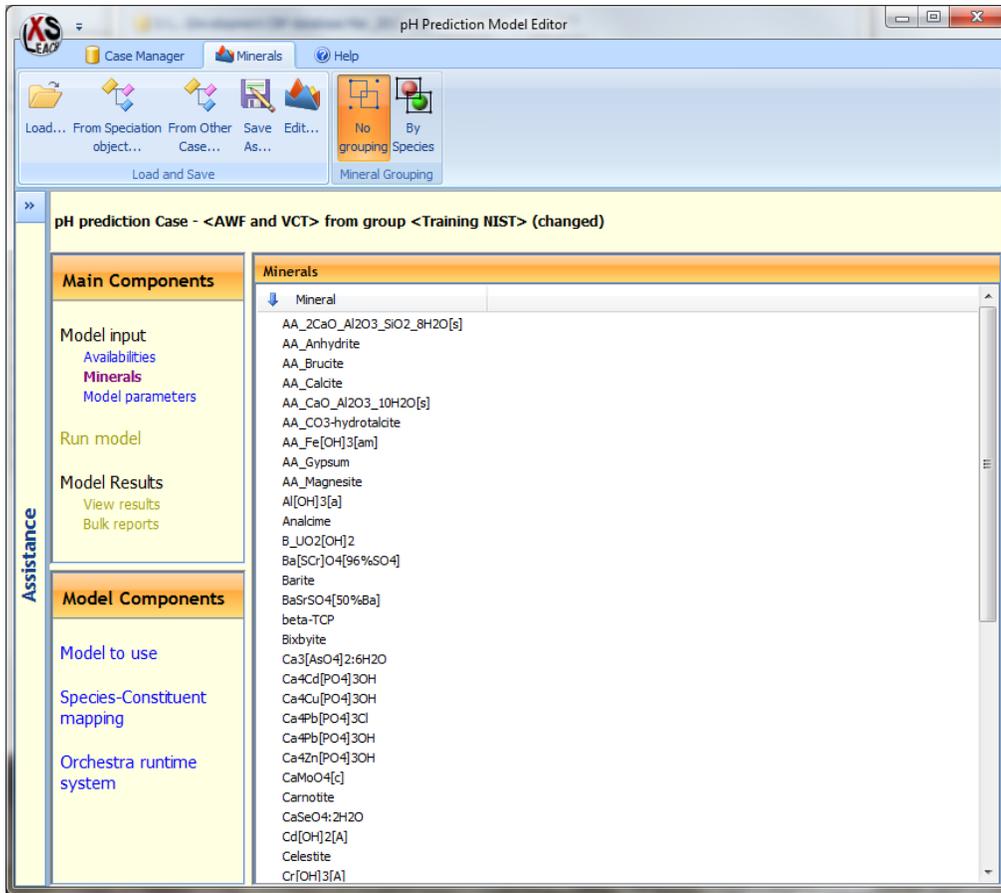
The **Mineral** list can be displayed in two modes: **No grouping** (alphabetical) and grouping **By Species**.

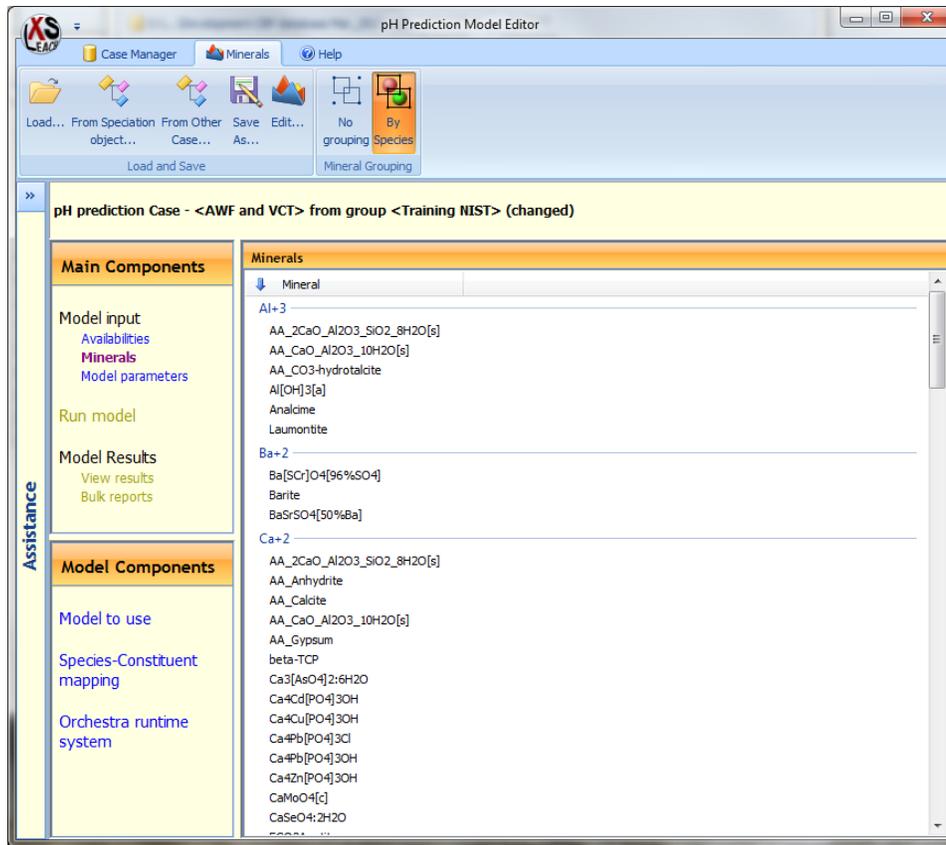
Here we select the second option: **From a Speciation Object**.

Select case **Training NIST** from the **Speciation case manager**. Then select **AWF and VCT**. A message will pop up:

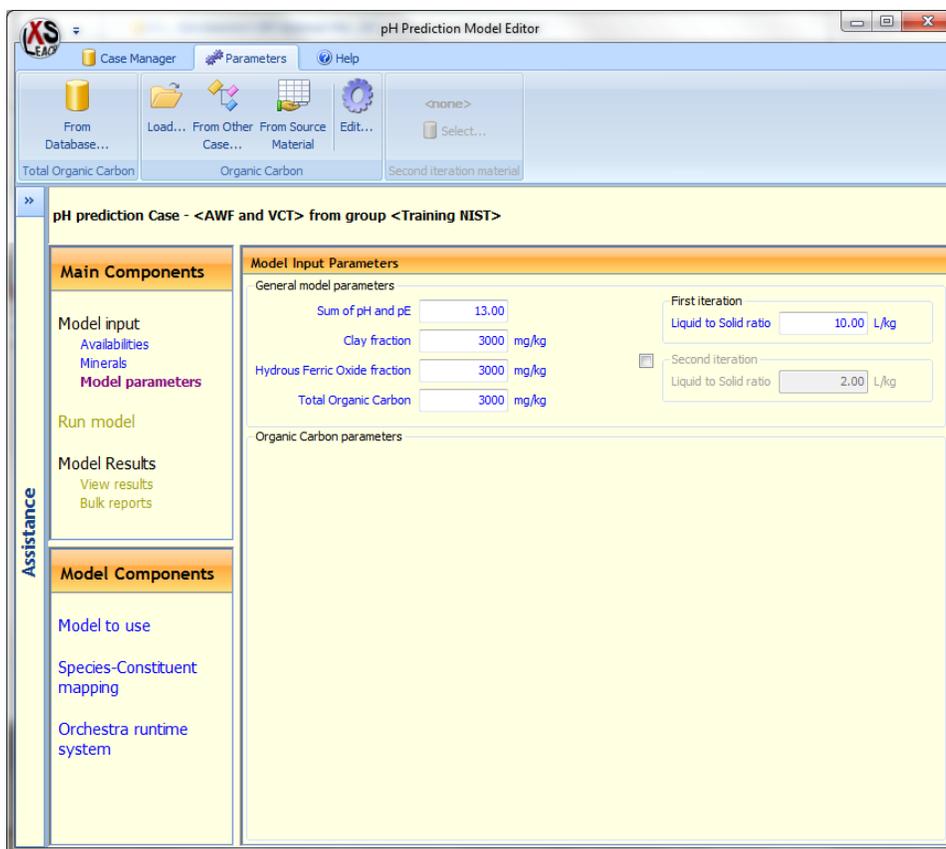


This option gives the possibility to edit the mineral selection. Let's accept the selection by clicking **No**. The mineral sets can be shown in alphabetical order and by Species (See below).





The next step is to incorporate the **Model parameters** into the run.



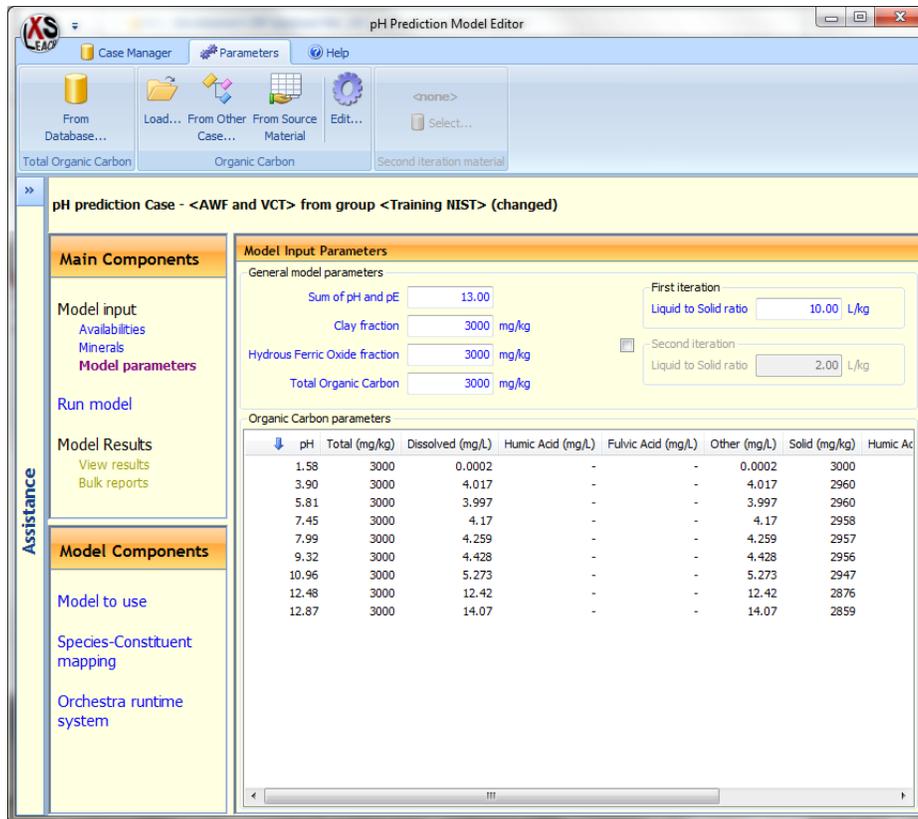
The default values for clay, hydrated iron oxide and total organic carbon can be modified with actual measurements of these parameters (ISO standard 21268 parts 1-5).

The  $pe+pH$  is a measure for the redox state of the material. A value as low as 4 – 6 reflects reducing conditions. A  $pH+pe$  of 8 – 10 indicates mildly reducing conditions. While oxidized conditions prevail for  $pe + pH > 13$ .

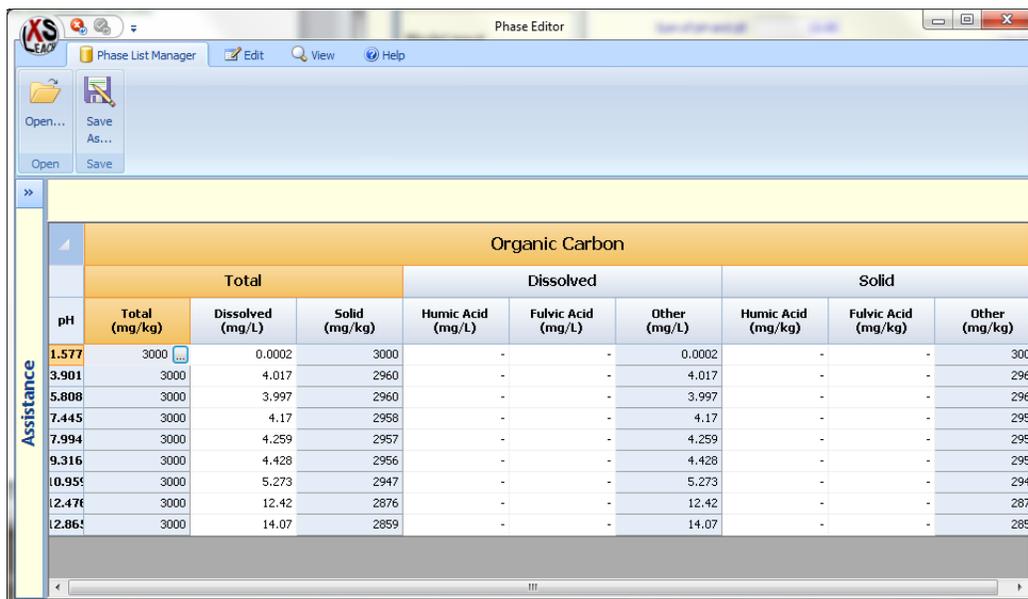
Organic matter is special as there is both dissolved and particulate organic matter. Several metals and radionuclides have a high affinity for organic matter surfaces. Association with dissolved organic matter will increase the mobility of otherwise immobile substances. In DOC complex forms metal are less toxic to organisms, as they cannot release the substance from the organic matter. As organic matter degrades, it will produce dissolved organic matter. Organic matter is present everywhere and thus its role cannot be ignored. The organic matter allows distinguishing between different forms of organic matter and reactive fractions thereof.

Default values for organic matter and its distribution can be provided at a later stage for use in concrete and waste form studies.

Here the base organic matter info is taken from the source material (measured DOC or TOC in eluates of the pH dependence test)



The **Organic matter editor** allows you to define the reactive fraction of DOC for interaction with trace components. As a default value, 20 % can be used, when no data on the actual distribution are available.



By clicking on **View** it is possible to toggle between absolute and percent values. It is easier to work with percent values.

The screenshot shows the 'Phase Editor' window with a table titled 'Organic Carbon'. The table has columns for pH, Total (%), Dissolved (%), Solid (%), Humic Acid (%), Fulvic Acid (%), Other (%), Humic Acid (%), Fulvic Acid (%), and Other (%). The data rows show various pH values and their corresponding percentages for Total, Dissolved, and Solid phases, along with the composition of the dissolved phase.

pH	Total			Dissolved			Solid		
	Total (%)	Dissolved (%)	Solid (%)	Humic Acid (%)	Fulvic Acid (%)	Other (%)	Humic Acid (%)	Fulvic Acid (%)	Other (%)
1.577	100	6.667E-05	100	20	-	80	-	-	100
3.901	100	1.339	98.66	20	-	80	-	-	100
5.808	100	1.332	98.67	20	-	100	-	-	100
7.445	100	1.39	98.61	-	-	100	-	-	100
7.994	100	1.42	98.58	-	-	100	-	-	100
9.316	100	1.476	98.52	-	-	100	-	-	100
10.95	100	1.758	98.24	-	-	100	-	-	100
12.47	100	4.14	95.86	-	-	100	-	-	100
12.86	100	4.69	95.31	-	-	100	-	-	100

By hitting the green button at the top left, the settings are saved in the case. Sometimes an error message occurs. Ignore this and save again.

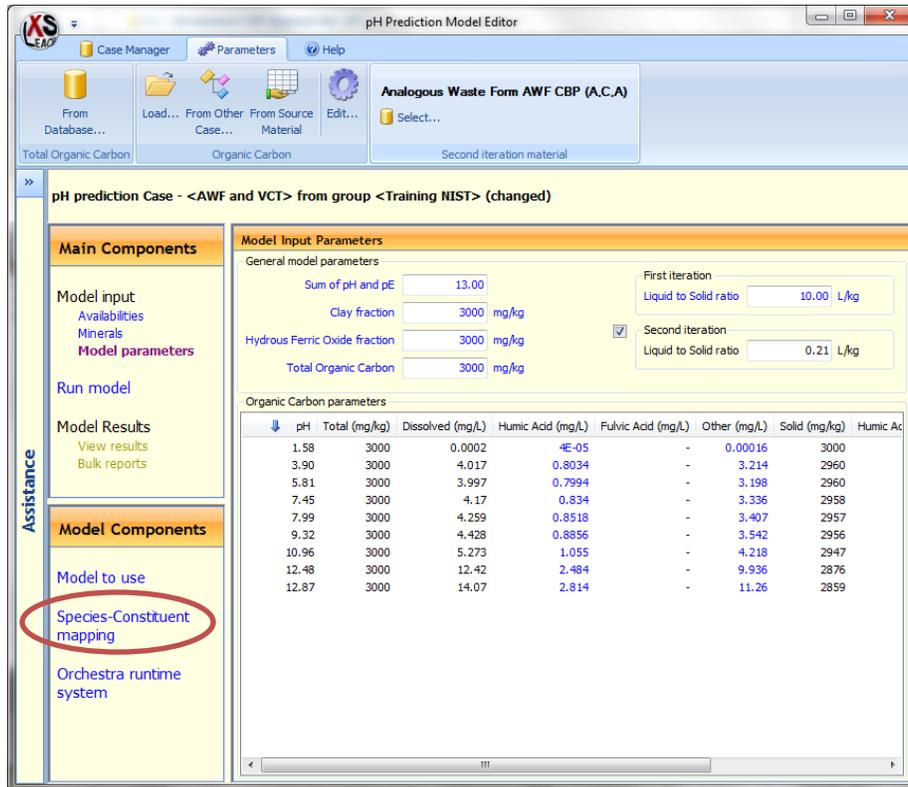
The screenshot shows the 'pH Prediction Model Editor' window. It displays 'Model Input Parameters' and 'Organic Carbon parameters'. The 'Model Input Parameters' section includes 'General model parameters' and 'Organic Carbon parameters'. The 'Organic Carbon parameters' section shows a table of results for various pH values, including Total (mg/kg), Dissolved (mg/L), Humic Acid (mg/L), Fulvic Acid (mg/L), Other (mg/L), and Solid (mg/kg).

pH	Total (mg/kg)	Dissolved (mg/L)	Humic Acid (mg/L)	Fulvic Acid (mg/L)	Other (mg/L)	Solid (mg/kg)	Humic Ac
1.58	3000	0.0002	4E-05	-	0.00016	3000	
3.90	3000	4.017	0.8034	-	3.214	2960	
5.81	3000	3.997	0.7994	-	3.198	2960	
7.45	3000	4.17	0.834	-	3.336	2958	
7.99	3000	4.259	0.8518	-	3.407	2957	
9.32	3000	4.428	0.8856	-	3.542	2956	
10.96	3000	5.273	1.055	-	4.218	2947	
12.48	3000	12.42	2.484	-	9.936	2876	
12.87	3000	14.07	2.814	-	11.26	2859	

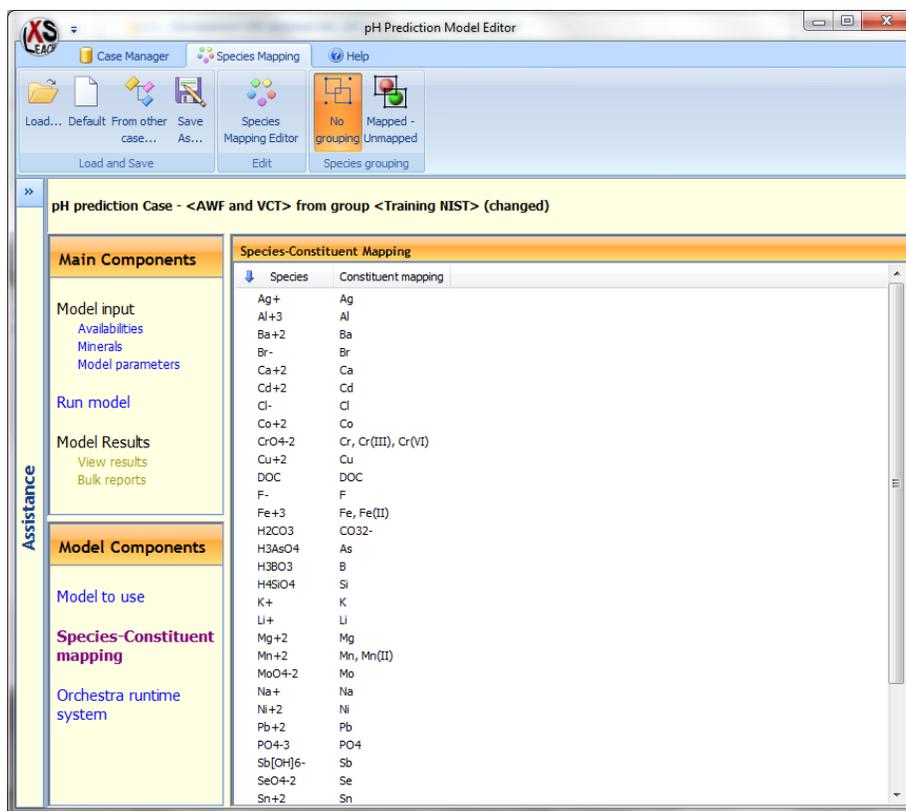
The L/S (liquid to solid ratio (L/kg) to be used is given by the pH dependence test as 10. It is possible to run a low L/S in parallel to the L/S=10 condition to assess to what extent the model result at L/S=10 adequately described the release at low L/S. This condition can be selected by hitting the tick mark at

**Second iteration.** If this condition is selected a **Second iteration material** needs to be selected. For this material the L/S to reflect porewater needs to be selected. Generally a value of 0.2 - 0.3 is adequate.

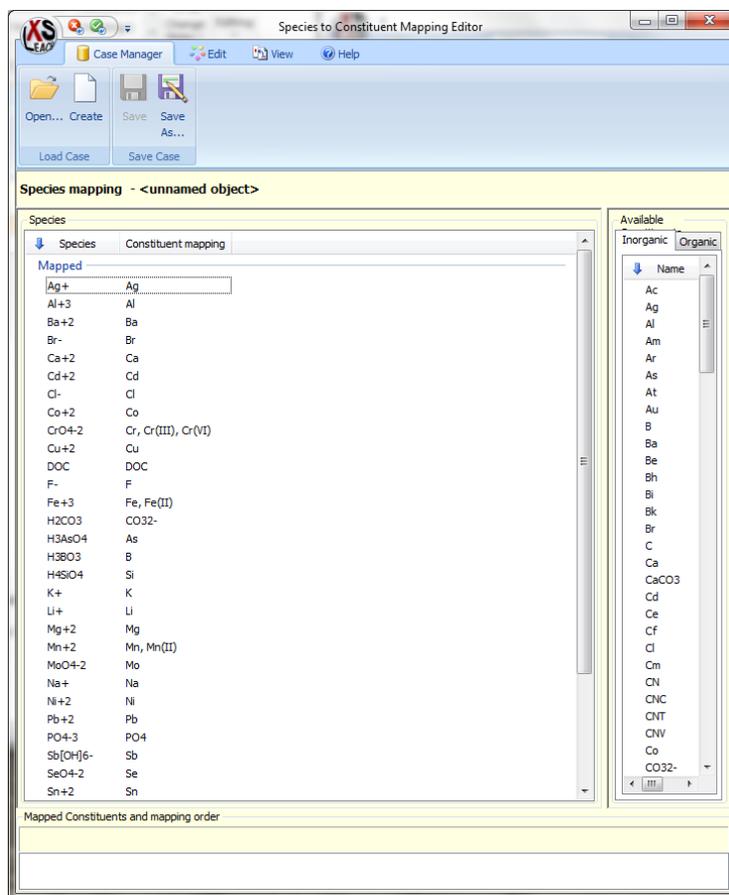
Hit the **Select...** button in tab group **Second iteration material**. The **Sample Selector** will show up. Choose the percolation test of sample **Analogous Waste Form Awf CBP (C,1,1)**.



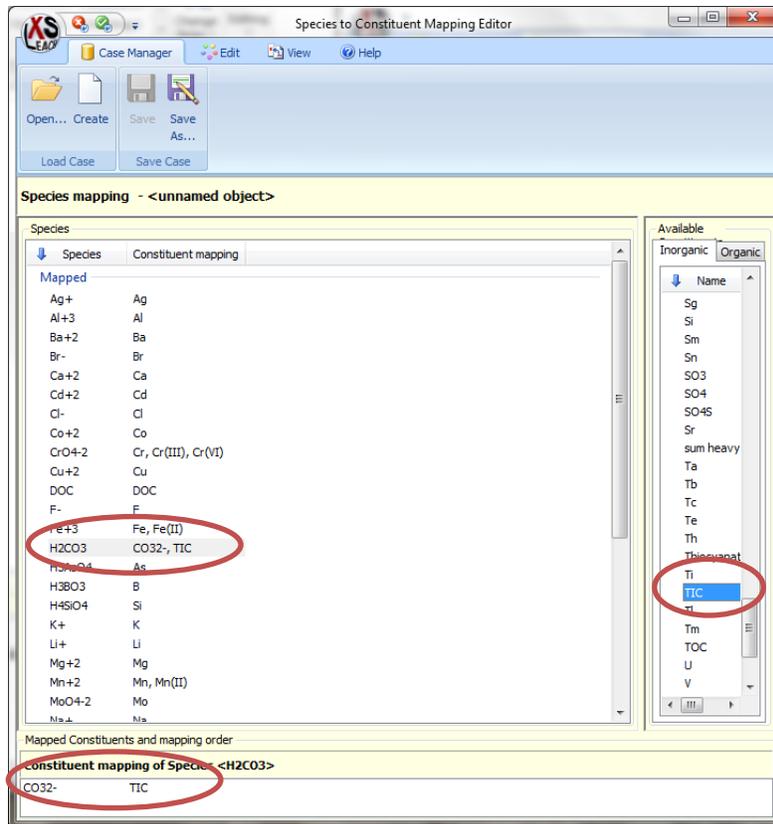
Before the run is actually started, it is good to check that all species in the model are adequately mapped. This is done by hitting **Species-Constituent mapping**.



Hit **Species mapping editor** to verify that all species are mapped adequately. If not, they won't be part of the modeling run.



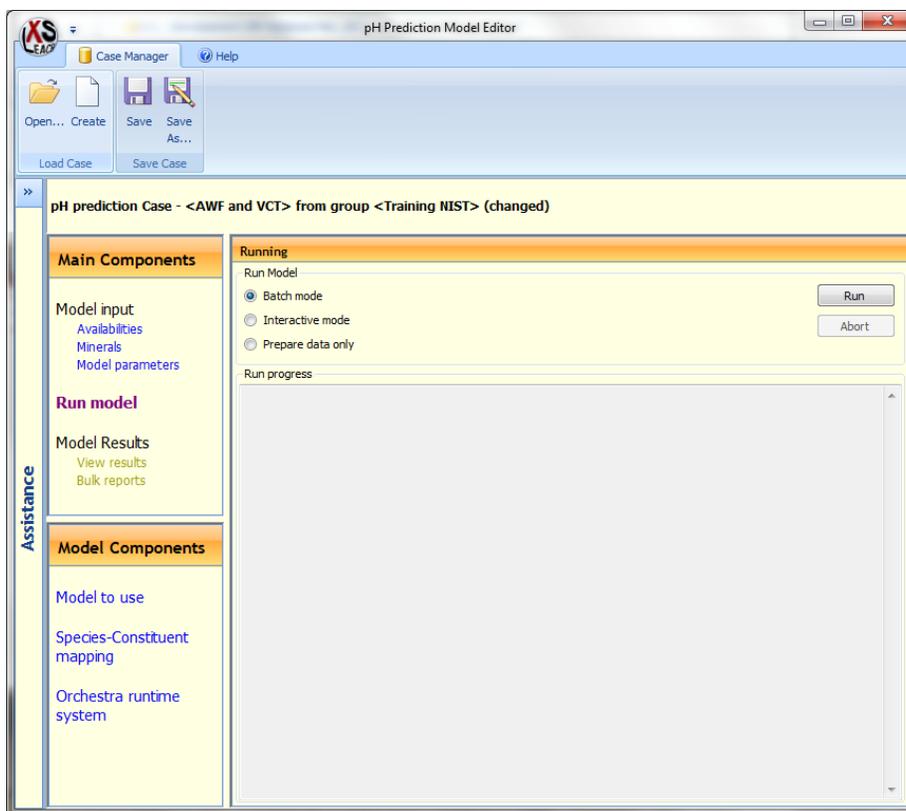
To map TIC on carbonate: click on **H2CO3** and double click on **TIC**.



Hit the green button at the top left of the pane.

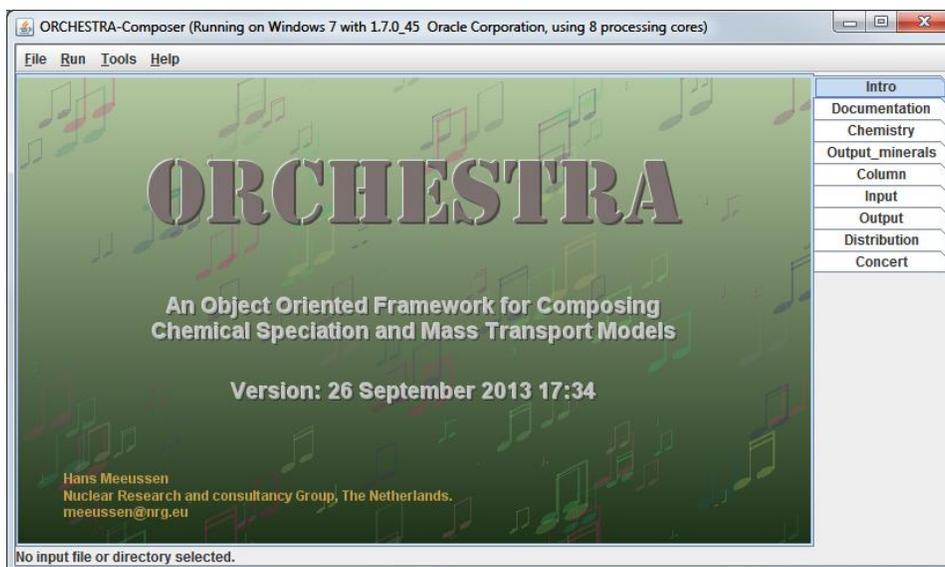
The settings can now be saved by clicking on the **Save button** at the **Case Manager** level (top bar).

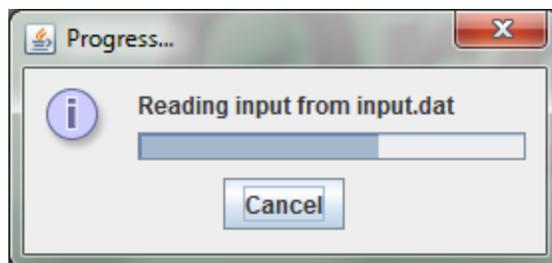
Now all is set to run the model. Click **Run model**.



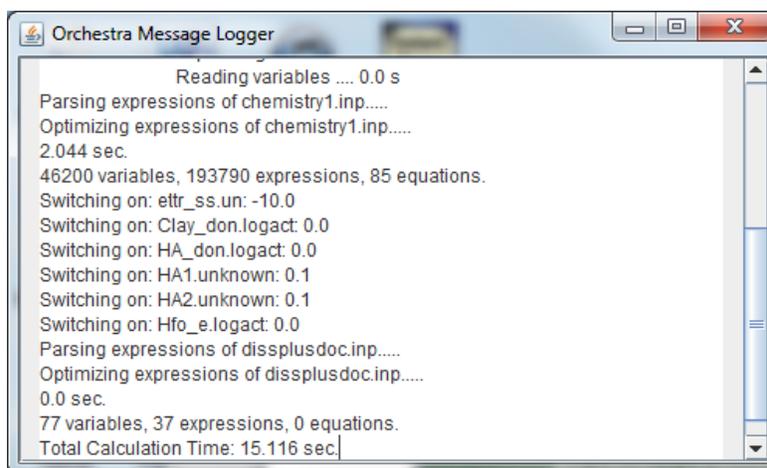
The model can be run either in **Batch mode** or **Interactive mode**. For this model **Prepare data only** is not so functional, unless the process of importing data and modifying the model run needs to be continued at a later time.

To understand what is happening in the background it is useful to run Orchestra interactively. Hit **Run** to start the model.

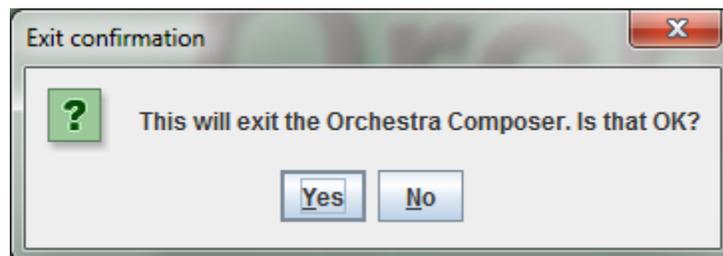




A progress bar will show up, indicating the progress of the model calculations. A log of actions that are taken during calculations is shown as well:

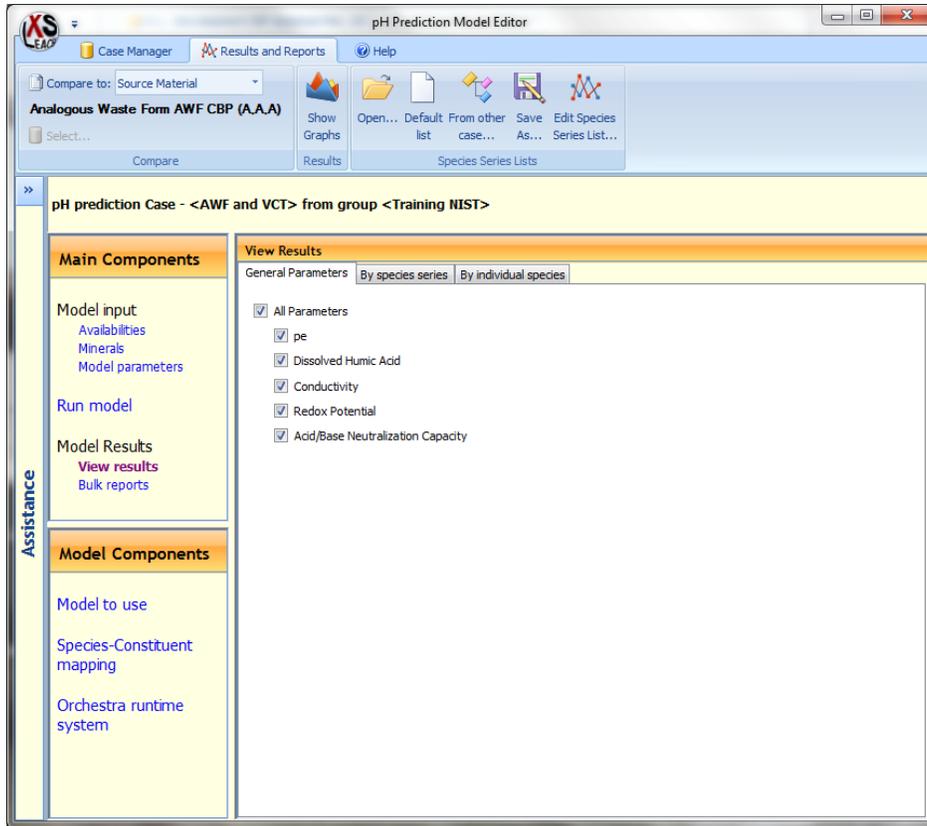


To close Orchestra and return to LeachXS, hit the cross on the top right hand corner of the main window. Confirmation will be asked:



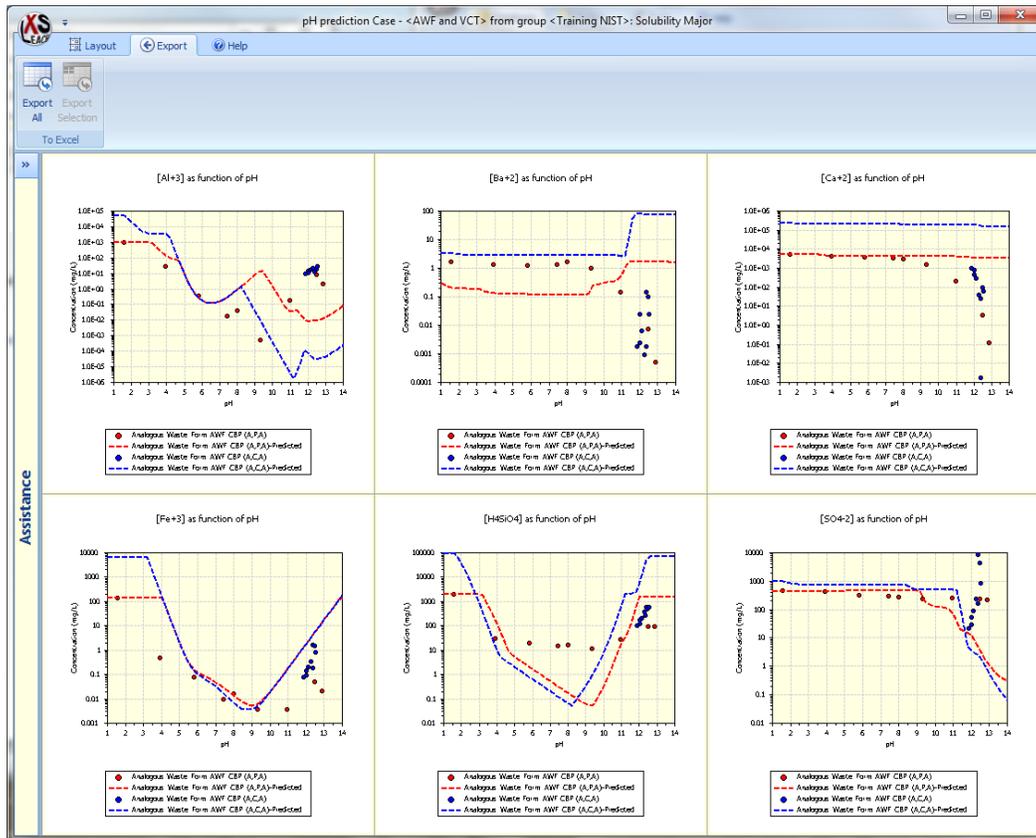
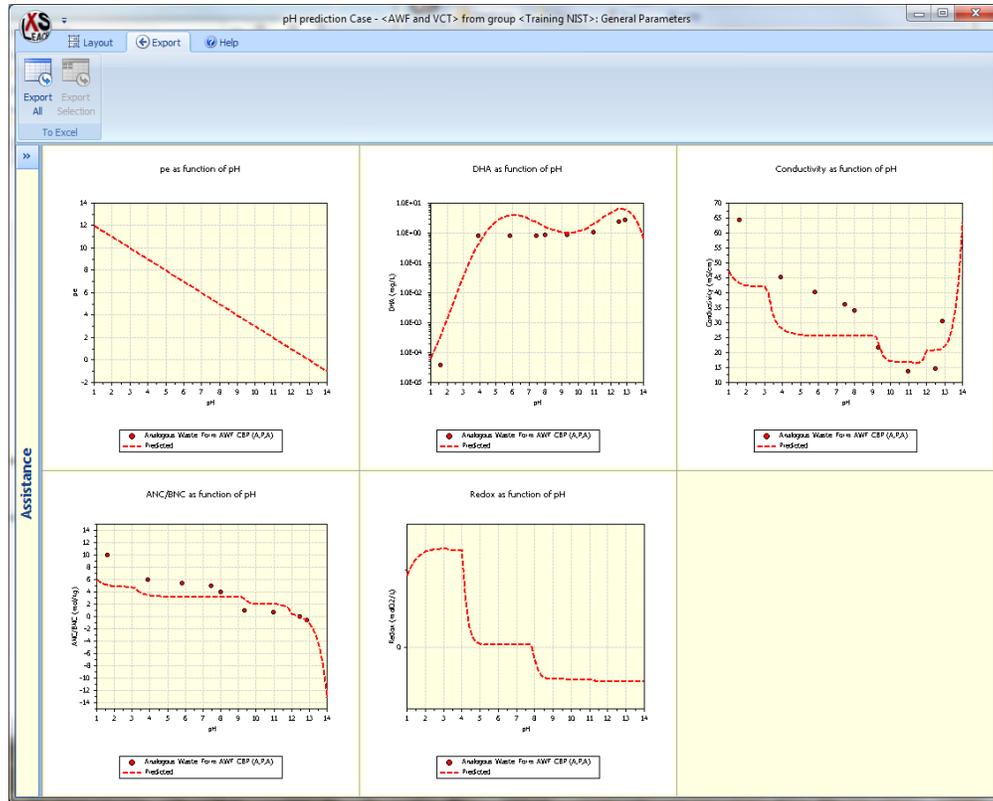
Hit **Yes** in the confirmation screen that pops up to close Orchestra and transfer the model output data to LeachXS.

Hit **Save** to save the results of the run. Hit **View** to visualize the model results.



Tick **Show graphs** to view the results of **General parameters**, **By species series** or **By Individual species** respectively.

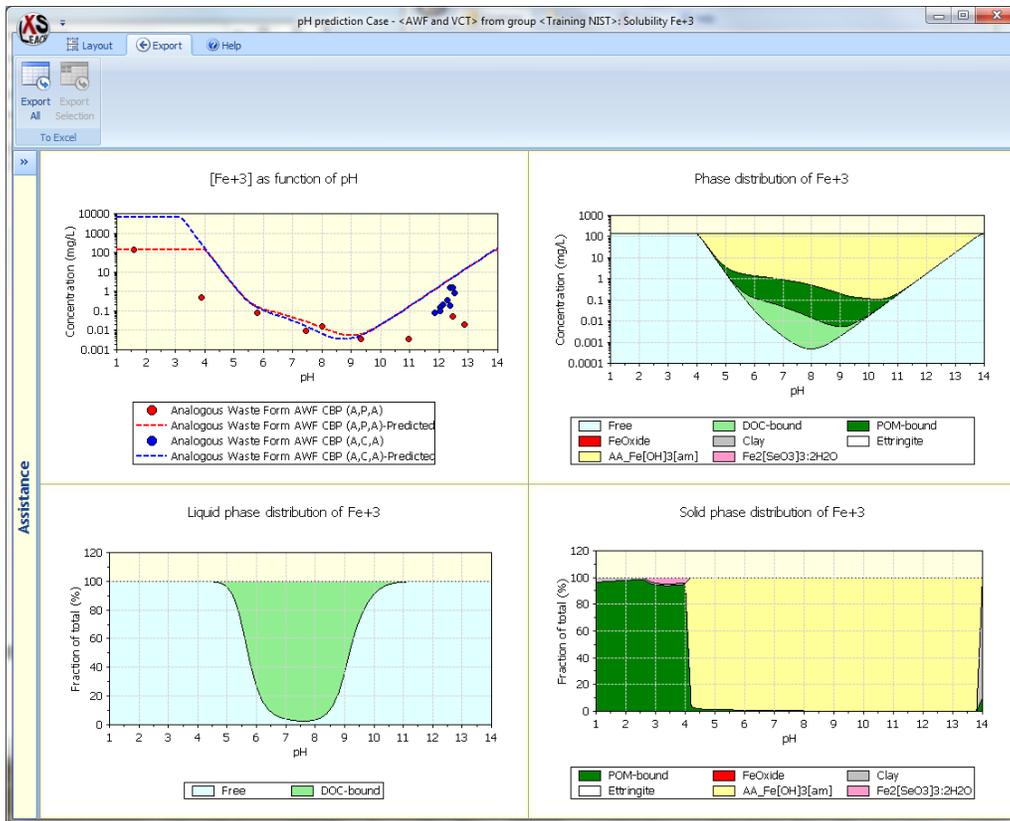
Here are examples of the various views.



The red dots are the pH dependent leaching test data (Method 1313). The blue dots are the percolation test data (Method 1314). If the data overlap, the conclusion is that the substance is solubility controlled and pH and redox are more important controlling factors of release than L/S (liquid to solid ratio).

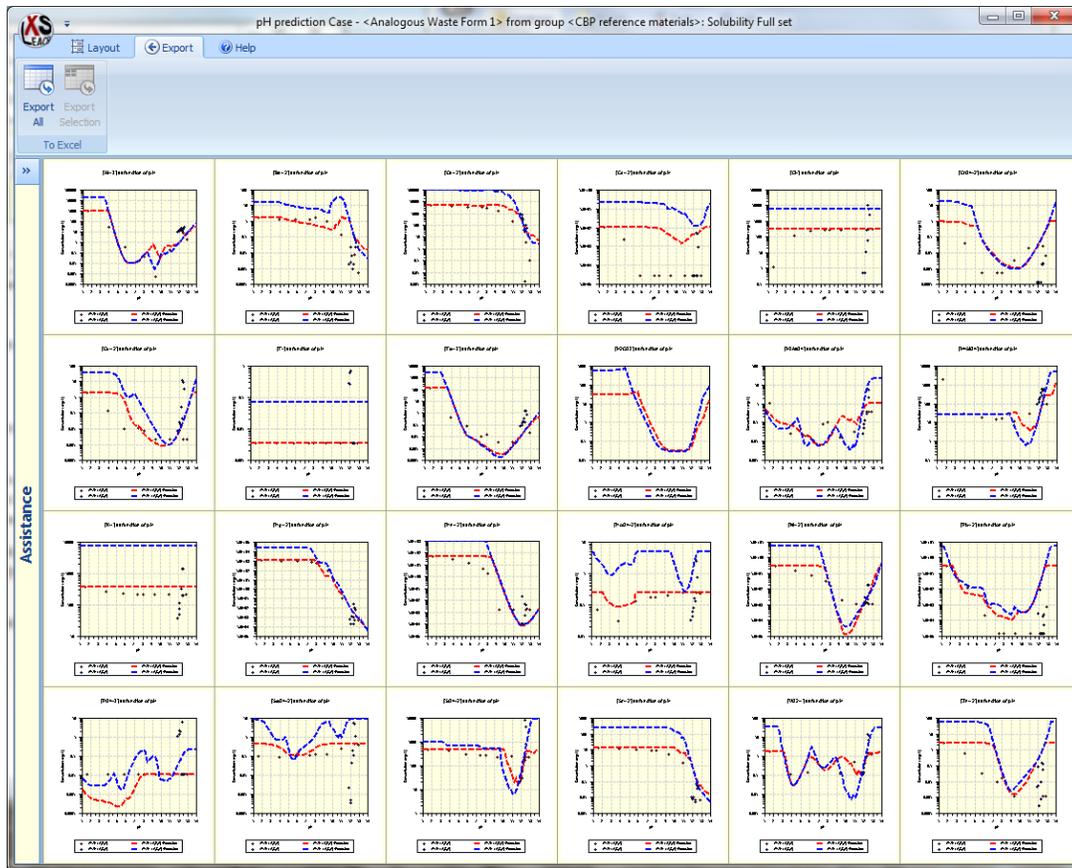
This is a very crucial observation for long term prediction potential.

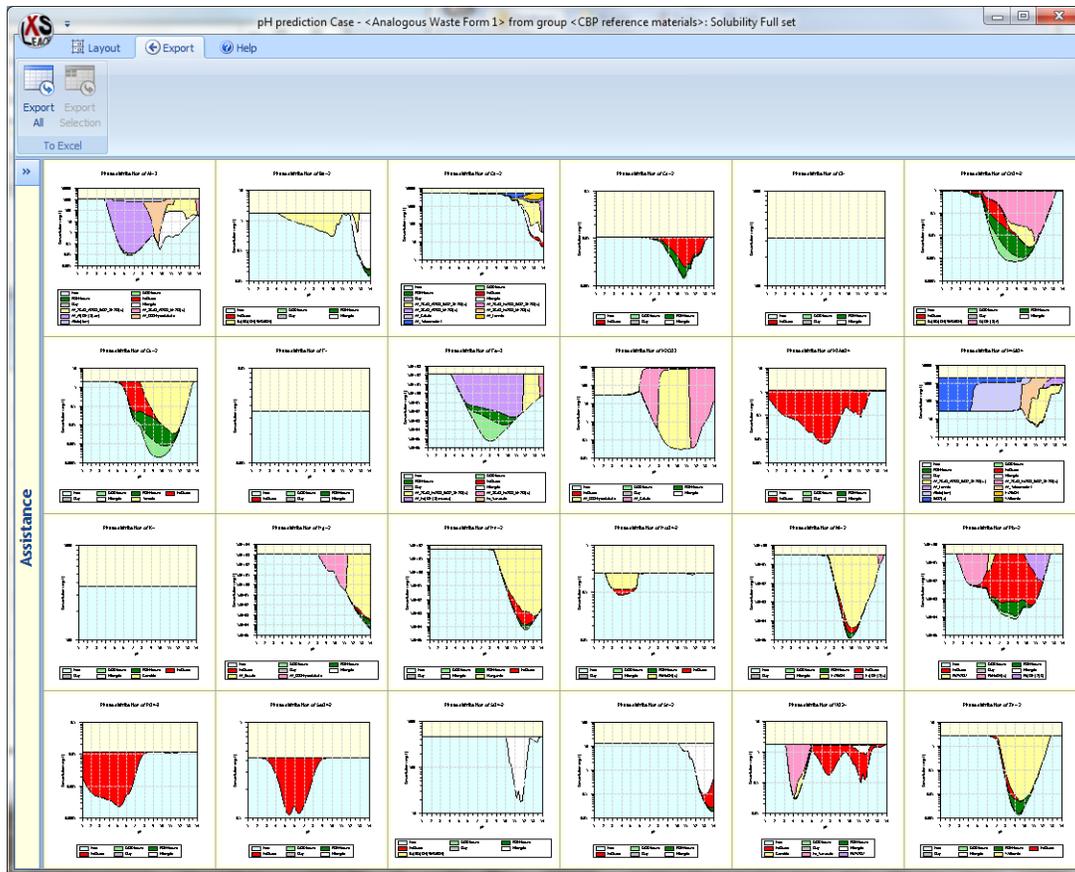




In an iterative approach the description can be optimized to describe all major, minor and trace substances in an optimized condition.

An optimized fit is shown for AWF (Waste form) below and will be made available at the training, as well as optimized model runs for all other CBP materials.





From these further modifications can be modeled, such as imposed reducing conditions, carbonation, addition of radionuclides, change in model parameters like HFO (hydrated iron-oxide content, variations in organic matter content, changes in trace element content, etcetera.

The pH dependence test modeling in combination with the percolation test covers a wide range of pH and L/S conditions and results in a Chemical Speciation Fingerprint (CSF) that can be used as basis for subsequent modeling of mass transfer cases.

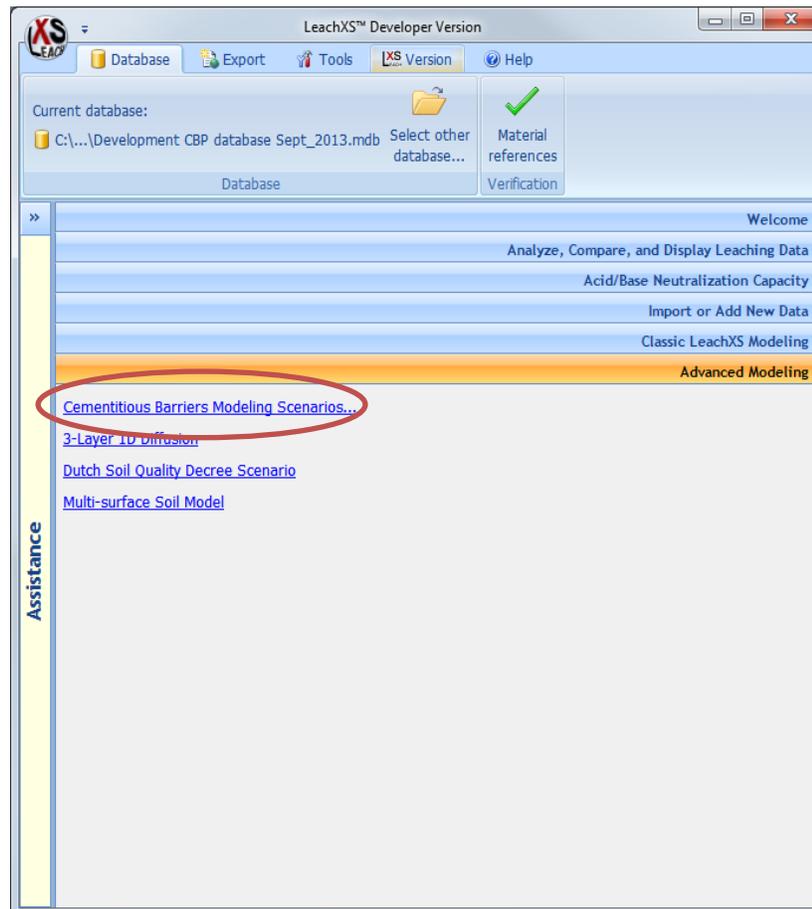
The CSF consists of element availabilities, reactive surface quantification (clay, Iron oxides, and organic matter), minerals and redox status.

## **Tank Model**

(No description available yet...)

## Advanced Modeling

The most advanced models that are disclosed in LeachXS are displayed in the Advanced Modeling roll-up menu. In particular, all models that are developed in the Cementitious Barriers project can be found here.

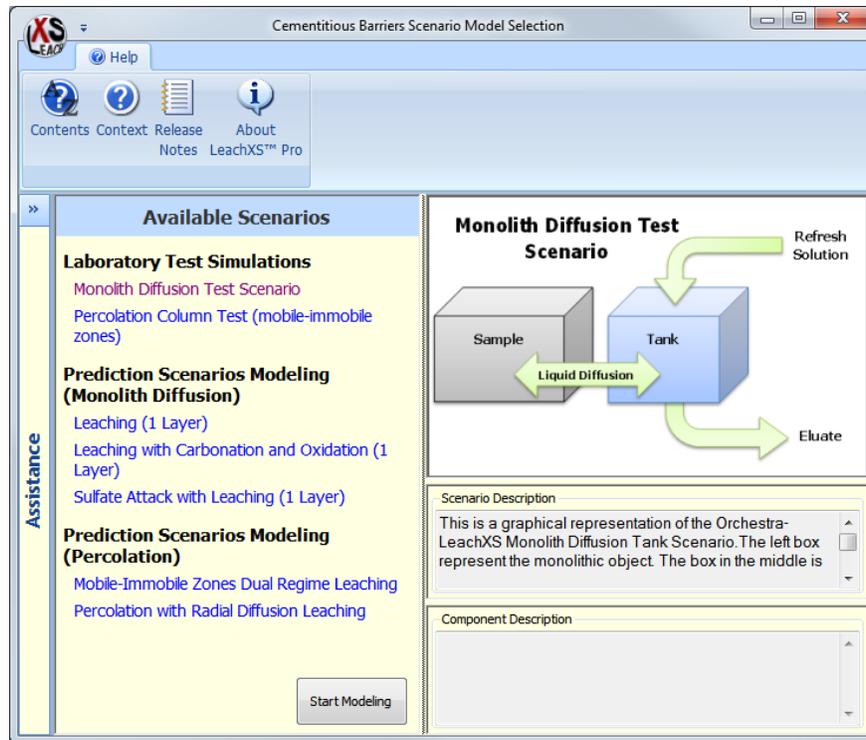


### Cementitious Barriers Modeling Scenarios ...

The development of scenarios for the Cementitious Barriers Partnership (CBP) follows the following general path:

- Within ORCHESTRA, a conceptual model is developed to describe sub-scenarios for CBP-relevant problems in HLW tank closure, waste vault disposal, spent fuel pool storage, and D&D activities.
- After preliminary testing, the model is implemented in LeachXS to allow easy data input preparation and output handling in graphical tabular and export mode.

The family of CBP models is accessed through the [Cementitious Barriers Modeling Scenarios ...](#) link.



If you click on one of the available scenarios, a schematic diagram of the selected scenario will appear in the top right pane. In the example above, the **Monolith Diffusion Test Scenario** has been clicked. You can adjust the size of the window. You can also enlarge or reduce the size of every pane by dragging its border up, down, left or right.

The models that have been developed are categorized in:

- **Lab test simulations**

The currently implemented scenarios are:

- *Monolithic Diffusion Test Scenario*  
Simulates tank test leaching results
- *Percolation Column Test (mobile-immobile zones)*  
Simulates column test results considering a dual regime equilibrium/convection approach

- **Prediction scenarios for monolithic diffusion**

Simulates leaching from single systems of containing monolithic materials with options for physical/chemical degradation from:

- *Leaching (1 Layer)*
- *Sulfate Attack with Leaching (1 Layer)*  
The sulfate attack model is a model developed for the CBP to address degradation of the cement barrier by elevated sulfate levels in contact with the barrier either from within or outside the barrier. The subject has been one of the subjects worked out by Sohini Sarkar

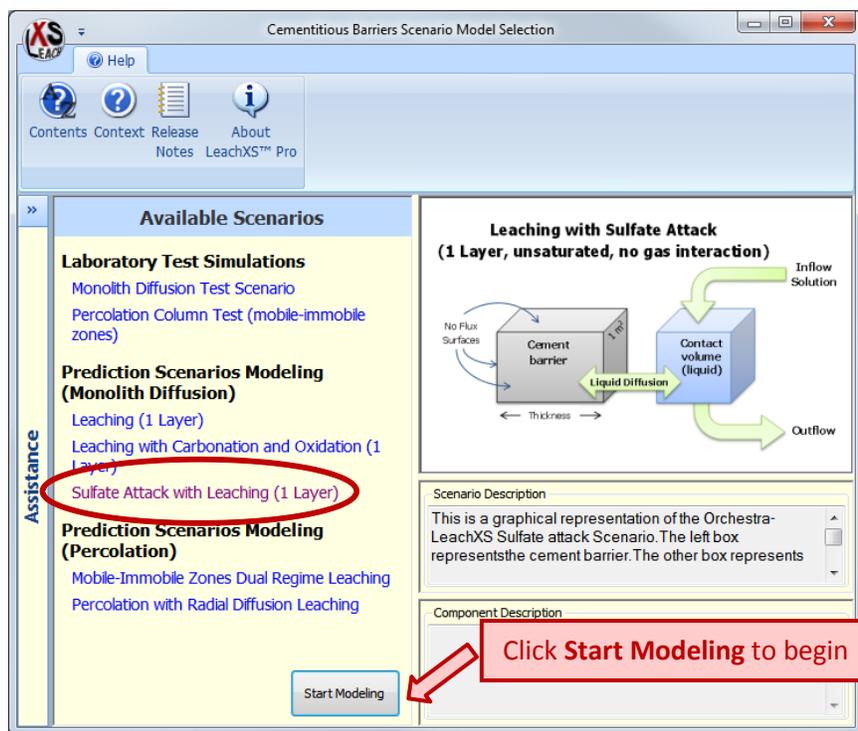
for her Thesis at VU. It is one of a series of sub-models to be implemented in LeachXS to be used through the GoldSim Bridge in GoldSim simulations.

- *Leaching with Carbonation and Oxidation (1 Layer)*
- **Prediction scenarios for percolation**

The currently implemented scenarios are:

- *Mobile-immobile Zones Dual Regime Leaching*
- *Percolation with Radial Diffusion Leaching*

To begin the sulfate attack modeling process, highlight a sulfate attack modeling the **Available Scenarios** pane and click on **Start Modeling**.



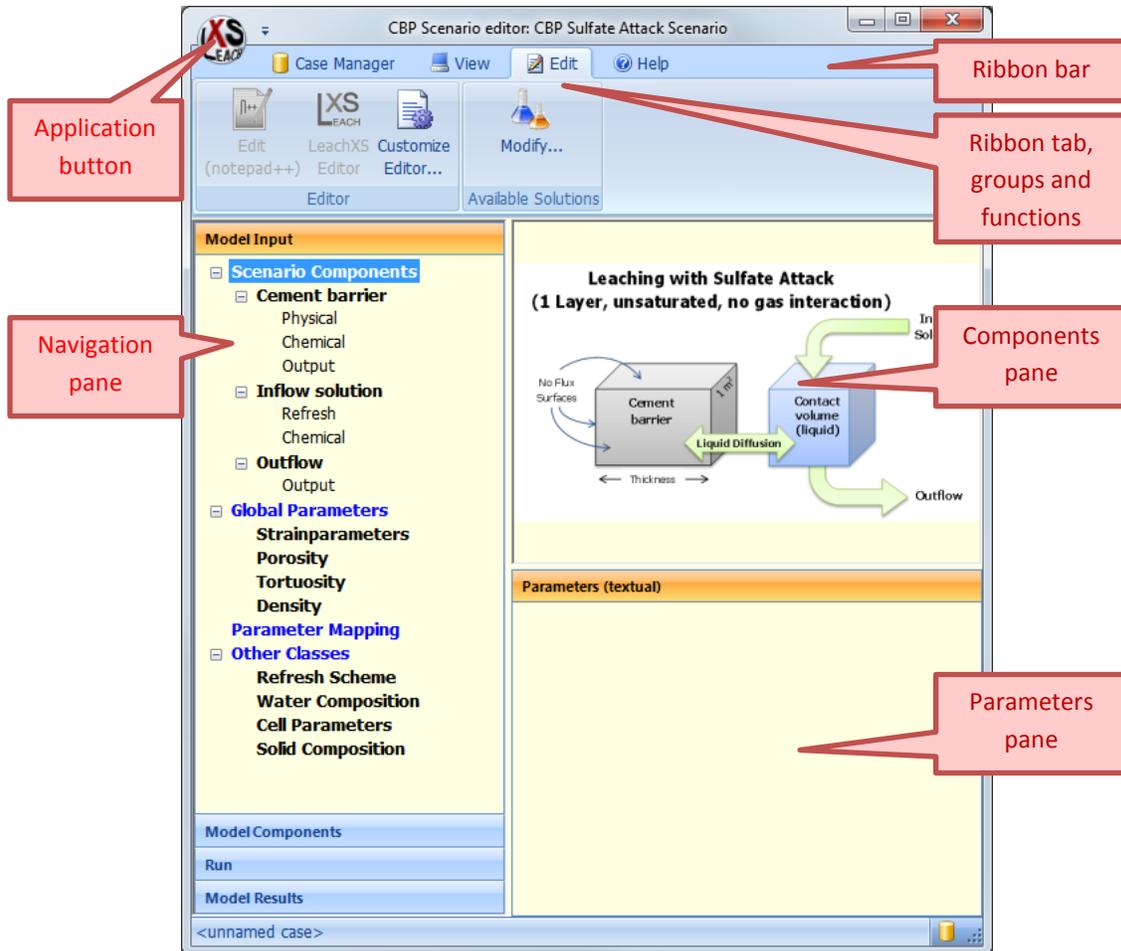
The **CBP Scenario Editor** will show up. The editor will assist you in:

- Editing input data for a model;
- Running the model;
- Showing model results;
- Saving your work;
- Opening previously saved sessions.

## The CBP Scenario Editor

The **CBP Scenario Editor** is a framework for working with CBP scenarios. It designed to have a consistent look and feel for all CBP models, although some parts of the editor may not be available for a specific model. For instance, the option to select a monolithic lab test that is to be simulated will only be available for a lab test simulation model and not in any prediction scenario for monolithic materials.

Below is an overview of all the elements that are part of the editor.



The description below summarizes the main functions of the editor. In order to see all options that are described, check the box **Show Advanced Options** on ribbon tab **View** in the ribbon bar.

### Scenario Editor components

#### Navigation pane

This pane is used to navigate through all information of the model that can be edited or shown. It will also assist you in running the model and showing results. The pane is divided in four sections, grouping

similar aspects of the model together. You can expand a section by clicking on its header. If you do so, the clicked section will expand itself, while other sections are collapsed.

Section **Model Input** shows all building blocks of the model and the input data associated with them. Every phrase in the section is a link. Clicking it will reveal the data associated with it.

Section **Model Components** shows configuration data for the model: the files that comprise the entire model, the Orchestra files needed to run a model and more. You'll probably won't visit this section, unless you are an advanced user.

Section **Run** contains options to run the model.

Section **Model Results** will enable you to make selections in the model results to be displayed and reported.

### **Components pane**

The model picture pane shows the same schematic picture of the model as the one that was displayed in the **Model Chooser**. It can be used as an alternative to navigate through the scenario components. If the **Model Input** panel or **Model Results** panel is expanded, clicking on a segment of the picture will select the corresponding scenario component in the panel.

### **Parameters pane**

The content of this pane depends on what section of the navigation pane is selected. When the **Model Input** section is expanded, a description of the selected entry is shown. If you have checked the box **Show Advanced Options** on ribbon tab **View** in the ribbon bar, you'll see that part of the Orchestra input file that contains input data for the selected entry. When the **Model Components** section is expanded, you'll see details of the specific model component you have selected. When the **Run** section is expanded and the model is running, you'll see details about the progress of the run. When the **Model Results** section is expanded, it will contain options to specify what results are to be shown.

### **Ribbon bar and its elements**

The ribbon bar contains all functions you can use to manage your model input and show results and reports. All functions are organized in different ribbon tabs. Within a ribbon tabs, ribbon groups are used to group functions that belong logically together.

### **Application button**

Clicking on the application button will reveal two lists. The left list contain general functions that are applicable to many windows and the right list contains the most recent cases that you have used for the particular type of model you are working with.

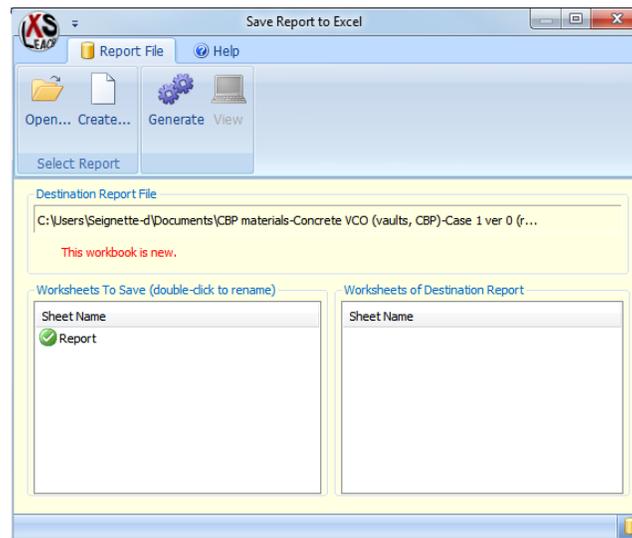
## Organizing your work

The CBP Scenario Editor offers you facilities to save all changes you made. All input data, model files and model components like minerals and Orchestra files are bundled into one document called a **Case**. Cases can be saved for later use and opened again. The ribbon tab group **Case Manager** gives access to the LeachXS **Case Manager**, which helps you saving and opening cases. You can read more about cases and the **Case Manager** in chapter “LeachXS Cases and Case Management” on page 100.

Every CBP model contains a number of cases that you can use as a template. Use the **Open...** button on the ribbon tab **Case Manager** to select a template. After you have opened a template, the case is loaded into the editor. The same ribbon tab contains functions to save your edits.

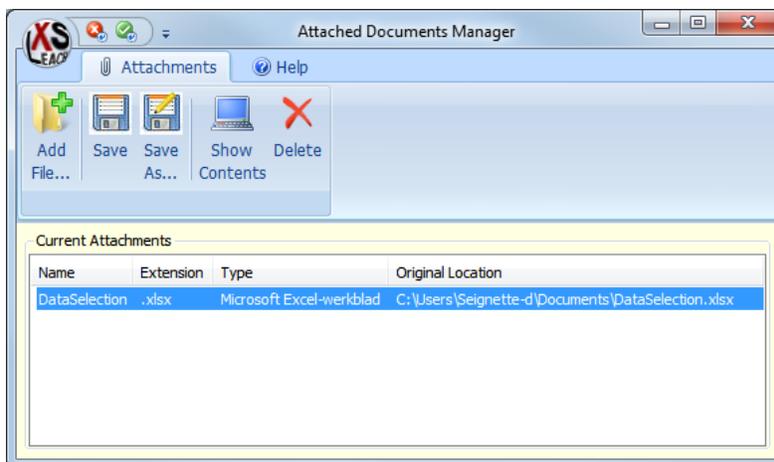
## Reporting and documenting

You can make a report of your case by pressing the **Report** button on ribbon tab **Case Manager**. The following dialog will show up:



The report will be created in a Microsoft Excel® workbook and worksheet of your choice. Use the **Open...** or **Create...** button to open an existing workbook or create a new one. The left pane shows the proposed worksheet name to create the report on. You can choose another name by double-clicking it. The right pane shows the worksheets that your chosen workbook contains. Press the **Generate** button to create the report. You can inspect the destination workbook by hitting the **View** button.

You can attach documents to your case for reference or documentation. Press the **Attached Documents** button on the **Case Manager** ribbon tab to organize your attachments with the **Attached Documents Manager**.



The pane named **Current Attachments** shows a list of attachments that are already included in your case. Use the **Add File...** button to add additional documents. Alternatively, you can drag files from an explorer window onto the **Current Attachments** pane. You remove documents by selecting them and press the **Delete** button. Press the **Show Contents** button to inspect a document you have selected. If you want to edit an attached document, use the **Save** button to save a copy of the attachment to the location that is listed in the **Original Location** column. Alternatively, you can use the **Save As...** button to specify a different location. After editing the document, drag it to the pane or use the **Add File...** button. Note that the document will be added to the list. You should remove the original file by selecting it and pressing the **Delete** button.

*Note that your attachments are not linked to your case. They are actually copied into it.*

## Navigation pane: Model Input

The **Model Input** section displays the Orchestra input file in a structured manner. This file (which is typically named leachxs\_parameters.txt) is formatted and organized in blocks in such a way, that both LeachXS and Orchestra can interpret it. All blocks in the input file are organized in the following categories:

- Scenario Components.**

The blocks in this category correspond with the segments in the graphical representation of the modeled case. For the chosen model, the segments are the **Cement barrier**, the **Inflow solution** and the **Outflow**. The data for every segment may be organized in separate blocks, such as physical parameters, chemical parameters or output parameters. Other blocks may be present, depending on the model. Chemical data is usually composed of concentrations or availabilities. Other non-chemical parameters are collected in the physical data block. Output parameters usually denote time series with times the model outputs results.
- Other Components.**

The blocks in this category are segments that play a role in the model, but are not represented in the graphical representation of the model.

- **Other Parameters.**  
This category may contain blocks containing parameters that do not belong to a particular segment or component, but are parameters to the model as a whole.
- **Parameter Mapping.**  
It may not be desirable to represent model parameters with the name and unit of measurement that Orchestra uses. The parameter mapping block contains a list of these variables, together with a corresponding LeachXS name, unit of measurement and a conversion factor to convert an Orchestra variable to a LeachXS variable. Note that this list usually is composed in the design phase of the Orchestra model and need not be modified.
- **Other Classes.**  
This category contains all blocks in the input file that do not belong to any of the other categories.

Every data type in this section has a dedicated editor. Chemical and physical data can be edited with the **Model Data Editor**, refresh data with the **Refresh Editor** and output data with the **Output Times Editor**.

## Navigation pane: Model Components

The screenshot displays the LeachXS CBP Scenario editor window for a "CBP Sulfate Attack Scenario". The interface includes a menu bar (Case Manager, View, Edit, Help), a toolbar with icons for Edit, LeachXS Editor, Customize Editor, Load model files, and Modify, and a status bar at the bottom showing "<unnamed case>".

The main workspace is divided into three sections:

- Model Input:** Contains a "Model Components" section with links for "Model to use", "Orchestra System", "Species-Constituent Mapping", and "Minerals".
- Diagram:** A schematic titled "Leaching with Sulfate Attack (1 Layer, unsaturated, no gas interaction)". It shows a "Cement barrier" block with "No Flux Surfaces" on its top and bottom, and "Thickness" indicated by a double-headed arrow. To its right is a "Contact volume (liquid)" block. "Inflow Solution" enters from the top right, and "Liquid Diffusion" is shown as a double-headed arrow between the blocks. "Outflow" exits from the bottom right.
- Minerals Table:** A table listing various mineral reactions with their names, reaction constants, and chemical equations.

Name	Reaction Constant	Reaction
AA_Fe[OH]3[am]	3.981E+16	AA_Fe[OH]3[am] + 1 H2O -> 1 Fe[OH]4+ + 1 H+
BaSrSO4[50%Ba]	1.663E+08	BaSrSO4[50%Ba] -> 0.5 Ba+2 + 1 SO4-2 + 0.5 Sr+2
beta-TCP	8.433E+28	beta-TCP -> 3 Ca+2 + 2 PO4-3
Cem07_Al[OH]3[am]	5.728E+13	Cem07_Al[OH]3[am] + 1 H2O -> 1 Al[OH]4+ + 1 H+
Cem07_Brucite	1.482E-17	Cem07_Brucite + 2 H+ -> 2 H2O + 1 Mg+2
Cem07_C2AH8	3.664E-15	Cem07_C2AH8 + 2 H+ -> 2 Al[OH]4+ + 2 Ca+2 + 5 H2O
Cem07_C2ASH8	2.539E+17	Cem07_C2ASH8 -> 2 Al[OH]4+ + 2 Ca+2 + 3 H2O + 1 H2SiO4-2
Cem07_C2FH8	4.018E-11	Cem07_C2FH8 + 2 H+ -> 2 Ca+2 + 2 Fe[OH]4+ + 5 H2O
Cem07_C2FSH8	2.542E+21	Cem07_C2FSH8 -> 2 Ca+2 + 2 Fe[OH]4+ + 3 H2O + 1 H2SiO4-2
Cem07_C3AH6	7.047E-36	Cem07_C3AH6 + 4 H+ -> 2 Al[OH]4+ + 3 Ca+2 + 4 H2O
Cem07_C3FH6	1.472E-31	Cem07_C3FH6 + 4 H+ -> 3 Ca+2 + 2 Fe[OH]4+ + 4 H2O
Cem07_CAH10	3.162E+07	Cem07_CAH10 -> 2 Al[OH]4+ + 1 Ca+2 + 6 H2O
Cem07_Calcite	6.375E-09	Cem07_Calcite + 2 H+ -> 1 Ca+2 + 1 H2CO3
Cem07_Gypsum	3.828E+04	Cem07_Gypsum -> 1 Ca+2 + 2 H2O + 1 SO4-2
Cem07_Portlandite	1.609E-23	Cem07_Portlandite + 2 H+ -> 1 Ca+2 + 2 H2O
Cem07_Syngenite	6.31E-08	Cem07_Syngenite -> 1 Ca+2 + 1 H2O + 2 K+ + 2 SO4-2

The **Model Components** section shows parts of the heart of the model and some interface definitions between Orchestra and LeachXS. These parts are usually not of interest or importance to a regular end user. The categories to edit offered here are:

- **Model to use**  
The Orchestra model is composed of a number of files that define relevant parameters, chemistry and definitions. These files together are called the "model". Files in the model can be edited,

replaced or removed, and extra files can be added. This function is normally of importance for a model designer only.

- **Orchestra System**

The Orchestra system is a set of files that form the heart of the Orchestra engine that is capable of performing the instructions that are comprised in a model [a better description needed]. Files can be added, replaced or removed, and extra files can be added. This function is normally of importance for a model designer only.

- **Species-to-Constituents Mapping**

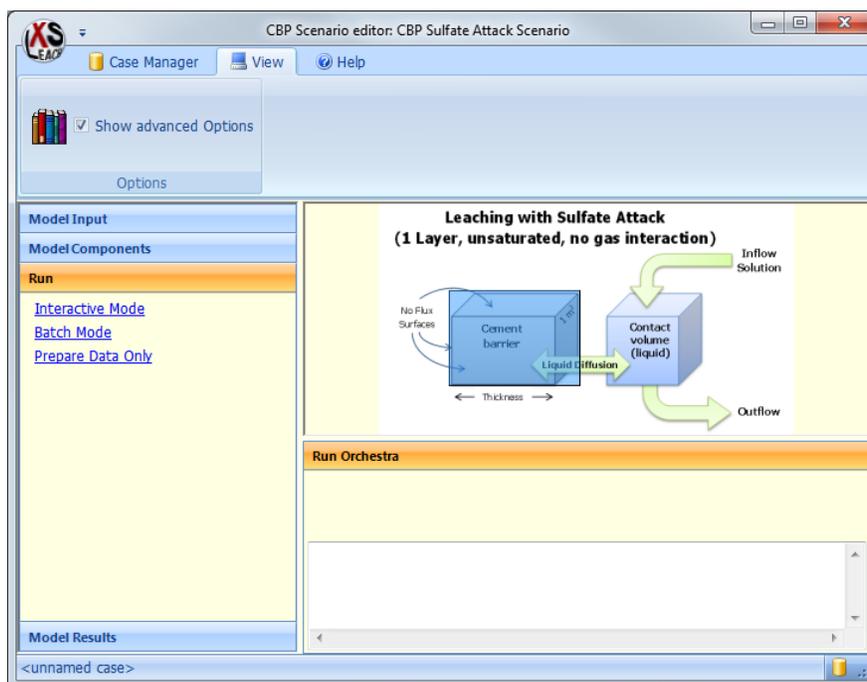
Some model parameters, like concentrations and availabilities, can be obtained from a LeachXS database with leaching data. The name giving of constituents like Na, As or Ba is different from the entities in Orchestra. The Species-to-Constituents Mapping defines which Orchestra species corresponds to which LeachXS constituent. This function is normally of importance for a model designer only.

- **Minerals**

Mineral reactions play an imported role in many models. The set of minerals that take part in the model can be defined and edited here.

The first two items will be visible only if the box **Show Advanced Options** on ribbon tab **View** in the ribbon bar is checked.

## Navigation pane: Run



The **Run** section shows the different ways to run the model. Currently, the options are:

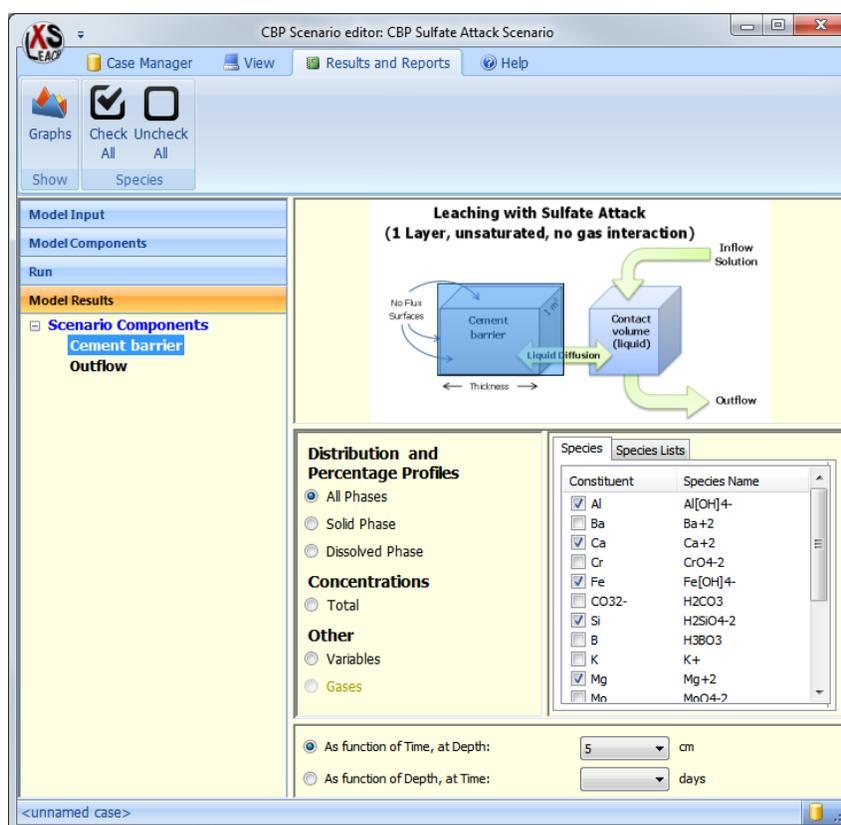
- **Interactive Mode**

Clicking this link will start Orchestra in interactive mode. Orchestra is started and execution is suspended until the Run button is clicked in the Orchestra user interface.

- **Batch Mode**  
Clicking this link will start Orchestra in batch mode. Orchestra is started for immediate execution. No user interface will show up.
- **Prepare Data Only**  
Clicking this link will not start Orchestra, but instead, a directory is created and all model files and Orchestra system files are stored in an appropriate directory structure, fit for running Orchestra outside of the LeachXS environment. This function is normally of importance for a model designer only.

The first and last option is visible only if the box **Show Advanced Options** on ribbon tab **View** in the ribbon bar is checked.

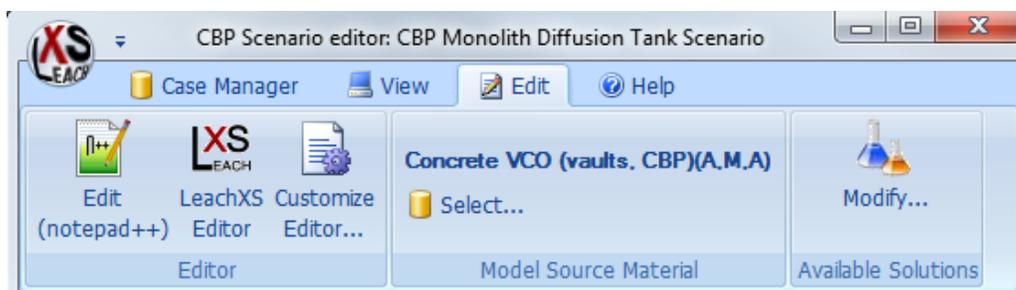
## Navigation pane: Model Results



The **Model Results** section helps you to select the results you want to inspect. It shows all scenario components and reveals what results can be obtained after selecting a specific scenario component.

## Editing your scenario

The **Edit** tab of the ribbon bar contains all functions to edit your scenario. What functions are available depends on what part of your model is selected. If you have selected anything in the **Model Input** section in the navigation pane, the tab may show something like this:



Tab group **Model Source Material** will only be present if you have opened a scenario for simulating a lab test. By pressing the **Select...** button you can select an existing lab test. The geometry and other physical parameters of the model will be set to the geometry and physical parameters of your selected test.

You can define standard solutions that can be used by your model. Press the **Modify...** button on the **Available Solutions** ribbon tab to define them. If, for example you are editing a model that simulates a monolithic diffusion test, you can use the solutions you have defined here for refreshing the tank.

You can edit a specific part of your scenario data by using the **LeachXS Editor** button on the **Editor** tab group. This will start an editor that is designed for the part of your scenario you selected.

## The Data Editor

The Data Editor is designed to edit chemical or physical data. For instance, if you select any entry with chemical parameters in the Model Input section of the Navigation pane, the editor may show up like this:

Nr	Ag mg/kg	Al mg/kg	Ba mg/kg	Br mg/kg	Ca mg/kg	Cd mg/kg	Co mg/kg	Cr mg/kg	Cu mg/kg	F mg/kg	Fe mg/kg	CO32- mg/kg	Si mg/kg	mi
Data 1	1	5372	26.93	0.08702	5.559E+04	0.06233	1.287	16.43	7.193	312.1	1750	2174	1.265E+04	

The editor may show several sections, depending on the content of the chemical parameters. These are the sections:

- Solid Constituents**  
 All constituents that are defined in the solid phase of the chemical parameter block are shown, together with their values, in mg/kg. There may be several rows of values, depending on how the block of chemical parameters is modeled. You can edit every single cell that represents a concentration. You can also obtain concentrations or availabilities for certain cells from the LeachXS

database. First, select the cells you want to fill from the database. You can select a range of cells, an entire row (click on the row header) or the entire grid (click the top left cell in the grid). Next, click tab **Chemical Data** and the **Availability or Total Content...** button on the **From Database** tab group. Next, select a test from the database: the selected cells will be filled from the selected test.

*Note: if there are constituents in your selection that did not have any availability data, the editor will inform you about the constituents that were not found in the database before the found constituents are filled. After you have acknowledged the message, the values of the constituents that were found in the database are updated and colored blue. The other values will not be updated and retain their black color.*

- **Dissolved Constituents**  
All species that are defined in the gas phase of the chemical parameter block are shown, together with their values; in mg/L. Edit them as desired.
- **Gas Constituents**  
All species that are defined in the gas phase of the chemical parameter block are shown, together with their values, in volume percentages. Edit them as desired.
- **Additional Specifications**  
All other, non-concentration variables in the parameter block are shown here. Edit them as desired. When you are finished, press the green checkmark in the title bar to save your changes. LeachXS will rewrite the input file for the model. You should be aware of the fact that any previously generated model results will become invalid.

## The Refresh Scheme Editor

The **Refresh Scheme Editor** is designed to edit refresh data. For instance, if you select any entry with refresh parameters in the **Model Input** section of the Navigation pane, the editor may show up like this:

Order	Duration (days)	Volume (L)	Flowrate (mL/h)	Start At (days)	Stops At (days)
0	0.25	2.08	0	0	0.25
1	0.75	2.08	0	0.25	1
2	1.25	2.08	0	1	2.25
3	1.75	2.08	0	2.25	4
4	5	2.08	0	4	9
5	7	2.08	0	9	16
6	20	2.08	0	16	36
7	28	2.08	0	36	64

The grid below the ribbon bar shows all the information needed to define the refresh steps. The pane at the very bottom of the window shows an impression of the relative lengths of each step. Clicking on a segment of this pane will select the corresponding step in the grid.

### Edit functions

If you double-click on a value in one of the columns **Duration**, **Volume** or **Flowrate**, you can alter its value.

The **From Database...** function on the **Fetch Scheme** tab group lets you pick a test material, whose refresh scheme will replace the current one.

The **Define Range...** function on the same tab group gives you the option of quickly generate a list of times. You can define a list of evenly distributed time steps, a list of times where each successive time increases with a constant factor, or just a list of times at you liking by typing a space separated list of times. See "List Generator" on page 147 for details.

With the functions on the **Add/Remove steps** tab group, you can add or insert a step or remove selected or all steps.

You can change the order of the steps by using the **Move Up** and **Move Down** buttons in the **Move Steps** tab group.

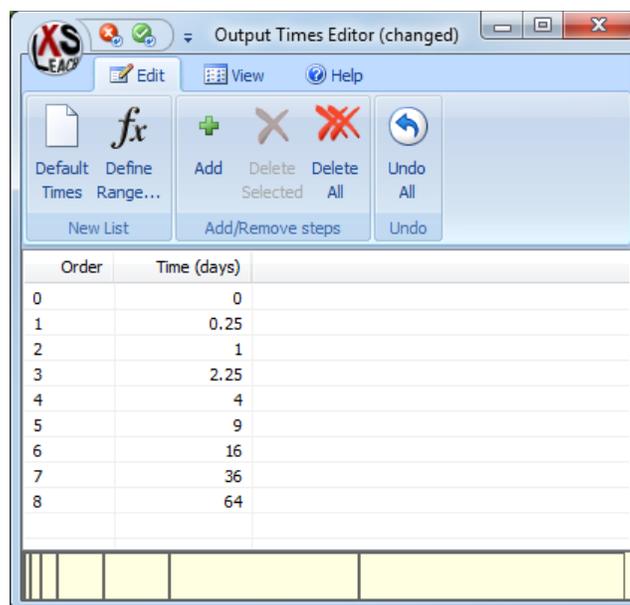
You can undo all your actions and revert to the list as it was when starting the editor by pressing the **Undo All** button.

### View functions

You can change the time unit by clicking the appropriate button on the **View** tab.

## The Output Times Editor

The **Output Times Editor** assists you in editing the times model results are recorded. You can use this editor if you have selected **Output** parameters in the **Model Input** panel.



The title bar contains buttons to close the editor and save (green button) or abandon (red button) changes. The text in the bar indicates if you have changed any data or not.

The ribbon bar contains functions to edit the times (the **Edit** tab) and to alter the way the data is displayed (the **View** tab).

The grid below the ribbon bar contains the list of times. Apart from the functions on the **Edit** tab, you can alter a time by double-clicking on the entry you want to change.

The bar at the bottom of the window gives you an indication of the relative lengths of the times in the list.

### **Edit functions**

If you double-click on a time step in the list, you can alter its value. Note that the list will be sorted immediately after you have changed it, so that the steps are in ascending order.

The **Default Times** function on the **New List** tab group replaces the current list with the list of times that might be appropriate for the model.

The **Define Range...** function on the same tab group gives you the option of quickly generate a list of times. You can define a list of evenly distributed time steps, a list of times where each successive time increases with a constant factor, or just a list of times at you liking by typing a space separated list of times. See "List Generator" on page 147 for details.

With the functions on the **Add/Remove steps** tab group, you can add a step or remove selected or all steps.

You can undo all your actions and revert to the list as it was when starting the editor by pressing the **Undo All** button.

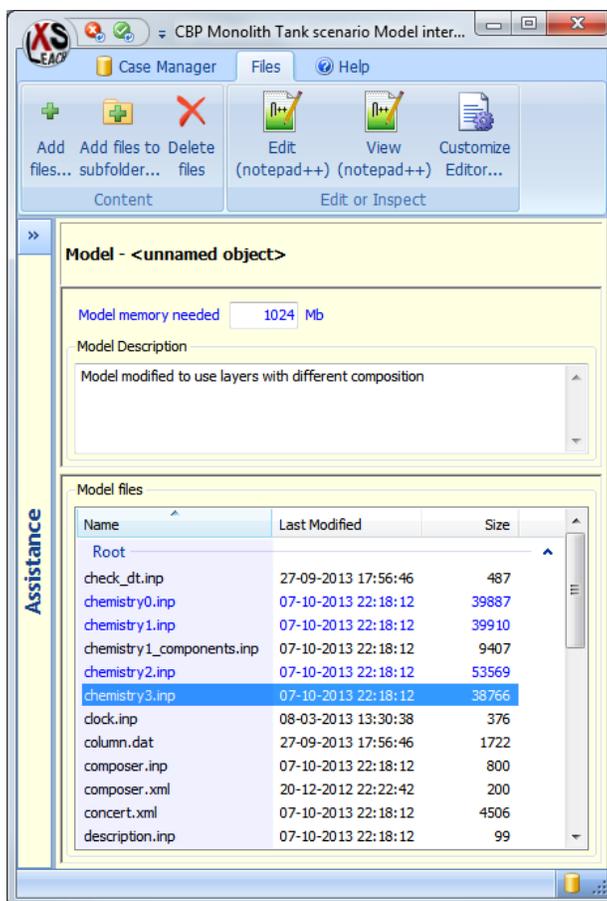
### **View functions**

You can change the time unit by clicking the appropriate button on the **View** tab.

## **The Model Files Editor**

If you have selected the **Model to use** section of the **Model Components** navigation pane, you will be able to modify the set of files that comprise the model you chose. You can add, edit view and delete files from the model and you can set the amount of memory the model is allowed to use.

*Note that this is possible only if the box **Show Advanced Options** on ribbon tab **View** in the ribbon bar is checked.*



The title bar contains buttons to close the editor and save (green button) or abandon (red button) any changes.

The ribbon bar contains functions to add files to or remove files from the file list (the **Contents** tab group) and to view or edit a selected model file (**Edit or Inspect** tab). You can also save the model as a separate object for use in other model cases or load one from disk. These functions are present in the **Case Manager** ribbon tab. Note that you can also add files by dragging files from any Windows Explorer window and drop them on the file list.

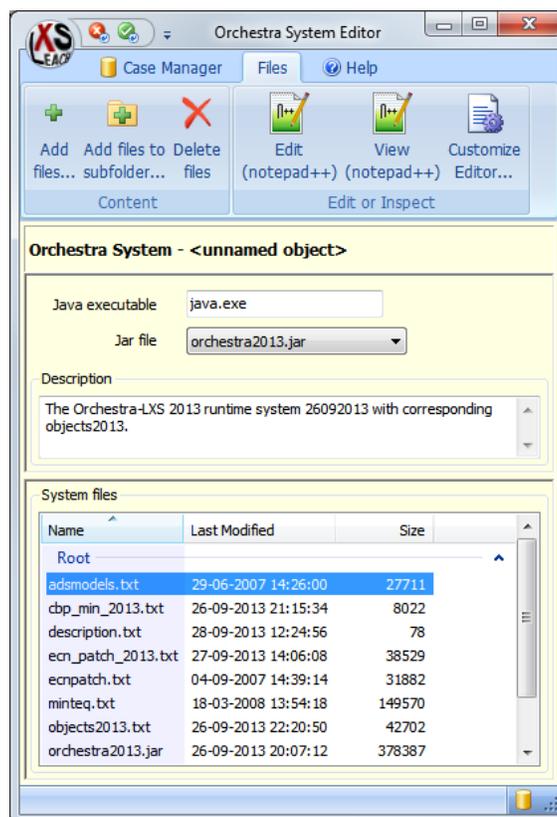
The pane below the ribbon bar shows the amount of memory the model is allowed to use and a model description. You can edit both the memory and the description.

The bottom pane shows the list of files make up the model. The files that form the core of the model are colored blue.

### The Orchestra System Editor

If you have selected the **Orchestra System** section of the **Model Components** navigation pane, you will be able to modify the set of files comprising the Orchestra system that is included with your case.

Note that this is possible only if the box **Show Advanced Options** on ribbon tab **View** in the ribbon bar is checked.



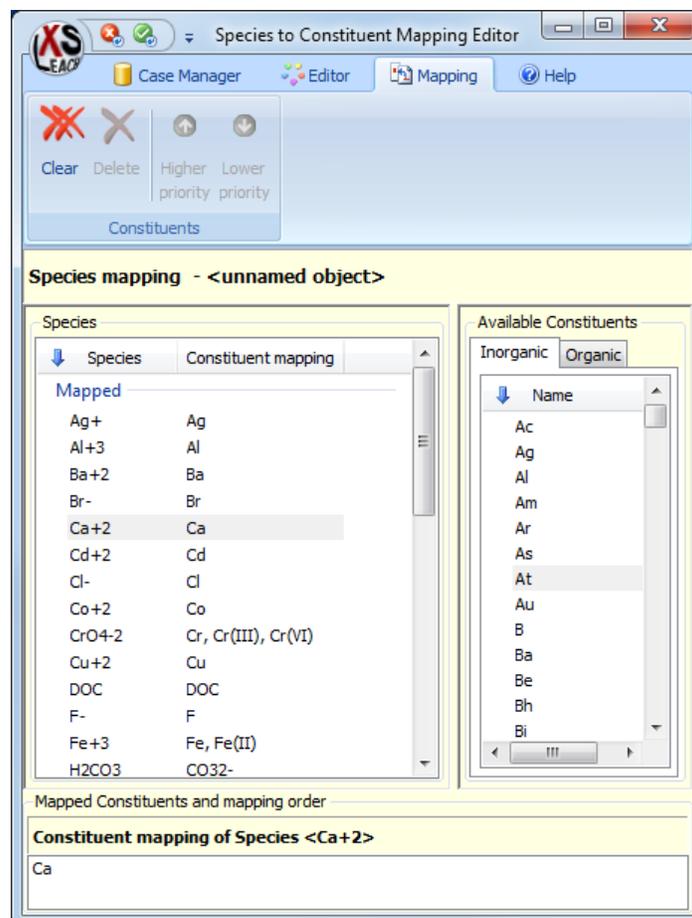
Most functions of this editor are the same as the ones in “The Model Files Editor” on page 91. In addition, you can specify the **Orchestra jar** file this is to be executed for running a model and how the **Java executable** is called in your system.

### The Species Mapping Editor

Orchestra uses species in its chemistry, whereas LeachXS uses constituents. When assigning concentrations or availabilities to Orchestra species, a LeachXS database can be used as source. In order to assign values to species correctly, a mapping should exist that maps an Orchestra species to a LeachXS constituent.

If you have selected the **Species-Constituent Mapping** section of the **Model Components** navigation pane, you will be able to modify this mapping by pressing the **LeachXS Editor** button on the **Edit** tab of the ribbon.

The **Species Mapping Editor** lets you inspect or adjust the mapping of all species of the model you use to constituents. You can assign one or more constituents to a species. If you assign more than one constituent, the order of constituents is of importance. When assigning a concentration from a LeachXS database to a species, LeachXS will walk through the list of assigned constituents. The first constituent in the list that has a concentration will be used.



The title bar contains buttons to close the editor and save (green button) or abandon (red button) changes.

The ribbon bar contains functions to edit the mapping (the **Edit** tab group), to group species (the **View** tab group) and to save or load existing mapping definitions to or from disk (the **Case Manager** tab group).

The left pane below the ribbon bar (**Species** pane) shows the mapping of all species, whereas the right pane (**Available Constituents** pane) contains all available LeachXS constituents you can use for mapping.

The bottom pane (**Mapped Constituents** pane) shows the constituents that are mapped to the species that is selected in the left pane.

To assign one or more constituents to a species, first select a species in the **Species** pane. Then, look up an appropriate constituent in the **Available Constituent** pane and double-click it. The constituent will be added to the list of mapped constituents in the **Mapped Constituents** pane.

To remove a mapped constituent, first select the species containing the constituent to remove. Then select the constituent in the **Mapped Constituents** pane and click on the **Delete** button in the **Edit** tab, tab group **Constituent**.

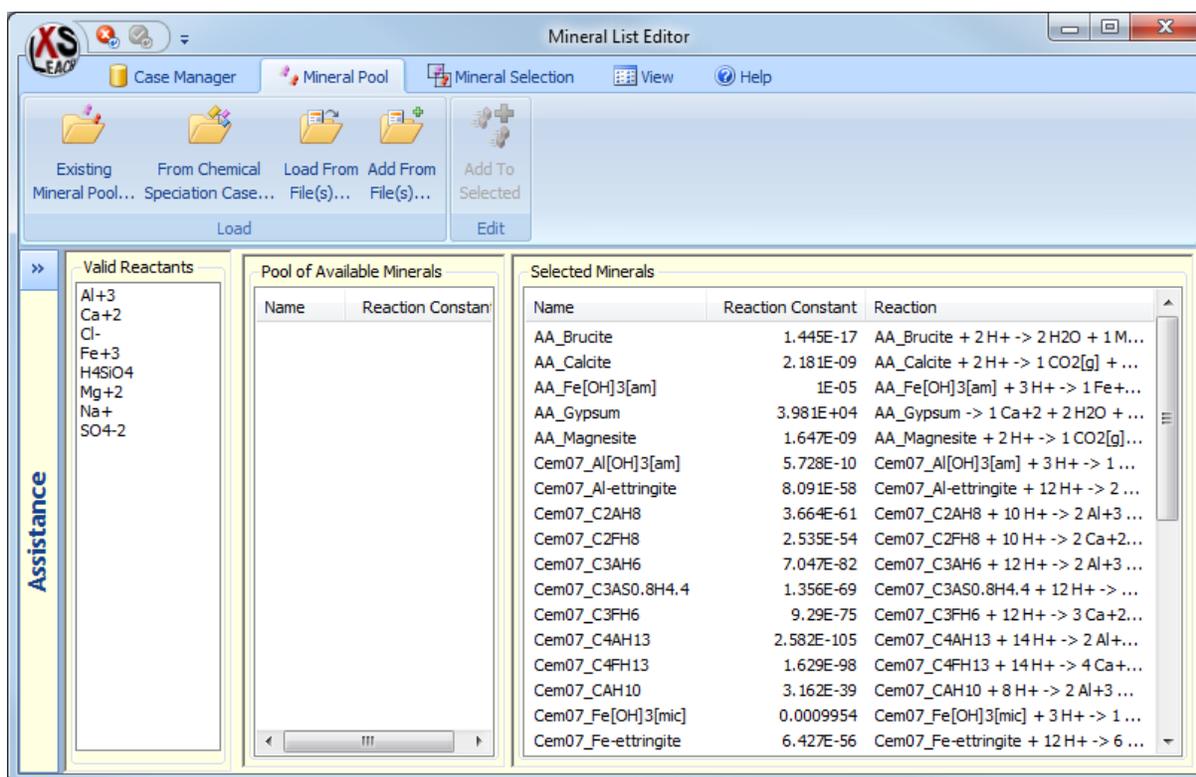
If you want to change the order the constituents are mapped for a species that is mapped to several constituents, select the subject species, then select a constituent in the **Mapped Constituents** pane and use one of the buttons in the **Constituent** tab group to change the priority of the constituent.

While manipulating the entire mapping, it may be handy if species are grouped according to their mapping. The **Species grouping** buttons on the **View** tab let you group or ungroup the list of species.

## The Minerals Editor

Minerals play an important role in the modeling process. You can change the list of minerals that are used in the model with the *Minerals Editor*. Select the **Minerals** section of the **Model Components** navigation pane, and press the **LeachXS Editor** button on the **Edit** tab of the ribbon. The **Minerals Editor** will appear.

To ease the process of selecting appropriate minerals, the editor contains two lists. One list contains all the minerals that comprise the selection you want. The other list contains a pool of minerals. You can load minerals from a mineral source to this pool. From the pool, you can compare mineral definitions with definitions in the list of selected minerals. You can also drag minerals from the pool to the selected minerals list.



The title bar contains buttons to close the editor and save (green button) or abandon (red button) changes.

The ribbon bar contains functions to fill the pool (**Mineral Pool** tab), edit the list of selected minerals (**Mineral Selection** tab), change the layout of the mineral lists that are displayed (**View** tab) and save your selection to disk (**Case Manager** tab).

Below the ribbon bar are three panes. The left pane (**Valid Reactants**) shows all the species in your model. The left pane shows the minerals that play a part in the model (**Selected Minerals**). The middle pane contains the minerals in the pool you have opened (**Pool of Available Minerals**).

### ***Using the Mineral Pool***

If you want to add minerals to your selection, you'll need the **Mineral Pool**. Once the pool is filled, you can start adding minerals. You can fill the pool from various sources. If you already have saved lists of minerals to disk, use button **Existing Mineral Pool...** from the **Load** group of ribbon tab **Mineral Pool**. Alternatively, you can select a **Chemical Speciation Case** you have created previously and use the minerals in it. Use button **From Chemical Speciation Case...** from the same tab group to select the case. Finally, you can use text files containing mineral definitions. The format of these files must be equal to the ones that are used to define the minerals of the Orchestra system.

### ***Organizing the minerals***

A number of view options are available to control how and which minerals are displayed in the pool and the list of selected minerals. The options are situated in tab **View** of the ribbon bar. You can display the minerals grouped by reactant or species. Press **By Reactant** of the **Grouping** tab group to group them. Note that the lists will grow considerably, because a certain mineral will show up in every reactant that has part in the mineral reaction.

When grouped by reactant, you can use the **Valid Reactants** pane to jump to the list of minerals having a certain reactant. If you select a reactant in this pane, the mineral lists are repositioned to show the minerals containing that reactant.

You can control the visibility of minerals that contain reactants that are not in the list of valid reactants. The tab group **Show Minerals Having Reactants...** you can choose:

<b>All</b>	All minerals are shown; minerals having at least one reactant that is not in the list of valid reactants are colored red.
<b>Having Any Available Reactant</b>	A mineral is shown only if it has at least one of its reactants in the list of available reactants. Again, minerals having at least one reactant that is not in the list of valid reactants are colored red.
<b>Having Available Reactants Only</b>	A mineral is shown only if all of its reactants are present in the list of available reactants. No minerals are colored red.

### Editing the list of selected minerals

Add minerals to your set by dragging selected minerals in the pool over the **Selected Minerals** pane and release them there. Alternatively, you can use **Add To Selected** on the **Edit** tab group of tab **Mineral Pool**. Pressing this button will copy selected minerals in the pool to your mineral set.

Added minerals from the pool are in no way connected to the pool anymore; you can fill the pool from another source and add minerals from that source as well, without losing added minerals from another pool.

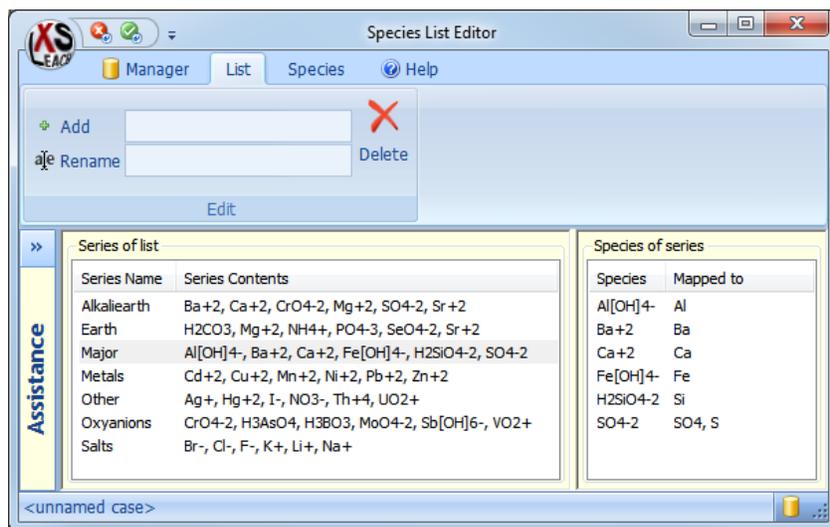
Take care with dragging minerals from the pool to your set: if a mineral in the set has the same name as one in the drag list, it will not be replaced, even if the reaction definition is different.

Remove minerals from your set by selecting the minerals to remove and pressing **Delete** from the **Edit** group of the **Mineral Selection** tab. Press **Clear** from this group to empty your set and **Undo All Changes** to restore the set to what it was when you opened the editor.

*Note that there is no way of adding a mineral by directly typing a mineral reaction. Instead, create a text file, type your reaction in the format equal to the format that is used to define the minerals of the Orchestra system. Then, open this file in the mineral pool and drag the mineral(s) to the set of selected minerals.*

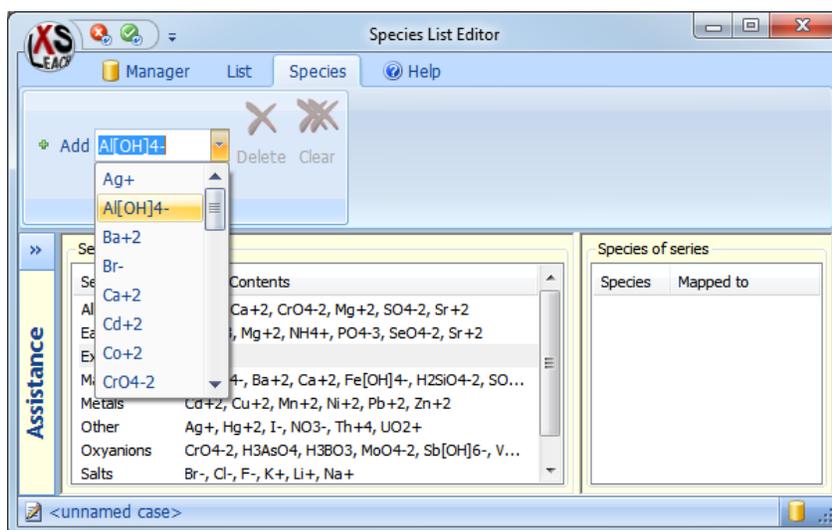
### The Species List Editor

If you want to see results of model calculations, you can select constituents by marking the checkboxes in front of the constituents that are present in tab **Species** of the **Parameters** pane if **Model Results** are visible in the **Navigation** pane. Alternatively, you can make predefined lists of species and select one to show results for all species in the list. Predefined species lists appear in tab **Species List**, next to the **Species** tab. To create, modify, load and save lists of species, use the **Edit...** button on ribbon tab **Results and Reports**. The **Species List Editor** will appear.



The left pane contains the species lists. The right pane contains the species that make up the list that is selected in the left pane. The **List** ribbon tab contains two fields. If you want to add a new list, type a name for the list in the **Add** field and hit the **Enter** key. If you want to give a list a new name, select it, type a new name in the **Rename** field and hit the **Enter** key.

You can add or remove species to or from a list by selecting the list and click in the **Species** of series pane. The **Species** ribbon tab will be activated.



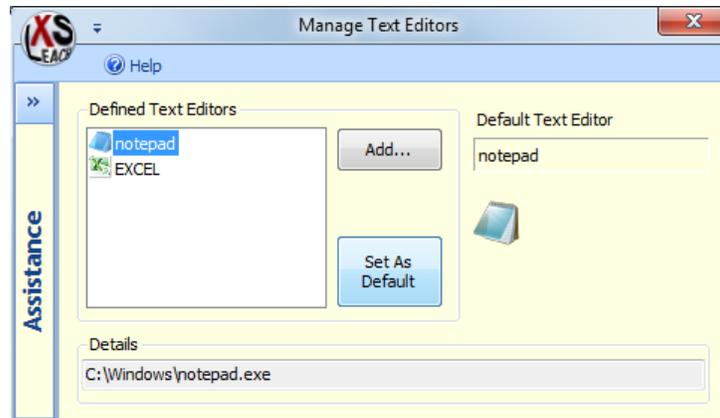
To add a species, select one from the **Add** list. To delete species, select them and press the **Delete** button.

You can save the set of lists to disk and save them for use at some other place or load an existing set. Select the **Manager** tab and press the **Save** or **Save As...** button to save the set or use the **Open...** button to load an existing one. The **Case Manager** will show up. See “LeachXS Cases and Case Management” on page 100 for details.

## Editing with a text editor

As an alternative to a dedicated data editor, you can edit data in your favorite text editor. The data will be presented in text, just as it is defined in the `leachxs_parameters` file. Only items in the **Model Input** navigation pane can be edited with a text editor. Note that this is possible only if the box **Show Advanced Options** on ribbon tab **View** in the ribbon bar is checked.

Before you can use it, you'll need to make it accessible from within LeachXS. Press button **Customize Editor...** from the **Editor** tab group of tab **Edit**. The following small dialog pops up:



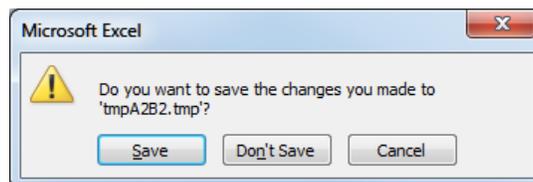
Press the **Add...** button and browse to the editor you want to use as text editor. In the above example, we've selected two editors as text editor: **Notepad** and **Microsoft Excel**<sup>®</sup>. Click on **Notepad** and press **Set As Default** to make **Notepad** your default text editor.

LeachXS will remember the editors you've selected to be candidates for a text editor, as well as the editor you have designated to be the default text editor.

This is what LeachXS will do if you want to edit a block of data with the text editor of your choice:

1. It will create a temporary file containing the data and remember the file size and time of creation.
2. It will start your editor with the file specification of the temporary file as argument.
3. It will wait until the editor is closed.
4. It will examine the file size and last modified time of the temporary file. If it is different with respect to the remembered size or time, it assumes the contents have been changed, and the subject block of data is replaced with the data in the temporary file.
5. It will dispose the temporary file.

Note that some editors might behave not quite as expected if they are closed while the file contents is edited. If, for instance, Microsoft Excel<sup>®</sup> is used to edit a file, closing Microsoft Excel<sup>®</sup> causes the following message to appear:



When the *Save* button is pressed, Microsoft Excel<sup>®</sup> forces you to give a different file extension for the file to save. In that case LeachXS does not detect any changes. For Microsoft Excel<sup>®</sup>, the appropriate action to take for saving edited data is:

Press *File->Save*, and answer *Yes* to the appearing question. Next, close Microsoft Excel<sup>®</sup> and answer *Don't Save* to the appearing question.

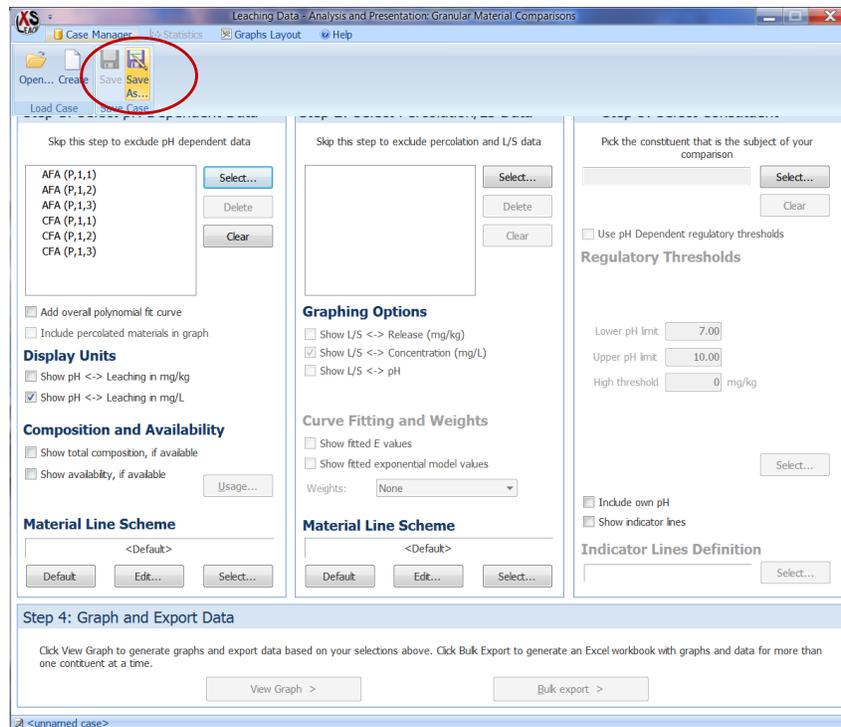
For other editors with an analogous behavior, you'll need to sort out the correct way to exit the editor yourself.

## LeachXS Cases and Case Management

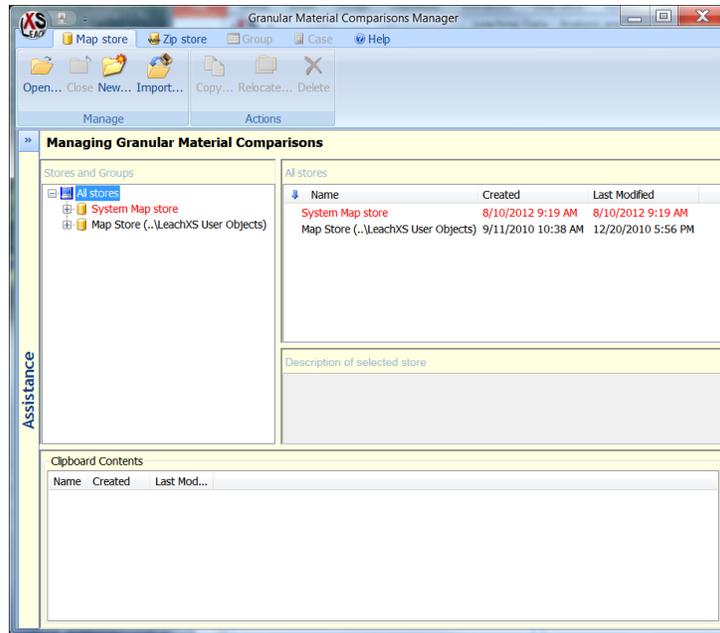
LeachXS allows the user to save any combination of selected materials and model outputs as a **Case** (i.e., a collection of files that may be recalled from a user-defined storage folder for later use or shared between users using the export/import features). **Cases** are saved in LeachXS using a browser window that allows access to the **Map Store-Group-Case** data structure. **Map Stores** and **Groups** are simply folders that allow the user to categorize their output and for LeachXS to recognize the saved data.

### Saving a Case

To save the current case, click on the **Case Manager** tab on the top menu and select the **Save As** icon in the ribbon menu.

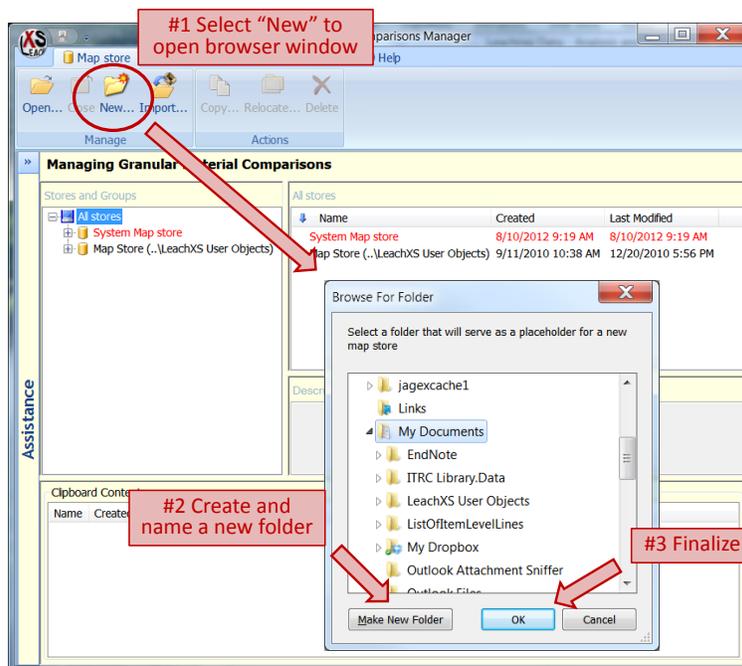


This action opens a pop-up window for storing user-defined items in LeachXS using the **Map Store** object. The tree structure in the upper left corner shows the currently defined map stores while the window on the upper right shows the current object within a highlighted map store. A **Map Store** file for **LeachXS User Objects** exists by default.



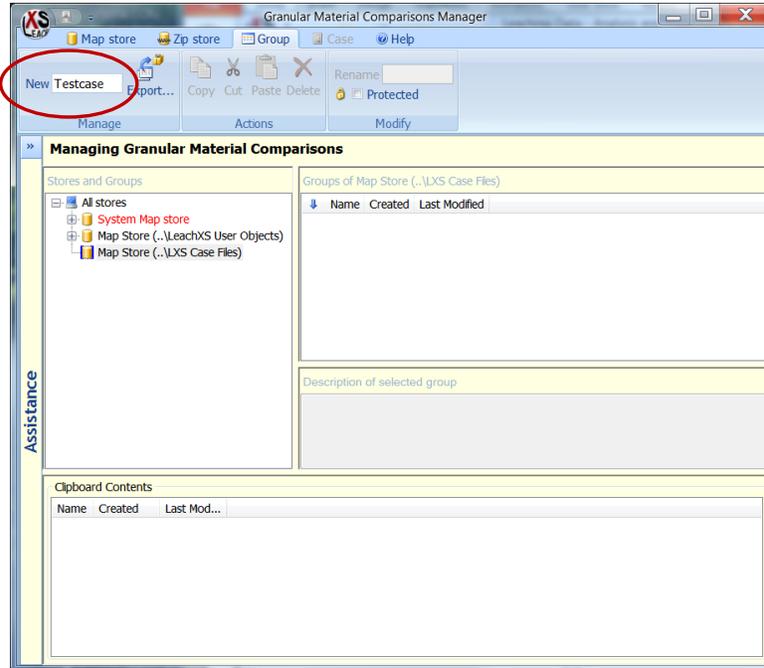
### Creating a New Map Store Folder

If no user-defined map store has been created for saving cases, create a new map store by clicking on **New** icon on the ribbon menu under the **Map Store** menu tab. Use the pop-up browser window to create a new folder by clicking the **Make New Folder** button and providing a name for the map store. Click the **OK** button to save the map store and display it in the tree structure.



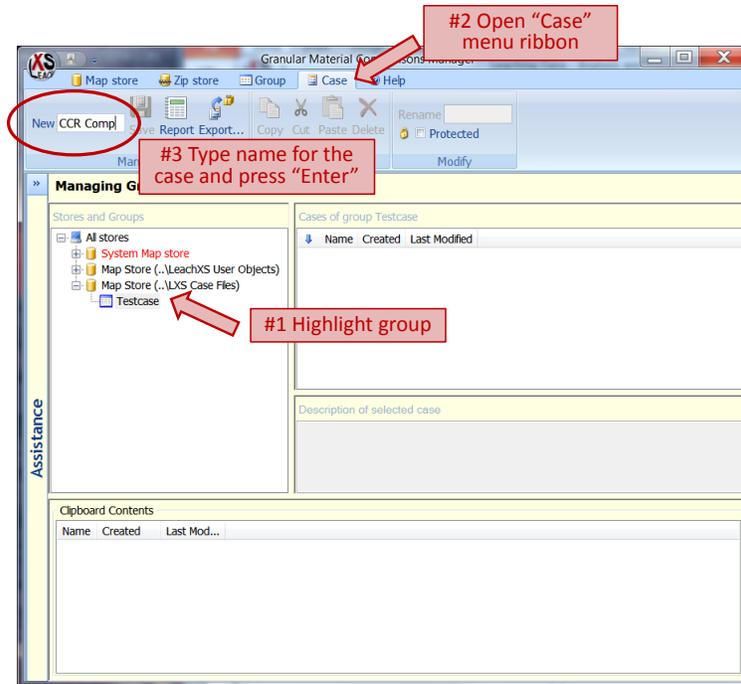
### Create a Group within a Map Store

Highlight the **Map Store** where cases are to be saved and then select the **Group** menu from the top menu bar. Create a new group by entering a folder name in the **New** field and pressing the **Enter** key on the keyboard.

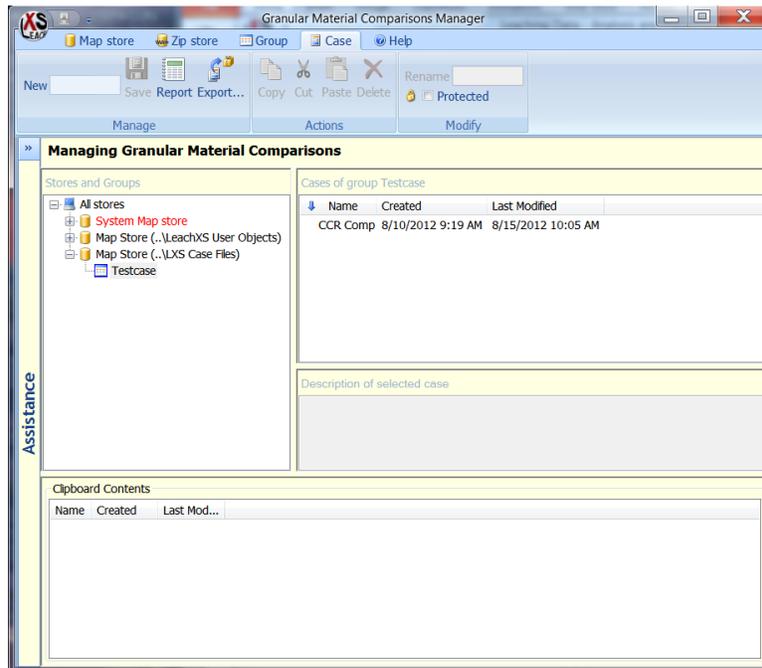


### Creating a Case within a Group

Highlight the group name in the left window to activate the **Case** menu tab on the menu bar. Create a case within the selected group by entering a case name in the **New** field and pressing the **Enter** key on the keyboard.

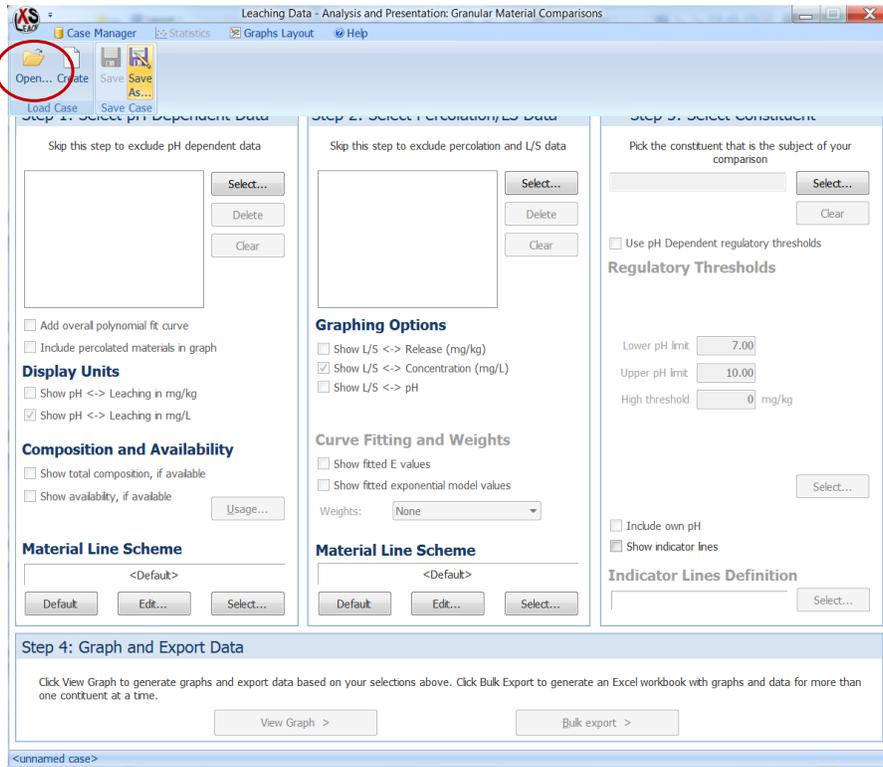


These actions results in the following window.

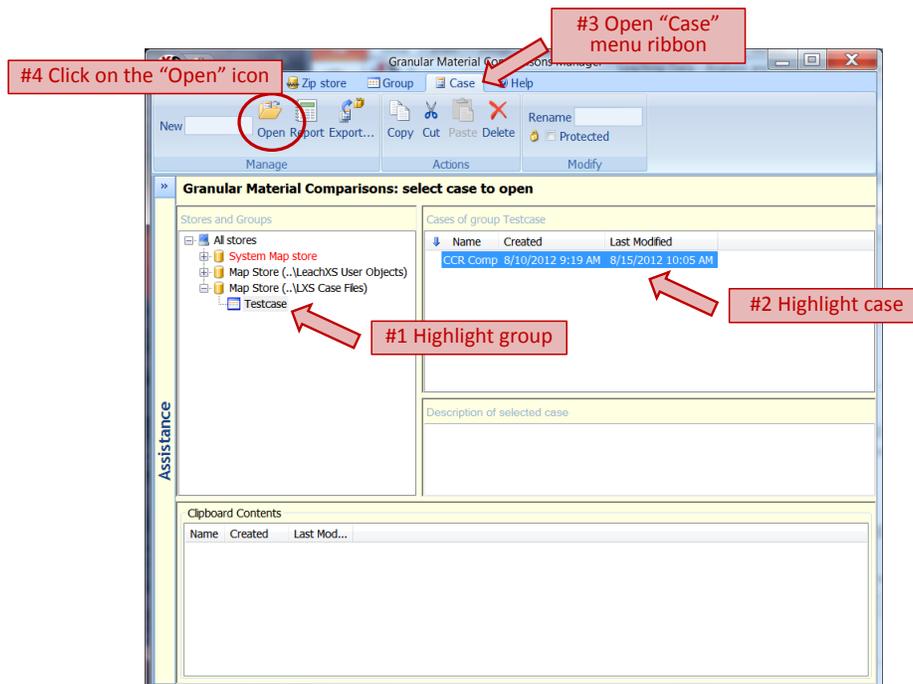


## Loading a Case from the Map Store

To recall a case from the map store into a comparison window, click on the **Case Manager** tab in the top menu bar and select the **Open** icon from the ribbon menu.

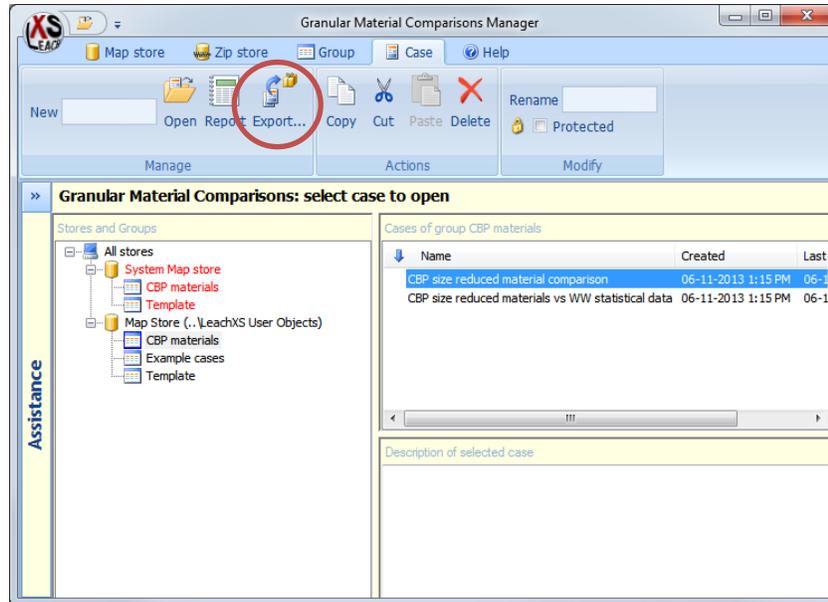


Use the tree structure to navigate to the target group and highlight the group name in the left hand box. Highlight the desired case in the right hand box and click on the **Open** icon in the ribbon menu of the **Case** menu tab.

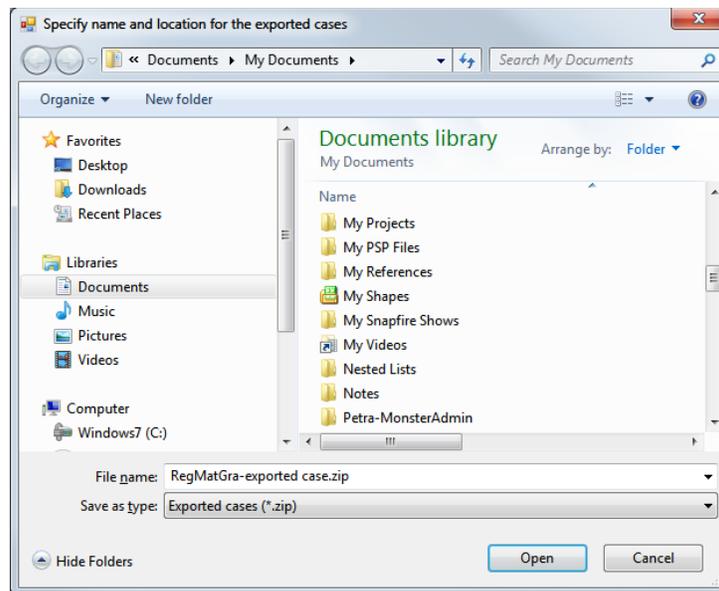


## Exporting a Case

If you want to share or hand over a case to another user, you can export a case. The other user can use the import function to add the case to his system. Any object type that is managed by the **Case Manager** can be exported. To export a modeling case, a comparison or any other object, open the **Case Manager** from the editor context of the object you want to export. For example, if you want to export a **Granular Materials Comparison** case, open the **Granular Materials Comparison** window from the main window of LeachXS and hit the **Open** button. Select the case you want to export and hit the **Export...** button.



The object to be exported will be packed into a zip file. A dialog will appear to enable you to specify a location and name for the zip file that will contain the object. Hit the **Save** button to save the zip file.



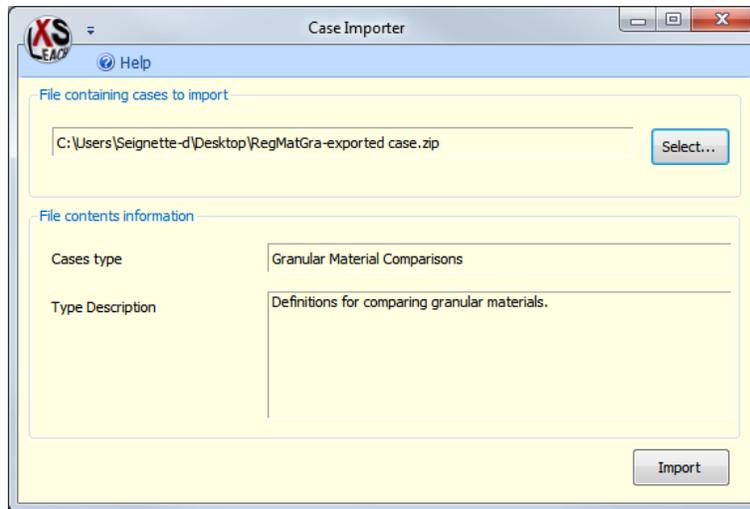
*Note: you can export more cases at a time by selecting a group or by selecting multiple objects within a group. All selected objects will be included in the zip file.*

## Importing a case

If you have received a zip file containing a case or object, you can import them in your own system. The import function is located in the ribbon bar of the main LeachXS window, in tab **Tools: Case Importer**.

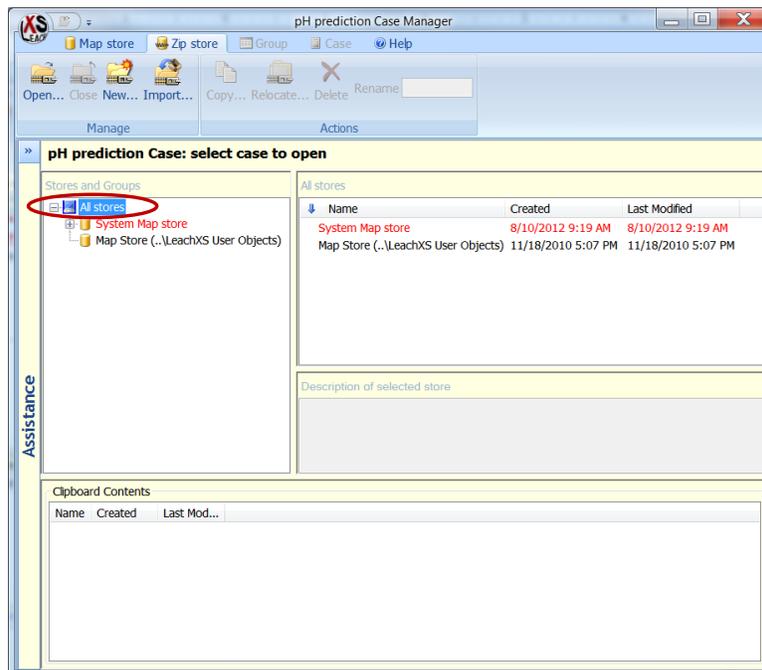


Click on this button. The **Case Importer** will show up. Press the **Select...** button to navigate to the zip file containing the case to be imported. The **Case Importer** will indicate what type of case the zip file contains. Hit the **Import** button to import the case into your own system.

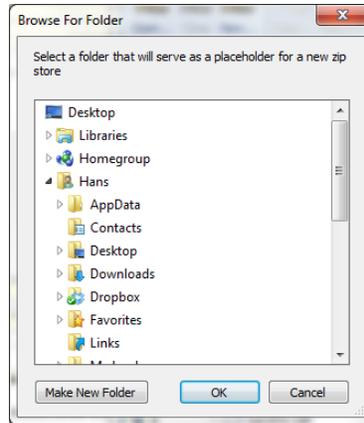


## Using a Zip Store to Compress Files

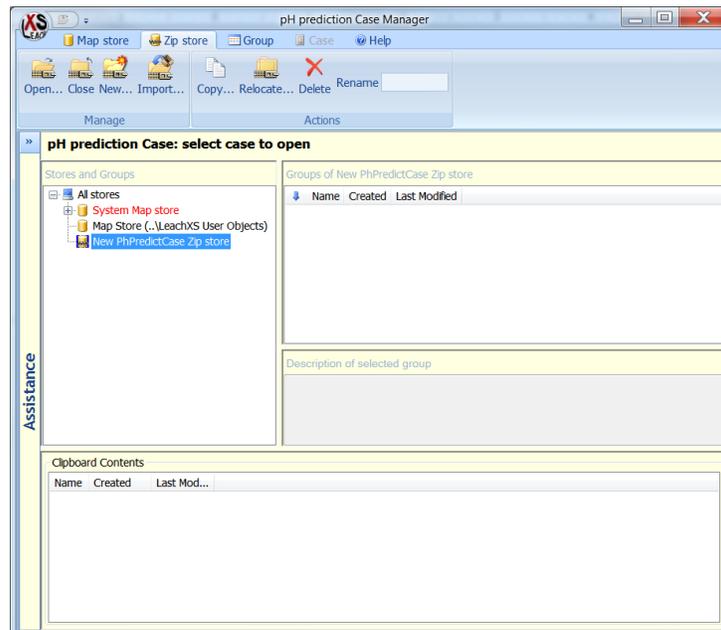
In a similar manner as the **Map Store**, a **Zip Store** needs to be created with the cases to be exported. A **Zip Store** is a folder where compressed or zipped files are stored. To create a new **Zip Store**, select **All Stores** in the list of **Stores and Groups** pane and click on the **Zip Store** tab in the top menu bar to activate the **Zip Store** ribbon menu.



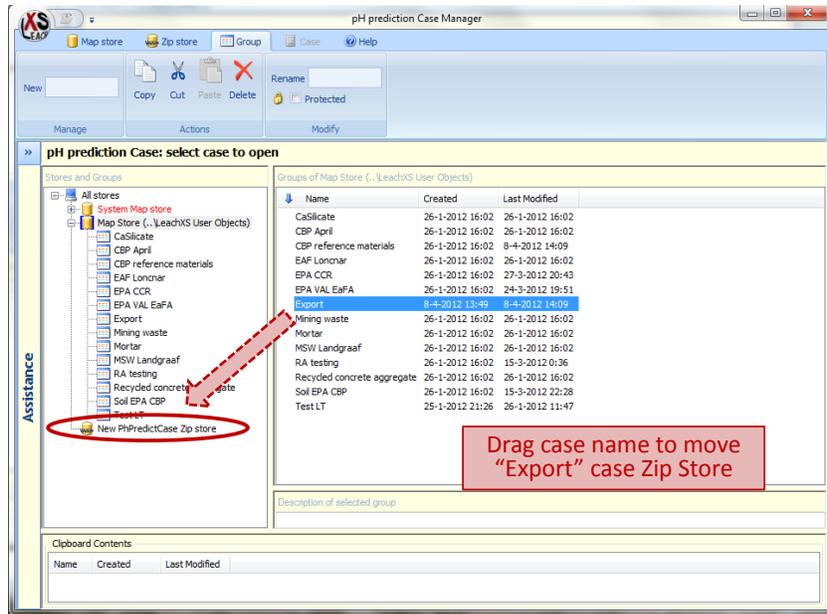
Click on the **New...** icon from the **Zip Store** ribbon menu and select the location where the zip file should be stored (e.g., the computer **Desktop** or a user file). Selecting the **Make a New Folder** button will create a folder for the new **Zip Store**. Click the **OK** button to finalize creation of the **Zip Store**.



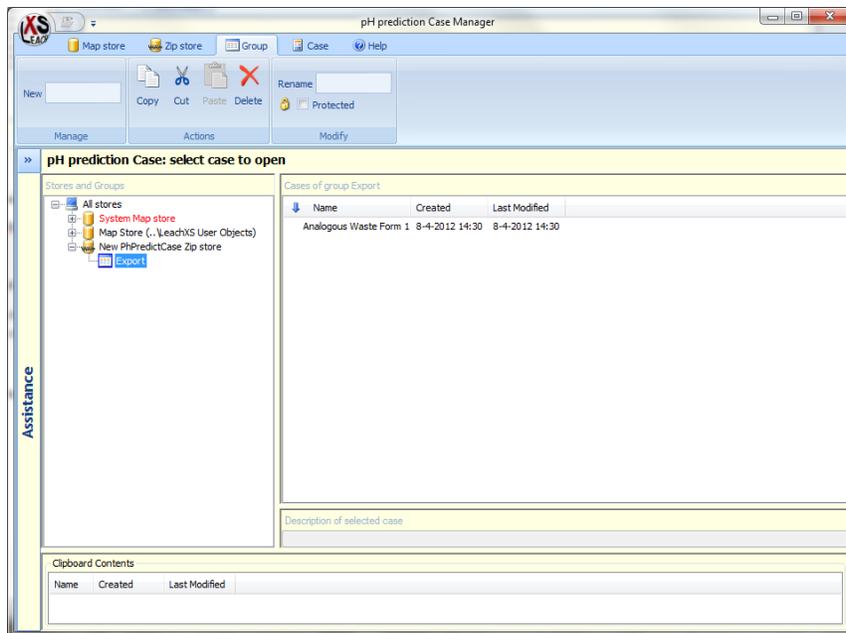
In the example below, a new **Zip Store** has been created and automatically named **New pH PredictCase Zip store**. The file can be renamed as desired; however, it is important that the case creator and the recipient of the case file know to what type of model the case belongs, as this is important for importing the case file in the proper model editor.



Navigate to the **Map Store** and select group **Export** from the **Groups of the Map Store** pane. Drag the group **Export** to the **Zip Store** titled **New pH PredictCase Zip store** to move the case to the **Zip Store** folder.

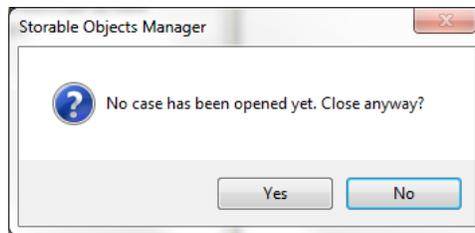


The newly-created **Zip Store** now contains the **Export** group from the **Map Store**.



The zip file in the **Zip Store** folder can be sent to another LeachXS user. Since all model components are embedded in the case this ensures that the other party has the exact same model and underlying settings and input data as the primary user.

The Model editor can be closed. Ignore the message and click **Yes**.



The created zip store will disappear (or can be deleted) as soon as the zip file has been sent to the receiving user, moved to another location, or renamed.

*Note: It is not possible to mix case files from different models within one zip file. This is because LeachXS will not be able to recognize the model when placed in the wrong model editor.*

## Statistical Evaluation of Data

---

Statistics functions embedded in LeachXS allow for calculation and display of statistical representations for multiple selected data series at critical points in the data set.

Statistical functions allow for calculation of:

- Mean
- Confidence intervals
- Prediction intervals
- Median
- Percentiles

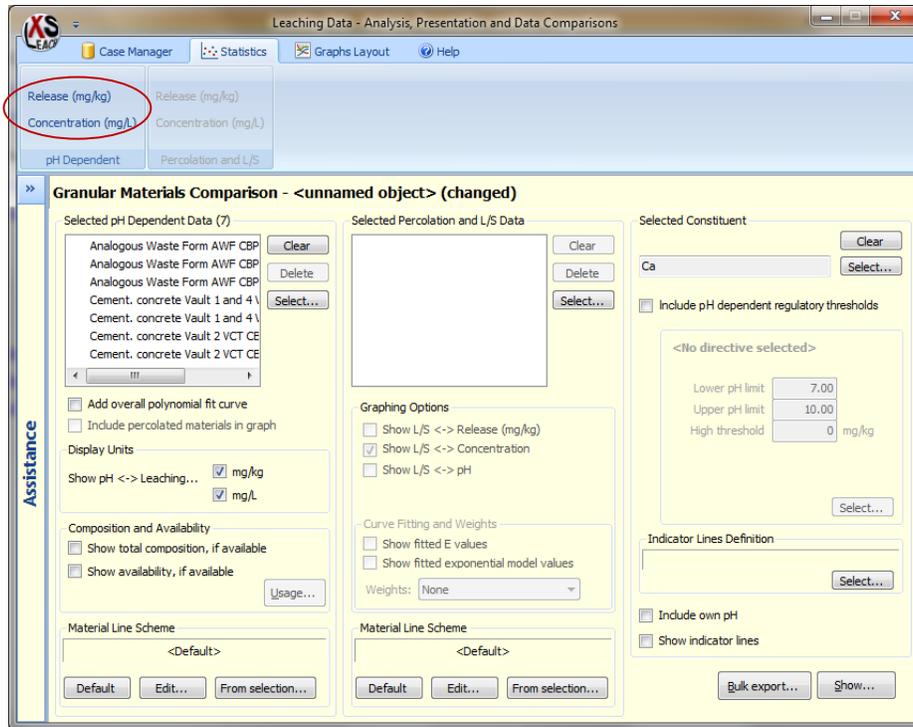
In many cases, calculation of statistics based on multiple testing results requires data interpolation/extrapolation to a consistent set of ordinate (x-axis) values. For example, the mean concentration of 3 pH-dependent replicate data series may be calculated at the target pH values. LeachXS offers several interpolation options (e.g., linear, spline, nearest value) that can be applied either directly to data sets or to log-transformed data.

There are two pathways for carrying out statistical analyses:

- From the **Analysis and Presentation** screen
- From the **Import or Add New Data** roll-up menu in the main screen

### Statistical Calculations from the Analysis and Presentation Screen

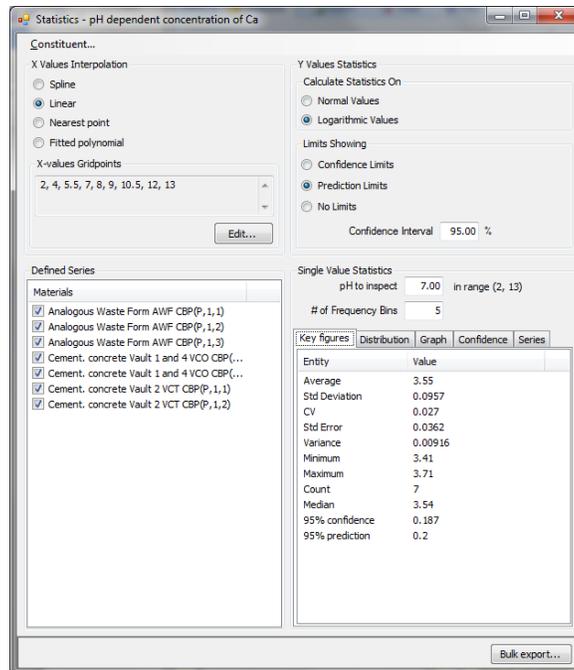
From the either of the **Analysis and Presentation** screens (either for **Granular Materials Comparisons** or **Monolithic Materials Comparisons**), click on the **Statistics** tab in the top menu bar and select either **Release (mg/kg)** or **Concentration (mg/L)** from the ribbon menu.



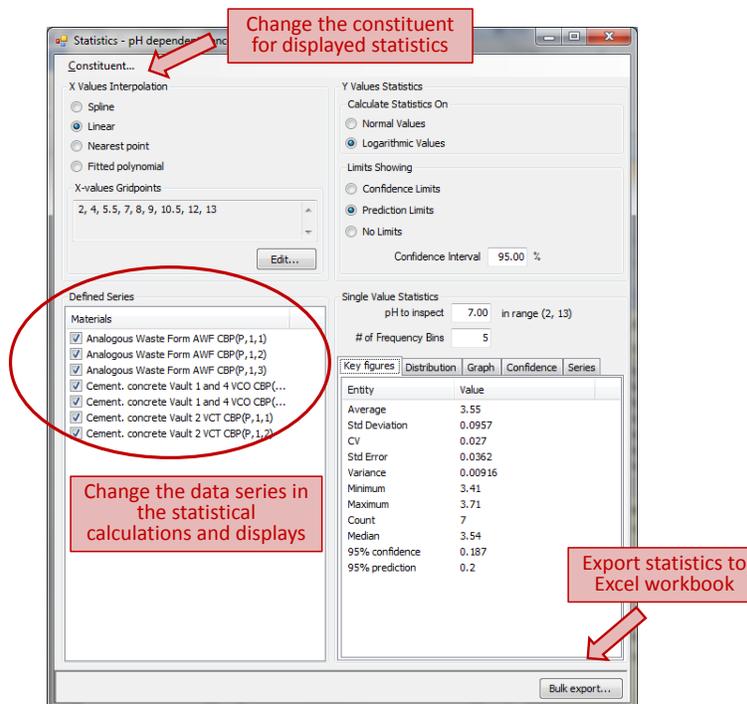
The following pop-up screen is displayed allowing the user to select the statistics and options for calculation. Options include:

- Basis for interpolation of X-values with editable target values for the grid points
- Basis for calculating Y-values statistics (i.e., whether statistics are calculated on the reported values or a log-transform of the values)
- Display options for **Confidence Limits**, **Prediction Limits** or **No Limits** (along with mean values).

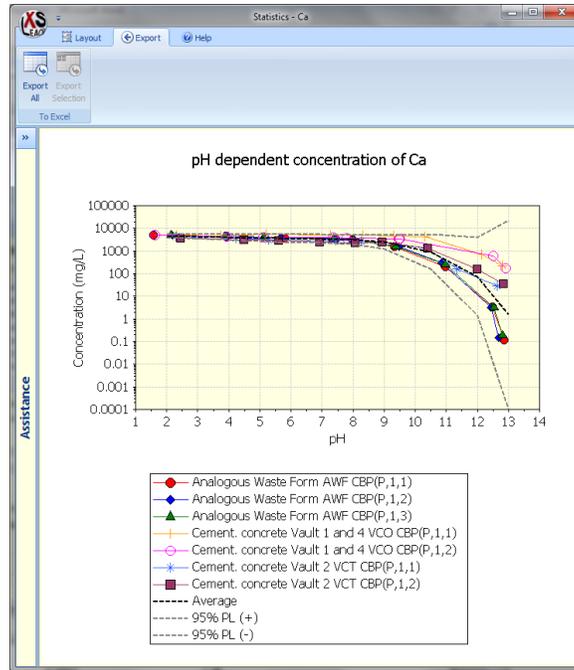
Statistical results are shown in the tabbed display at the lower right corner of the window with options for showing distributions, graphs, confidence intervals, etc.



The displayed constituent may be changed by clicking on **Constituent...** in the upper left hand corner of the window. The **Defined Series** panel allows for the user to vary what data series are used in the statistical calculations and display. The **Bulk export...** button will allow users to export selected statistics and associated graphs to a Microsoft Excel® file for multiple constituents.

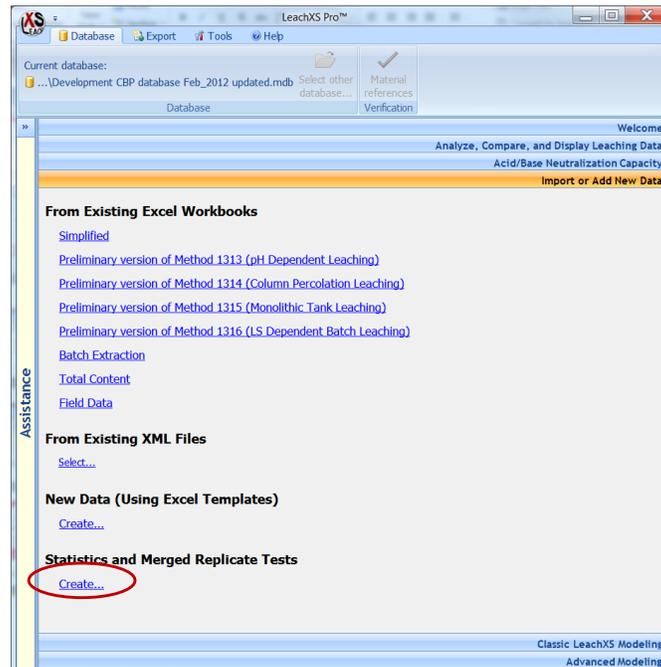


The screen below is an example display of the statistics results from the above case with the mean and 95% prediction limits displayed as dashed lines.

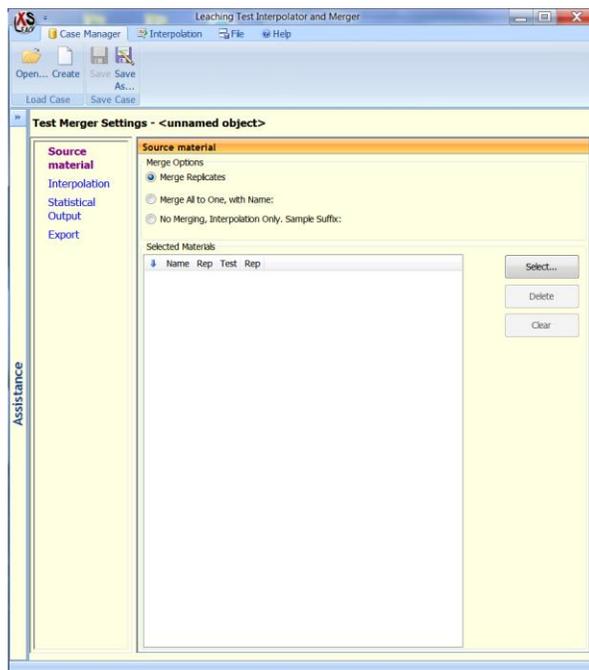


## Statistical Calculations from the Import or Add New Data Roll-up Menu

An alternative approach for accessing statistical functions is through the **Import or Add New Data** roll up menu on the main start up screen. This approach allows for development of more complex statistical analyses, and importing the statistical results as additional data sets into the database for display with the original data or as comparison lines with other data sets.



Under the header **Statistics and Merged Replicate Tests**, click on **Create...** to go the to the **Leaching Test Interpolator and Merger** screen.



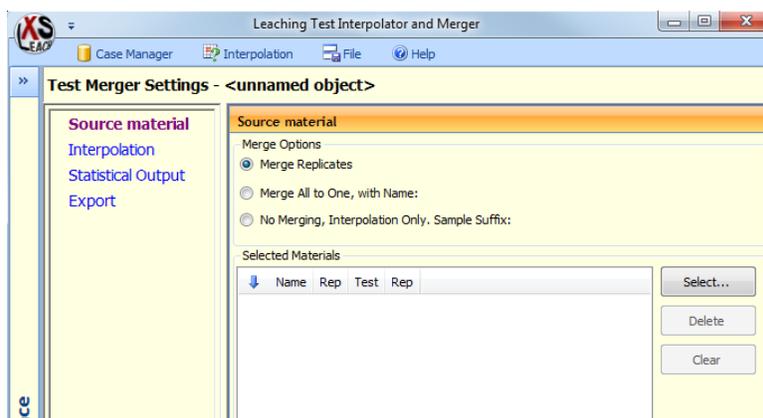
This tool has been designed to merge multiple existing leaching tests into one, the resulting test being the output of a statistical function.

For example, if you have three replicates of a pH dependence test, you can create a new test, the values being the average of the replicates. This new test can be saved and imported into a LeachXS database.

There are three main steps to take in the merging process. First, the tests to be merged are to be selected. After that, the tests need to be interpolated. Interpolation or extrapolation is necessary, because statistical data cannot be calculated if time, L/S or pH values of all selected tests are not the same. Finally, the desired statistical quantities to output need to be chosen.

The resulting data sets will be saved in Material Exchange XML format, so that you can import them into a LeachXS database.

## Step 1: Choosing source materials and merge options



From the left pane, select **Source material**. The top right pane shows the merge options you can choose:

- **Merge Replicates.**

If you have chosen multiple materials each having multiple test replicates, the replicates are merged on a per material basis. In this case you will have an additional set of statistical quantities at your disposal.

- **Merge All to One.**

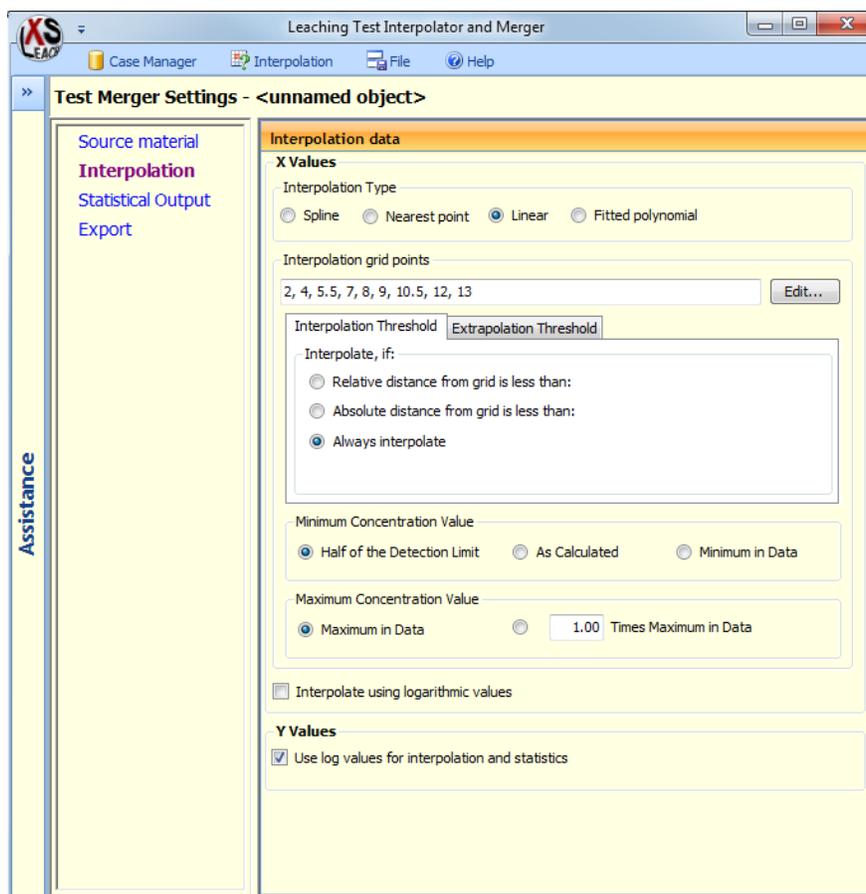
All tests you have selected will be merged into one test. You can give the material to create a name of your liking.

- **Interpolation only.**

In this case, the tests won't be merged, but every test will be interpolated only. You can give a suffix that will be appended to each material you have selected.

The bottom right pane will show the materials and tests you have selected. Press the **Select...** button to pick the materials and tests. See "The Sample Selector" on page 121.

## Step 2: Interpolation



As you can see in the right pane, there are many options to control the interpolation process. The options appear if you click on **Interpolation** in the left pane.

The **Interpolation Type** controls how time, pH or L/S values are interpolated. Usually, **Linear** interpolation will do fine, but if the values of the test are very different from the target interpolation values, you can experiment with this option.

The **Interpolation grid points** are the target interpolation values. Press the **Edit...** button to edit them. See “Interpolation Grid Editor” on page 145 for details.

If you want to know which values will be interpolated and which will be extrapolated to the target interpolation values, given the current interpolation and extrapolation options, press the **Interpolation Preview** button on the ribbon tab page **Interpolation**. The **Interpolation Inspector** will show up:

	2	4	5.5	7	8	9	10.5	12	13
<b>Concrete VCO (vaults, CBP) (P,1,1)</b>	Ext	Int	Int	Int	Int	Int	Int	Int	Ext
<b>Concrete VCO (vaults, CBP) (P,1,2)</b>	Int	Int	Ext						
<b>Concrete VCT (vaults, CBP) (P,1,1)</b>	Ext	Int	Int	Int	Int	Int	Int	Int	Ext
<b>Concrete VCT (vaults, CBP) (P,1,2)</b>	Ext	Int	Int	Int	Int	Int	Int	Int	Ext

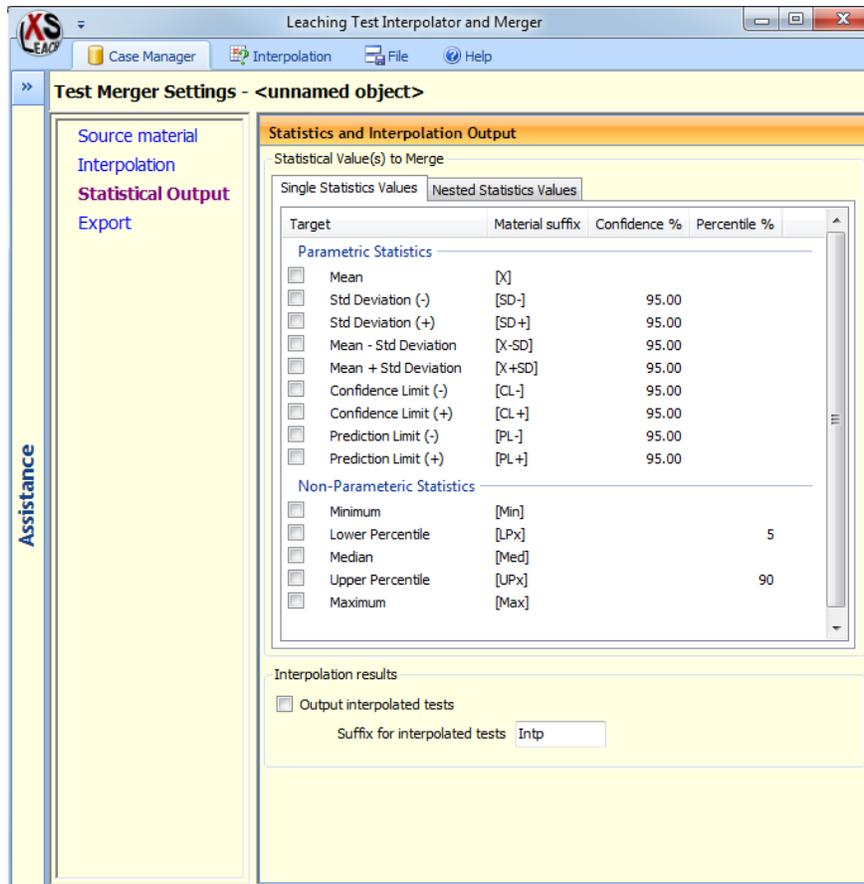
Legend

- Int The value is reached by interpolation
- Ext The value is reached by extrapolation
- <x> Not reachable by interpolation or extrapolation
- <!> Calculation not feasible

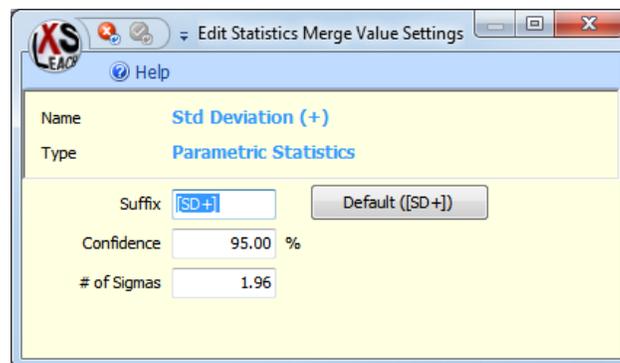
You can choose to perform the interpolation on the x-values on a logarithmic bases. This is especially appropriate for time and L/S values. Check the Interpolate using logarithmic values for this option. The way the concentration (y) values are interpolated can be controlled in the same way, using the **Use log values for interpolation and statistics**.

### Step 3: Choosing statistical quantities

There are about a dozen statistical quantities to choose from. They appear if you click on **Statistical Output** in the left pane.



You can check multiple values. Each value will be output as a separate material. The name of the material will be composed of the original name with a suffix appended. The default suffixes are listed, but you can change it by double-clicking an entry. When appropriate, you can change the confidence or percentile as well:

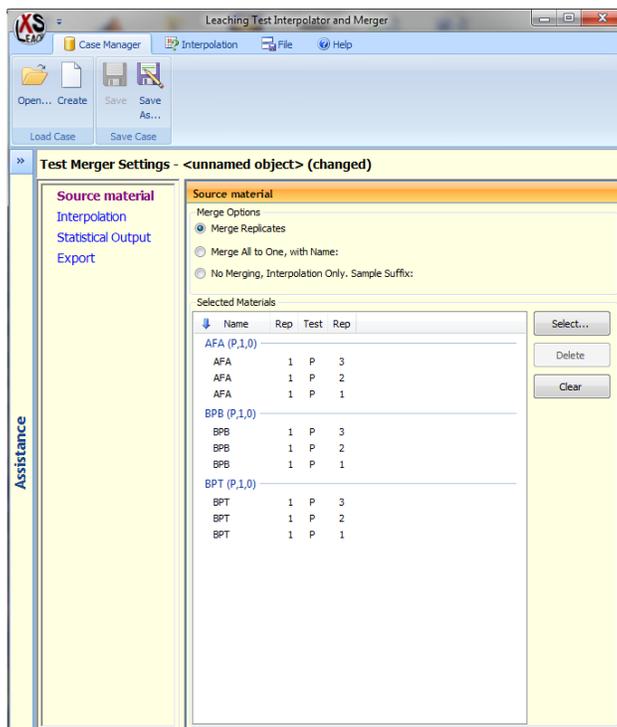


Below the list is an option to output the interpolated test along with the statistical values as separate materials.

If you have chosen the **Merge Replicates** option, you have additional statistical options in the **Nested Statistics Values** tab page.

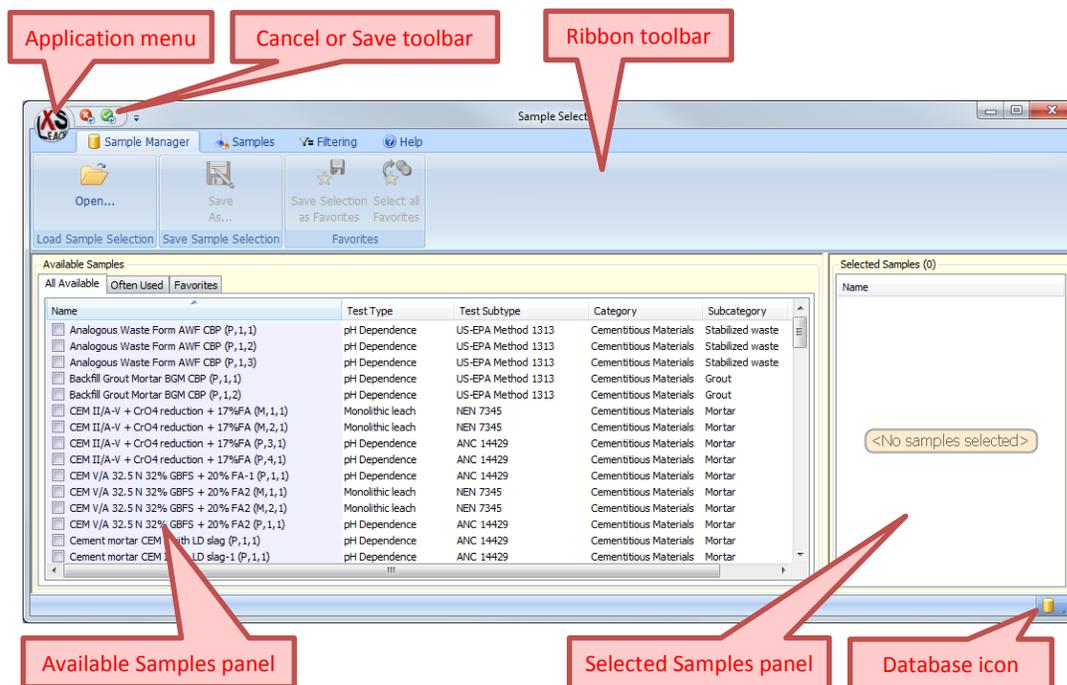
## Exporting the results

After you've set the options you want, you are ready to save the results in a Material Exchange XML file. Save the results by clicking the **Save to File** button on the **File** ribbon tab. Before you do that, you can choose to create a new file for the results, or append them to an existing file. You can specify this if you press the **Export** link in the left pane.



## The Sample Selector

The **Sample Selector** helps you selecting one or more leaching samples from the database.



- The **Application** menu contains functions to make screenshots and load recently used lists of leaching samples.
- The **Cancel or Save** toolbar contains two small buttons to leave the **Sample Selector**. The red one cancels your selection and the green one passes the selection to the module that called up the **Sample Selector**.
- The **Ribbon** toolbar contains functions that operate on lists or samples, grouped in ribbon tabs.
- The **Available Samples** panel contains leaching sample lists from which you can choose the desired samples.
- The **Selected Samples** panel contains all the samples that will be passed to the module that called up the **Sample Selector**.
- The **Database** icon shows information on the name and location of the active sample database if you keep the mouse steady on it.

### Basic Operation

The **Available Samples** panel displays a list of samples from the sample database. Not all samples in the database may show up. Only those samples that make sense within the context from which the **Sample Selector** is started will be visible. If you check a sample by clicking the checkbox, it will show up in the **Selected Samples** panel, indicating that the sample will be included in the list of desired samples. You

can also select samples by highlighting samples using the **Ctrl** and **Shift** key, and then hit the spacebar: all highlighted samples will show up in the **Selected Samples** panel.

The checkboxes will not always be present: if the **Sample Selector** is called from within a context that requires only one sample, there will be no checkboxes. In this case, you can select a sample just by clicking on it.

If you are done with selecting samples, click on the small green button with the checkmark on the **Cancel or Save** toolbar. The **Sample Selector** will close and pass the selected samples to its caller. If you want to leave the **Sample Selector** without using the selection, click on the small red button with the cross.

If there are not many samples in your database, the easiest way to select samples is just scrolling through the panel and checking the appropriate boxes. However, if you have a very large database with samples, there are many options to sort, group and filter the sample list in order to make it easier to find and select samples.

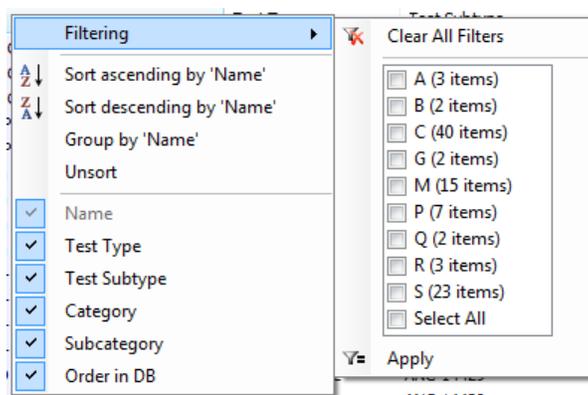
## Manipulating the Sample List

The **Available Samples** panel shows columns with extra information on the samples. There are columns showing the leaching test type, the test subtype, the material category, the subcategory and finally, an indication of the location of the location in the database. Samples last entered in the database have the highest location indication.

### Sorting, grouping and filtering samples

You can sort the list of samples by clicking on one of the column headers. The list is sorted according to the information in the column. Clicking the same column header again will reverse the sort order.

If you use the right mouse button to click on a column header, all grouping and filtering options show up in a small context menu:



This screenshot is made when the **Name** column was right-clicked.

To filter the list, check the appropriate initial characters of the sample names that appear to the right of the **Filtering** entry in the menu and click on the **Apply** button at the bottom of the list. Alternatively, you can click on the **Clear All Filters** entry if you want to remove a filter from a column.

To group the list, click on the **Group by '<column name>'** entry in the menu (in this example the column is the **Name** column). The list will look like:

Name	Test Type	Test Subtype
<b>A [3 items]</b>		
<input type="checkbox"/> Analogous Waste Form AWF CBP (P, 1, 1)	pH Dependence	US-EPA Metho
<input type="checkbox"/> Analogous Waste Form AWF CBP (P, 1, 2)	pH Dependence	US-EPA Metho
<input type="checkbox"/> Analogous Waste Form AWF CBP (P, 1, 3)	pH Dependence	US-EPA Metho
<b>B [2 items]</b>		
<input type="checkbox"/> Backfill Grout Mortar BGM CBP (P, 1, 1)	pH Dependence	US-EPA Metho
<input type="checkbox"/> Backfill Grout Mortar BGM CBP (P, 1, 2)	pH Dependence	US-EPA Metho
<b>C [40 items]</b>		
<input type="checkbox"/> CEM II/A-V + CrO4 reduction + 17%FA (M, 1, 1)	Monolithic leach	NEN 7345
<input type="checkbox"/> CEM II/A-V + CrO4 reduction + 17%FA (M, 2, 1)	Monolithic leach	NEN 7345
<input type="checkbox"/> CEM II/A-V + CrO4 reduction + 17%FA (P, 3, 1)	pH Dependence	ANC 14429
<input type="checkbox"/> CEM II/A-V + CrO4 reduction + 17%FA (P, 4, 1)	pH Dependence	ANC 14429
<input type="checkbox"/> CEM V/A 32.5 N 32% GBFS + 20% FA-1 (P, 1, 1)	pH Dependence	ANC 14429

Now, if you click a group heading, all samples in the group will be highlighted. Press the **spacebar** to select them. You can expand or collapse a group by double-clicking a group heading. You'll find buttons on the ribbon toolbar, tab **Samples** to expand or collapse all groups.

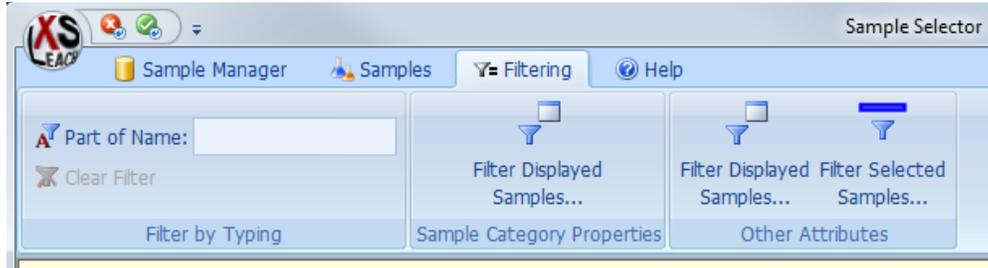
The grouping is temporary: if you click on another column heading, the list is ungrouped. If you want the grouping to remain, right-click on the grouped column heading and select **Lock grouping on '<column name>'** entry in the menu (in this example the column is the Name column). You can unlock grouping as well.

### Hiding or showing columns

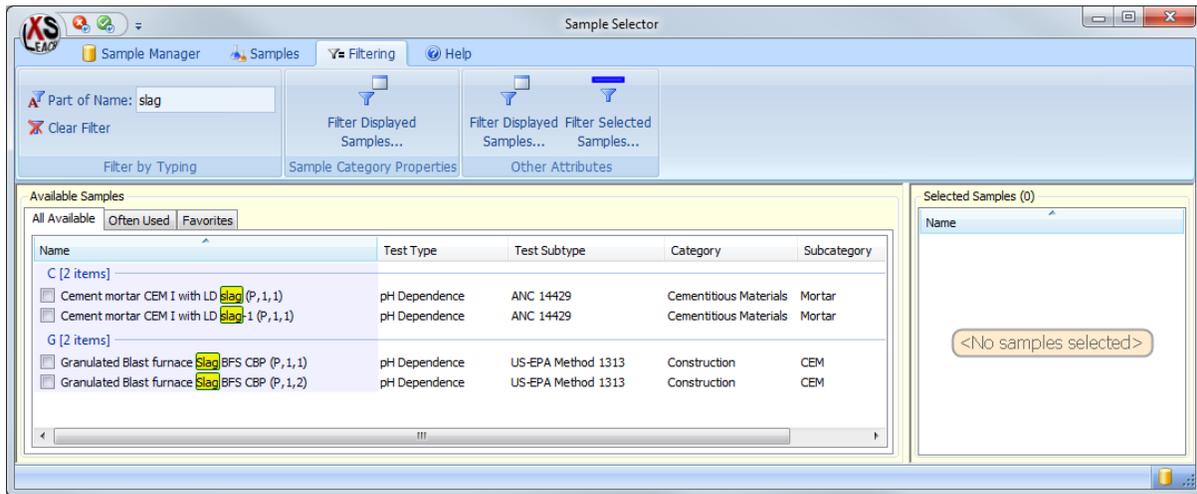
At the bottom of the context menu you'll see a list of column names. If you don't want hide columns, remove the check marks for the appropriate columns by clicking on them.

### More filtering

Besides filtering the list with the aid of the context menu, the **Filter** ribbon tab contains more filtering options:

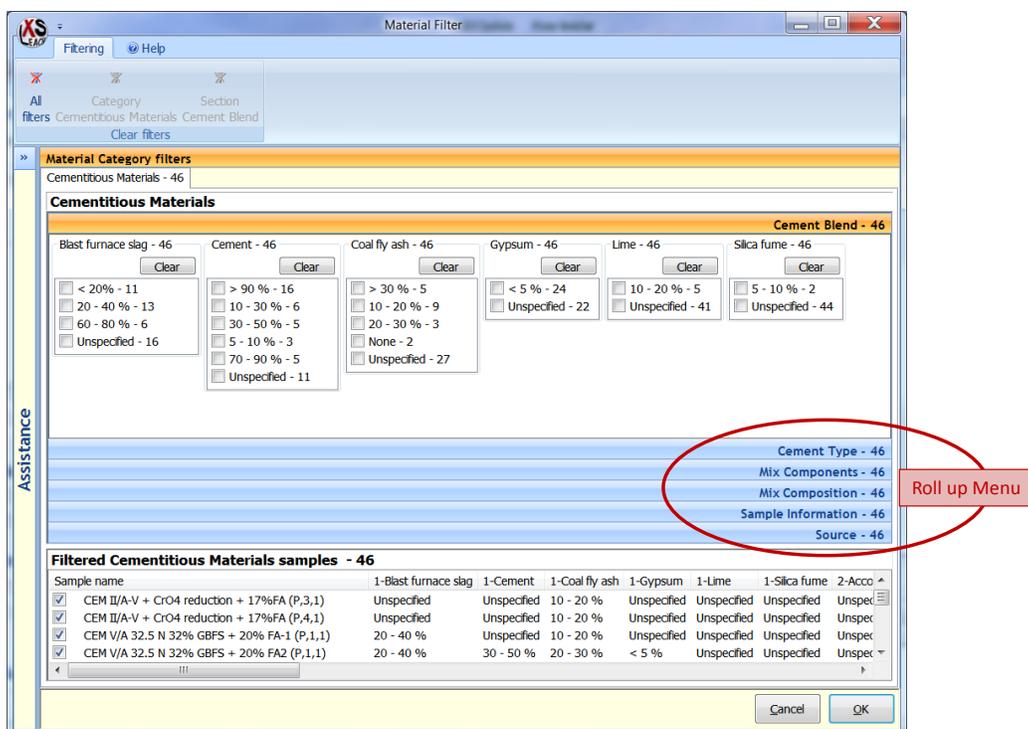


The **Filter by Typing** tab group contains a text box where you can type text. The sample names are filtered while you are typing text, showing only those samples that contain the text you type. For instance, if you type “slag”, the sample list will change to:



If you hit the **Enter** key in the text box or press the **Clear Filter** button, the filter is removed.

Database samples may have extra material properties. You can filter on these properties by clicking on **Filter Displayed Samples...** on the **Sample Category Properties** ribbon tab. A new filter dialog will appear:



The display box is divided into several filter categories by a roll up menu on the right side. In the example below, the following filter categories are shown:

- Cement Blend
- Cement Type
- Mix Components
- Mix Composition
- Sample Information
- Source

The filter categories for the US EPA CCR database ([USEPA CCR 12-2009 rev1.mdb](#)) will differ from this example, but the filtration of materials by filtration category is the same. At the bottom of the screen, LeachXS displays the materials corresponding to the filters applied. In the example shown above, no filters have been applied and 46 materials are available for display.

By selecting the appropriate roll up menus and checking the desired filter options, the database is filtered. When the desired data sets are located, click the **OK** button to accept the filtered materials and to return to the **Sample Selector**. The filtered samples will appear in the **Selected Samples** panel.

If you have knowledge about the internal sample database structure, you can also filter on values of a number of fields and tables in the database. These filter options are on the **Other Attributes** group on the **Filtering** ribbon tab.

## The Selected Samples panel

The **Selected Samples** panel contains the samples you have selected. On tab group **Edit** of ribbon tab **Samples** there are two buttons to manipulate the selection list. Button **Delete** will delete the highlighted samples from this panel, while button **Clear** will clear the entire list.

If you want to see where a selected sample is listed in the **Available Samples** panel, double-click on a sample. The sample in the **Available Samples** panel will scroll into view.

## Saving and loading sample lists

Sample lists can be saved for later use; if you foresee that you will use a list of selected samples more often, you can save the list with a name of your liking. Loading and saving lists is done with the **Case Manager**.

If you have created a list of selected samples and want to save the list, click on button **Save As...** on tab group **Save Sample Selection** of ribbon tab **Sample Manager**. The **Case Manager** will show up and enables you to save the list.

If you have opened the **Sample Selector** and want to use a list that you created and saved earlier, press button **Open...** on tab group **Load Sample Selection** of ribbon tab **Sample Manager**. The **Case Manager** will show up, assisting you in selecting your list.

A quick way to open a previously saved list is by selecting it from the **Recently Used** lists. You can show and select these lists by clicking on the **Application menu** (the round LeachXS logo).

You should be aware of the fact that a list of samples you load may not be loaded completely in the **Selected Samples** panel. The list may not (fully) show up in the following circumstances:

- The list you want to load contains many samples, but from the context of the **Sample Selector** you are allowed to select only one sample.
- The list you want to load contains leaching test samples that are not valid from the context of the **Sample Selector**. For instance, the list to load contains pH dependence test samples, while the context requires selection of monolithic diffusion test samples.
- The list you want to load contains samples from a different sample database than the one that is currently active.

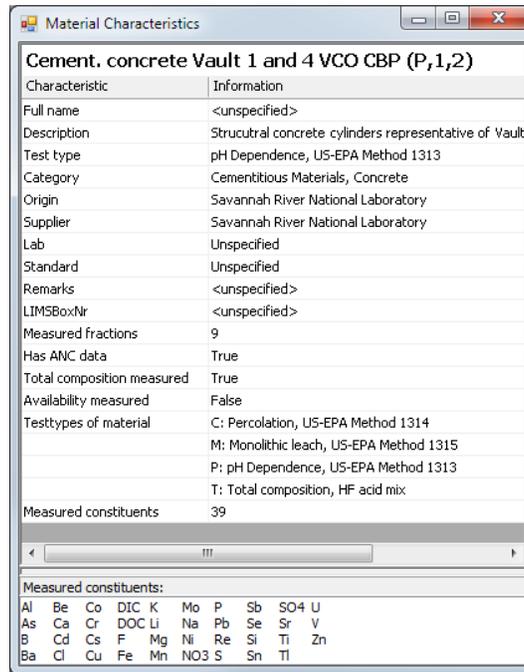
## Favorites list and often used samples.

You can make a list of selected samples your favorite list by saving the list with button **Save Selection as Favorites** on the **Favorites** tab group of ribbon tab **Sample Manager**. If you have designated a list of samples to be your favorite, you will always have these samples at your disposal, whenever you use the **Sample Selector**. The list will show up on tab page **Favorites** in the **Available Samples** panel.

The **Sample Selector** keeps track of the samples you selected and remembers the 60 most often used ones. They appear on tab page **Often Used** in the **Available Samples** panel.

## Revealing detailed sample information

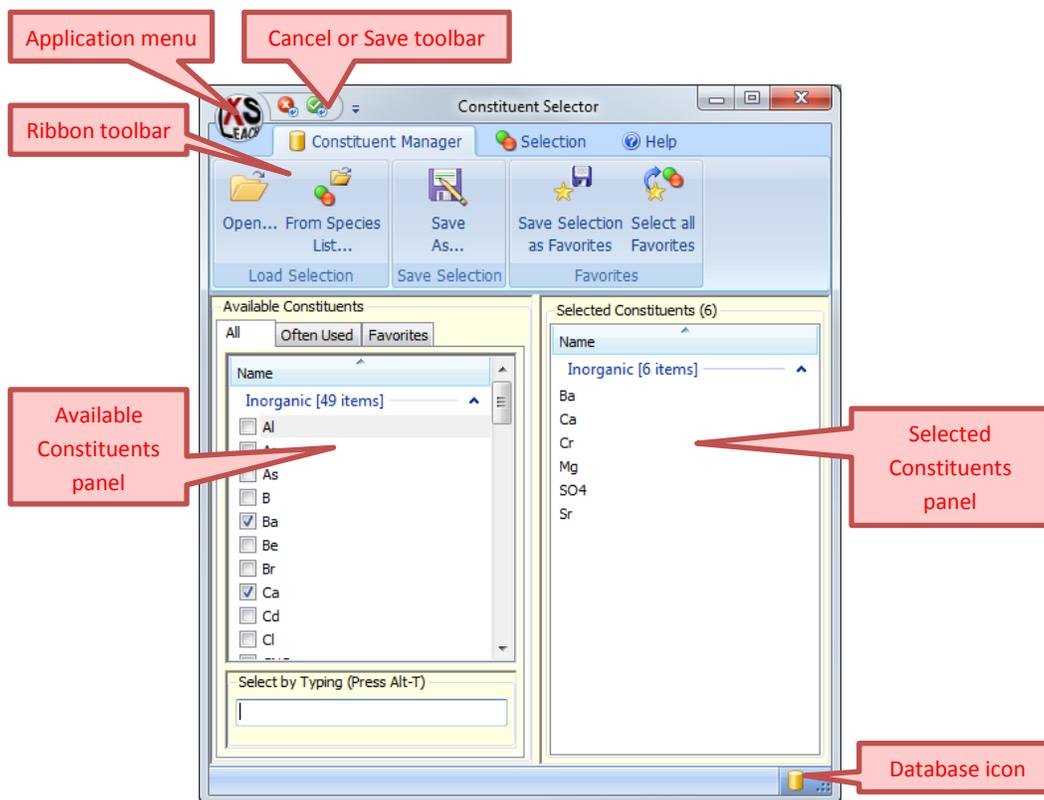
You can inspect more details of a sample by selecting it and press button **Show/Hide** on the **Sample Information** tab group of ribbon tab **Samples**. A window like the one below will pop up:



The window will stay on your screen until you press the **Show/Hide** button again or until you leave the **Sample Selector**. If you select another sample, the content of the window is refreshed with information of that sample. You can select a sample from any list you want: from any tab in the **Available Samples** panel or from the **Selected Samples** panel.

## The Constituent Selector

The **Constituent Selector** helps you selecting one or more constituents from the database.



- The **Application** menu contains functions to make screenshots and load recently used lists of constituents.
- The **Cancel or Save** toolbar contains two small buttons to leave the **Constituent Selector**. The red one cancels your selection and the green one passes the selection to the module that called up the **Constituent Selector**.
- The **Ribbon** toolbar contains functions that operate on lists or constituents, grouped in ribbon tabs.
- The **Available Constituents** panel contains constituent lists from which you can choose the desired constituents.
- The **Selected Constituents** panel contains all the constituents that will be passed to the module that called up the **Constituent Selector**.
- The **Database** icon shows information on the name and location of the active sample database if you keep the mouse steady on it.

### Basic Operation

The **Available Constituents** panel displays a list of constituents from the active database. If you check a constituent by clicking the checkbox, it will show up in the **Selected Constituents** panel, indicating that

the constituent will be included in the list of desired constituents. You can also select constituents by highlighting samples using the **Ctrl** and **Shift** key, and then hit the spacebar: all highlighted constituents will show up in the **Selected Constituents** panel.

The checkboxes will not always be present: if the **Constituent Selector** is called from within a context that requires only one constituent, there will be no checkboxes. In this case, you can select a constituent just by clicking on it.

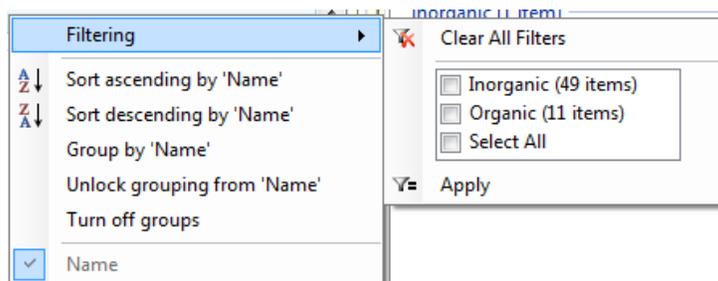
If you are done with selecting constituents, click on the small green button with the checkmark on the **Cancel or Save** toolbar. The **Constituent Selector** will close and pass the selected constituents to its caller. If you want to leave the **Constituent Selector** without using the selection, click on the small red button with the cross.

If there are not many constituents in your database, the simplest way to select constituents is just scrolling through the panel and checking the appropriate boxes. But there are also options to sort, group and filter the constituent list in order to make it easier to find and select constituents.

## Sorting, grouping and filtering constituents

You can sort the list of constituents by clicking on the column header. The list is sorted alphabetically. Clicking the same column header again will reverse the sort order.

If you use the right mouse button to click on the column header, all grouping and filtering options show up in a small context menu:



To filter the list, check one or more of the entries that appear to the right of the **Filtering** entry in the menu and click on the **Apply** button at the bottom of the list. Alternatively, you can click on the **Clear All Filters** entry if you want to remove the filter.

To group the list, click on the **Group by 'Name'** entry in the menu. The list will have two groups: **Inorganic** and **Organic**. You can expand or collapse a group by double-clicking on the group heading.

If you click a group heading, all constituents in the group will be highlighted. Press the **spacebar** to select them.

You can ungroup the list by clicking on **Turn off groups** in the context menu.

## Selecting by using Select by Typing

Another way of selecting constituents is to make use of the **Select by Typing** text box. First, move the focus to this text box by clicking on it or press **Alt+T**. Start typing the name of the constituent. While you are typing, the first constituent that matches will scroll into view. As soon as the characters you type matches a constituent (in a case insensitive way), the text color turns from red to black. Hitting the **spacebar** or **Enter** key will select the corresponding constituent and clears the text box, so that you can continue typing to select another constituent.

If the text remains red while you are typing, either no match or no full match is found in the constituent list. You can check if a partial match is found by looking at the selected constituent in the **Available Constituents** pane. The selected constituent will have a light gray background. If no partial match is found, no constituent will be selected. If a partial match is found, and if it is the constituent you want, select it by hitting the **spacebar** twice. The first hit will expand the selected constituent name in the text box and the second hit will select it.

## The Selected Constituents panel

The **Selected Constituents** panel contains the samples you have selected. On tab group **Edit** of ribbon tab **Selection** there are two buttons to manipulate the selection list. Button **Delete** will delete the highlighted constituents from this panel, while button **Clear** will clear the entire list.

## Saving and loading constituent lists

Constituent lists can be saved for later use; if you foresee that you will use a list of selected constituents more often, you can save the list with a name of your liking. Loading and saving lists is done with the **Case Manager**.

If you have created a list of selected constituents and want to save the list, click on button **Save As...** on tab group **Save Selection** of ribbon tab **Constituent Manager**. The **Case Manager** will show up and enables you to save the list.

If you have opened the **Constituent Selector** and want to use a list that you created and saved earlier, press button **Open...** on tab group **Load Selection** of ribbon tab **Constituent Manager**. The **Case Manager** will show up, assisting you in selecting your list.

A quick way to open a previously saved list is by selecting it from the **Recently Used** lists. You can show and select these lists by clicking on the **Application menu** (the round LeachXS logo).

If you use LeachXS for Orchestra modeling, you probably have used and created species lists. Species lists define the mapping of Orchestra species to LeachXS constituents. You can use a species list as list of selected constituents by using **From Species List...** button from tab group **Load Selection** of ribbon tab **Constituent Manager**.

### **Favorites list and often used constituents.**

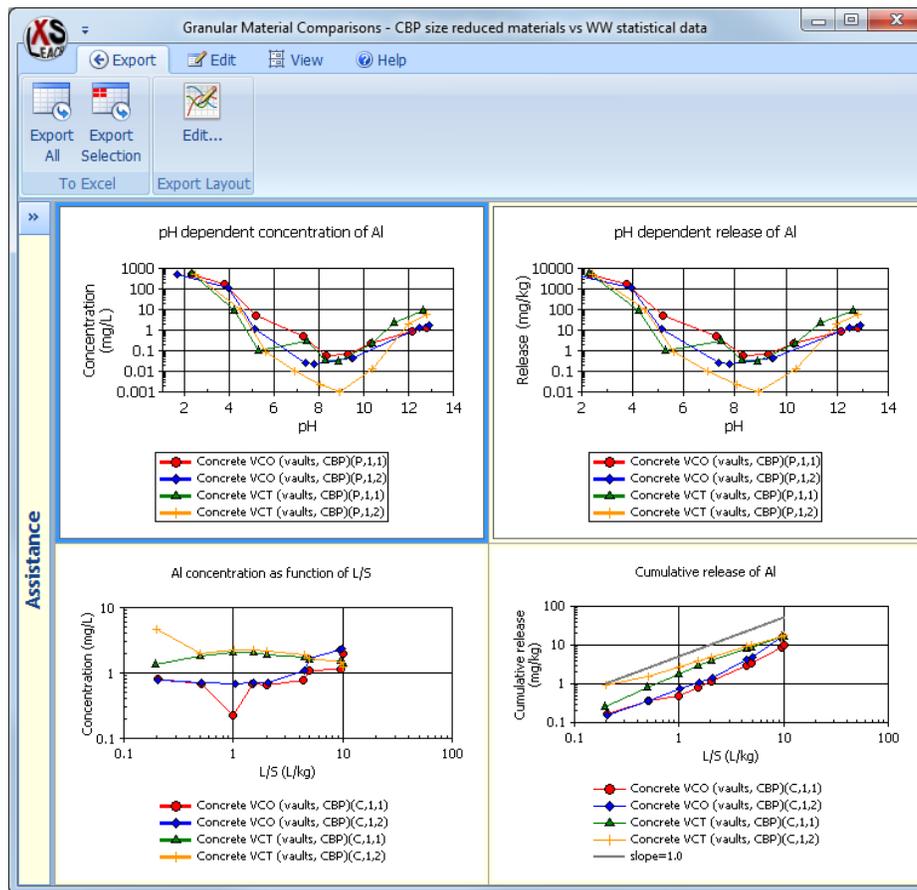
You can make a list of selected constituents your favorite list by saving the list with button **Save Selection as Favorites** on the **Favorites** tab group of ribbon tab **Constituent Manager**. If you have designated a list of constituents to be your favorite, you will always have these constituents at your disposal, whenever you use the **Constituent Selector**. The list will show up on tab page **Favorites** in the **Available Constituents** panel.

The **Constituent Selector** keeps track of the samples you selected and remembers the 30 most often used ones. They appear on tab page **Often Used** in the **Available Constituents** panel.

## Graph Window

The Graph window displays the results you have selected in a graphical way. It serves as a quick preview window before you export your results to a Microsoft Excel workbook.

You can copy any graph in the window to the Windows clipboard or save it to disk. You can inspect point values by moving the mouse pointer over a graph area. You can also change the graphical appearance of graphs a bit: you can zoom in a graph, reduce or enlarge the size of the legend font and change the appearance of the graph. For presentation purposes, you can save a graph on the Windows clipboard or a storage medium. All these functions are under the right mouse button.



## Highlighting a series

If there are many series in a graph, it may become difficult to distinguish series from each other. If you click on an entry in the legend, that entry and the corresponding series will be highlighted as long as the mouse button is pressed. The same will happen if you click on a marked point of a series. If the legend is not shown while highlighting a series, a small window will pop up with the name of the series.

## Viewing coordinates

When you move the mouse over the plot area of a graph, the exact coordinates of the mouse are displayed in the lower left corner of the graph. The coordinates are in the same scale as the plotted data. If you move the mouse pointer near a data point in a series, the coordinates will get the same color as the series color and the exact coordinates of the data point is displayed.

## Translating, scaling and zooming a chart

You can translate or scale a graph in any direction, or zoom in on a part of a graph. However, these manipulations will be canceled before you export the results to Microsoft Excel®.

You translate a graph by left-clicking the mouse button, while pressing the **Shift** key. If you click near the X-axis, you can translate along the X-axis. If you click near the Y-axis, you can translate along the Y-axis. Drag the mouse along the axis you chose to translate the graph.

*Note that translating along a logarithmic axis will probably not give any meaningful graphs.*

You scale a graph by left-clicking the mouse button, while pressing the **Ctrl** key. If you click near the X-axis, you can scale the X-axis. If you click near the Y-axis, you scale the Y-axis. Drag the mouse upward to get more detail and downward to get less detail.

*Note that scaling a logarithmic axis will probably not give any meaningful graphs.*

You zoom in on a graph by left-clicking the mouse button, while pressing the **Alt** key. Create a rectangle by dragging the mouse to another point. When you release the mouse button the graph is zoomed to the thus created rectangle.

You can restore the original scaling of the graph by pressing the **r** key, after you have clicked the graph to restore.

## Exporting results

The **Export** tab on the ribbon bar contains functions to export selected or all graphs to Microsoft Excel®. You can also change layout aspects of a graph to be exported. Select a graph and hit the **Edit...** button on the **Export** tab. See “General Options” on page 20 to find information on how to change layout aspects.

## General graph layouts

The **View** tab on the ribbon bar gives you a number of options to change the overall appearance of the **Graph Window**.

You can change how multiple graphs are laid out by pressing **Landscape** or **Portrait**.

If you have a lot of graphs, you may enlarge the plot areas of the graphs by not showing the legend, axis titles and axis labels. In tab group **Screen Appearance**, uncheck entries **Show Legend**, **Show Axis Titles** and/or **Show Axis Labels** to remove graph components.

You can zoom in to a particular graph by selecting it and pressing button **Zoom In** in the **Zoom Selection** tab group. The selected graph will fill the entire graph window. Press the **Zoom Out** button to return to the full page of graphs.

*Note that you can quickly zoom in to a particular graph by pressing and holding down the middle mouse button or scroll wheel. The full page is displayed again if you release the button.*

## Indicator Lines Editor

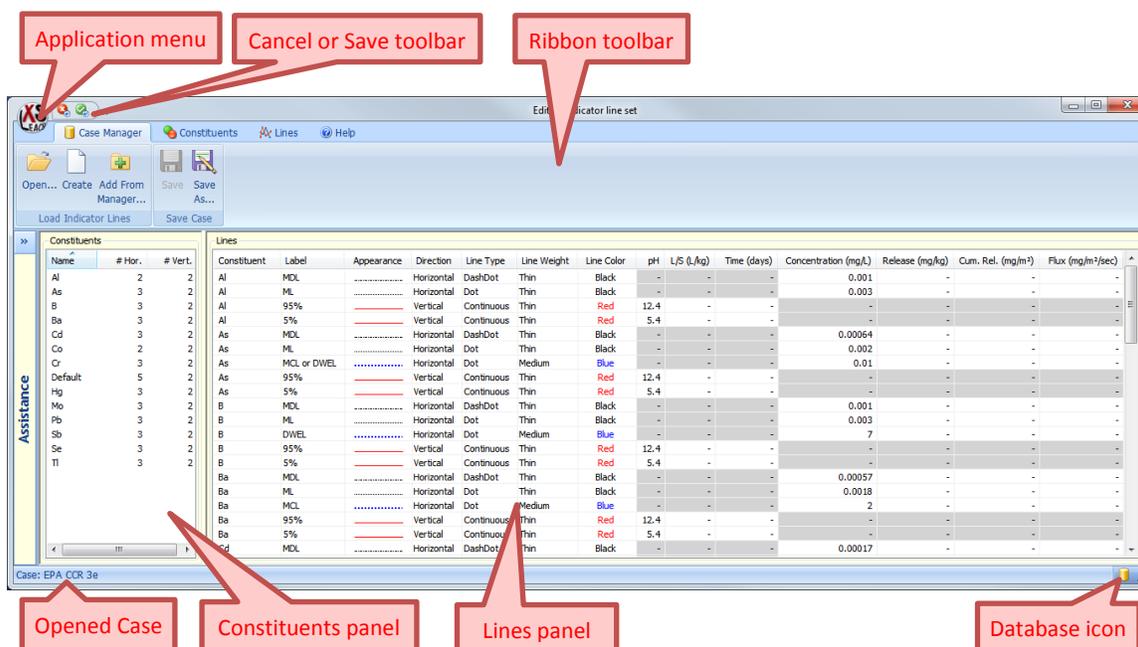
An indicator line is a LeachXS concept of a horizontal or vertical line to be shown in a chart. An indicator line belongs to a constituent, has properties to format the line and has a value that indicates at what position the line is to be drawn.

Indicator lines are typically used to show detection limits or regulatory directive values in a chart and are used in comparison cases. In LeachXS you can create indicator lines and save a set of lines for later use. You can edit the contents of indicator line sets and merge them with other sets. More than one indicator line per constituent can be present in a set.

When LeachXS draws a chart that shows data on a constituent, it scans all indicator lines the user has selected. LeachXS uses the following procedure to draw the appropriate indicator lines:

- First, only those lines are handled that belong to the subject constituent in the chart.
- From these lines, all are picked that have level values defined for the quantities that are plotted along the x-axis and the y-axis.

The **Indicator Lines Editor** looks like this:



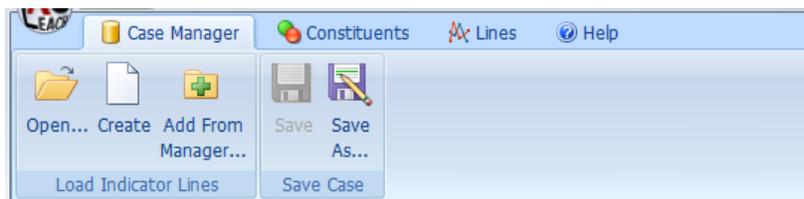
In the picture above, an existing set of indicator lines is already opened.

- The **Application** menu contains functions to make screenshots and load recently used lists of indicator lines.
- The **Cancel or Save** toolbar contains two small buttons to leave the **Indicator Lines Editor**. The red one cancels your editing and the green one passes the indicator lines to the module that called up the **Indicator Lines Editor**.

- The **Ribbon** toolbar contains functions that operate on the list of constituents or list of indicator lines, grouped in separate ribbon tabs.
- The **Constituents** panel displays all constituents that are present in the set of indicator lines, summarizing the number of horizontal and vertical indicator lines per constituent.
- The **Lines** panel shows all the lines and their definitions in the set.
- The **Opened Case** field shows the name of the set of indicator lines that is loaded from disk. If you have made changes in the set, an icon with a pencil in it will be present, like in the example picture. If you keep the mouse steady on the field, you'll see more details of the case.
- The **Database** icon shows information on the name and location of the active sample database if you keep the mouse steady on it.

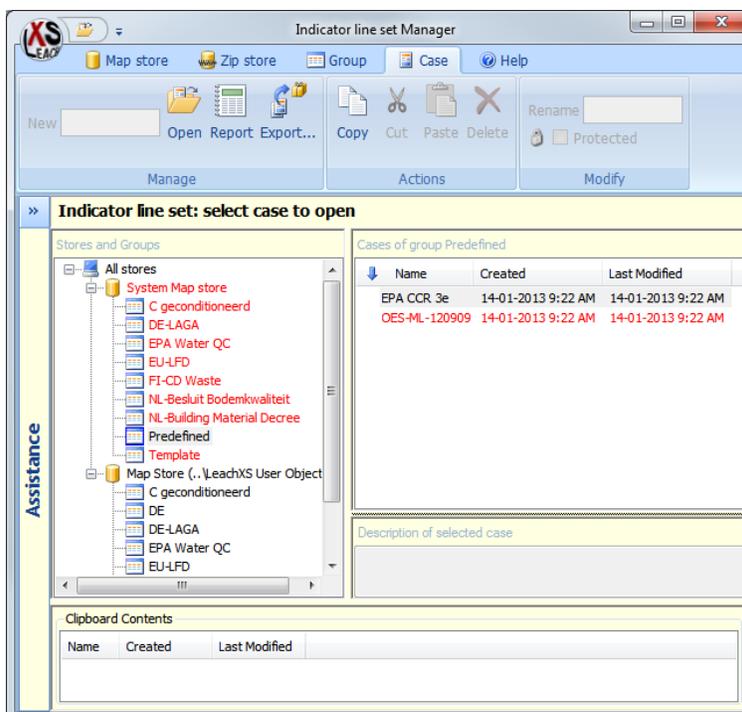
## Loading and saving indicator lines

All functions to load existing lines from disk or saving them are on the **Case Manager** tab on the ribbon toolbar.



From this toolbar, you can open an existing set of lines (**Open...**), create a new set from scratch (**Create**), or add a set of lines to the lines already present in the editor (**Add From Manager...**). The **Save** and **Save As...** buttons allow you to save the current set of lines.

Let's start with an existing set of indicator lines. Press the **Open...** button. The **Case Manager** will show up.



The red groups below **System Map** store are groups of indicator line sets that are shipped with LeachXS and are copied to your system during the installation process. Select group **Predefined** and then case **EPA CCR 3e** in the right pane. Press the **Open** button in tab group **Manage**. Alternatively, you can double-click the case name or press the small icon showing a folder in the small toolbar next to the **Application** menu. The **Case Manager** closes and the indicator lines are loaded into the **Indicator Lines Editor**. The editor should look more or less like the example picture at the beginning of this chapter.

## Organizing and editing indicator lines

In the **Lines** panel, all the indicator lines are shown. Every line has the following fields:

<b>Constituent Label</b>	The name of the constituent the line belongs to.
<b>Appearance</b>	Text to appear in the chart, near the line.
<b>Direction</b>	An indication of how the line will look like in the chart.
<b>Line Type</b>	The direction of the line.
<b>Line Weight</b>	The pattern of the line.
<b>Line Color</b>	The thickness of the line.
	The color of the line.

In addition, one or more fields can be used to specify the value of the line:

<b>pH</b>	A pH value.
<b>L/S (L/kg)</b>	A liquid to solid ratio.
<b>Time (days)</b>	A time.
<b>Concentration (mg/L)</b>	A concentration.
<b>Release (mg/kg)</b>	A release.

**Cumulative Release (mg/m<sup>2</sup>)** A cumulative release.  
**Flux (mg/m<sup>2</sup>/sec)** A flux.

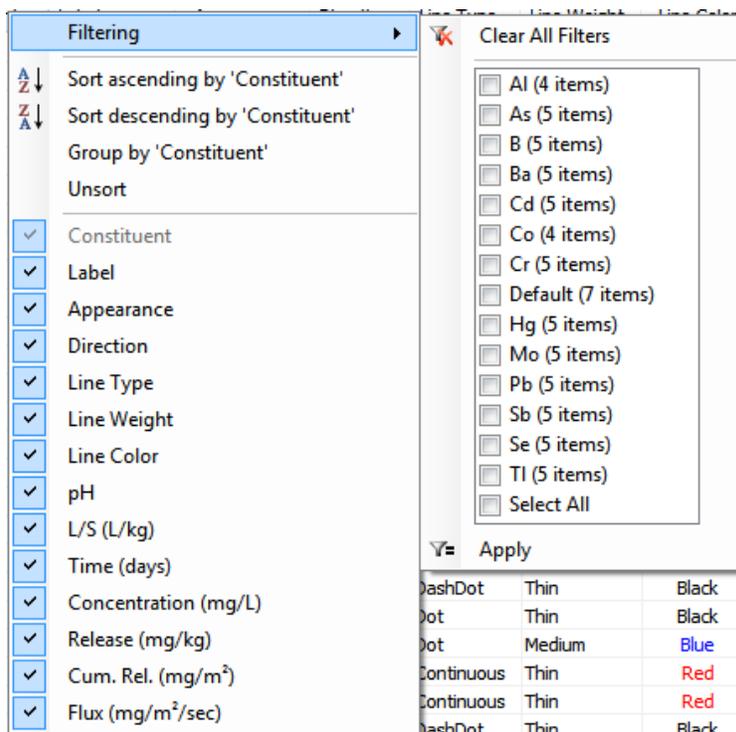
One of first three fields is usually used for vertical lines, since these quantities usually are plotted along the x-axis. The other fields are common for horizontal lines.

If you want to edit a line, click on the appropriate cell and type or choose a new value. The **Constituent** field and **Appearance** field are not editable.

### Sorting, grouping and filtering samples

You can sort the list of lines by clicking on one of the column headers. The list is sorted according to the information in the column. Clicking the same column header again will reverse the sort order.

If you use the right mouse button to click on a column header, all grouping and filtering options show up in a small context menu:



This screenshot is made when the **Constituent** column was right-clicked.

To filter the list, check the appropriate constituents that appear to the right of the **Filtering** entry in the menu and click on the **Apply** button at the bottom of the list. Alternatively, you can click on the **Clear All Filters** entry if you want to remove a filter from a column.

To group the list, click on the **Group by '<column name>'** entry in the menu (in this example the column is the Constituent column). The list will look like:

Constituent	Label	Appearance	Direction	Line Type	Line Weight	Line Color	pH	L/S (L/kg)	Time (d)
<b>Al [4 items]</b>									
Al	95%	—————	Vertical	Continuous	Thin	Red	12.4	-	
Al	5%	—————	Vertical	Continuous	Thin	Red	5.4	-	
Al	MDL	- - - - -	Horizontal	DashDot	Thin	Black	-	-	
Al	ML	.....	Horizontal	Dot	Thin	Black	-	-	
<b>As [5 items]</b>									
As	95%	—————	Vertical	Continuous	Thin	Red	12.4	-	
As	5%	—————	Vertical	Continuous	Thin	Red	5.4	-	
As	MCL or DWEL	.....	Horizontal	Dot	Medium	Blue	-	-	
As	MDL	- - - - -	Horizontal	DashDot	Thin	Black	-	-	
As	ML	.....	Horizontal	Dot	Thin	Black	-	-	
<b>B [5 items]</b>									
B	95%	—————	Vertical	Continuous	Thin	Red	12.4	-	
B	5%	—————	Vertical	Continuous	Thin	Red	5.4	-	
B	DWEL	.....	Horizontal	Dot	Medium	Blue	-	-	
B	MDL	- - - - -	Horizontal	DashDot	Thin	Black	-	-	

Now, if you click a group heading, all constituents in the group will be highlighted. You can expand or collapse a group by double-clicking a group heading. You'll find buttons on the ribbon toolbar, tab **Lines** to expand or collapse all groups.

The grouping is temporary: if you click on another column heading, the list is ungrouped. If you want the grouping to remain, right-click on the grouped column heading and select **Lock grouping on '<column name>'** entry in the menu (in this example the column is the Constituent column). You can unlock grouping as well.

### Hiding or showing columns

At the bottom of the context menu you'll see a list of column names. If you don't want hide columns, remove the check marks for the appropriate columns by clicking on them.

### Editing multiple lines

Sorting, filtering and grouping can be very convenient if you want to change an aspect of a selection of indicator lines. Suppose you want to change the line color of all horizontal indicator lines of Al and Cr to silver. First, filter the list on the desired constituents by using the filter options on the **Constituent** column: check constituents Al and Cr in the **Filtering** list and press **Apply**. Only the lines of these 2 constituents will be visible in the **Lines** panel. Now, group on line direction by right-clicking the **Direction** column and select **Group by 'Direction'**. The Lines panel will look like this:

Constitu...	Label	Appearance	Dire...	Line Type	Line Weight	Line Color	pH	L/S (L/kg)	Time (days)	Concentration (mg/L)
<b>Horizontal [5 items]</b>										
Al	ML	.....	Horizontal	Dot	Thin	Black	-	-	-	0.00
Al	MDL	.....	Horizontal	DashDot	Thin	Black	-	-	-	0.00
Cr	MCL	.....	Horizontal	Dot	Medium	Blue	-	-	-	0.
Cr	ML	.....	Horizontal	Dot	Thin	Black	-	-	-	0.0015
Cr	MDL	.....	Horizontal	DashDot	Thin	Black	-	-	-	0.000
<b>Vertical [4 items]</b>										
Al	5%	_____	Vertical	Continuous	Thin	Red	5.4	-	-	
Al	95%	_____	Vertical	Continuous	Thin	Red	12.4	-	-	
Cr	5%	_____	Vertical	Continuous	Thin	Red	5.4	-	-	
Cr	95%	_____	Vertical	Continuous	Thin	Red	12.4	-	-	

Now, click on the **Horizontal** group heading. All lines in this group will be selected. Press ribbon button **Edit Multiple Lines...** in group **Edit** of ribbon tab **Lines**. The **Multiple Lines Editor** will show up:

The Multiple Lines Editor dialog box is shown with the following fields:

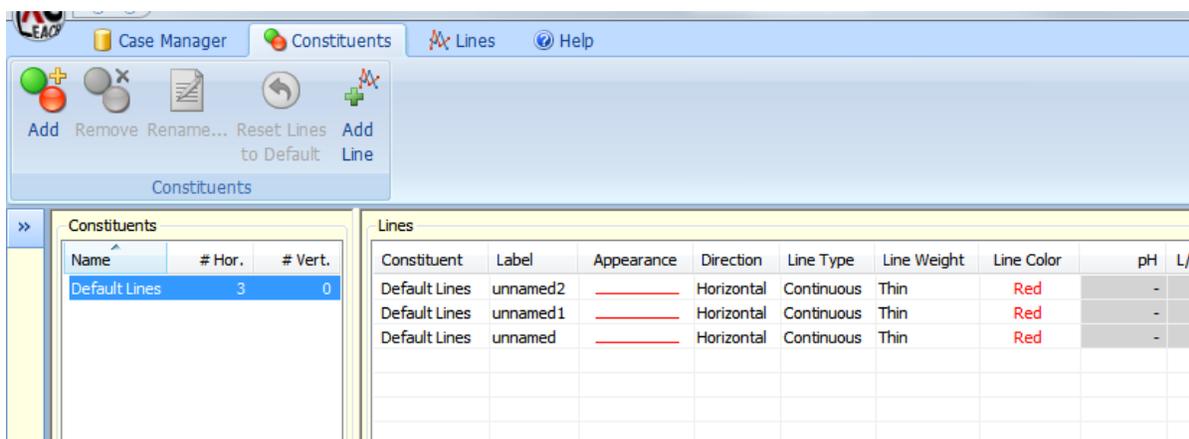
- Line Label:** Label (multiple values)
- Line Appearance:**
  - Line Direction: Horizontal
  - Line Type: (multiple values)
  - Line Weight: (multiple values)
  - Line Color: (multiple values) with a Change... button
  - Appearance: (multiple values)
- Horizontal Line Values:**
  - Concentration: (multiple values) - mg/L
  - Release: (multiple values) - mg/kg
  - Cum. Release: (multiple values) - kg/m<sup>3</sup>
  - Flux: (multiple values) - kg/m<sup>2</sup>/sec

The editor shows a list of all aspects of the selected lines. If any aspect in the lines is the same for all lines, the aspect is displayed. If not, the aspect is left empty and the phrase (multiple values) is written behind it. In this example, the lines only have the same line direction. Press the **Change...** button to the right of the **Line Color** field and find an appropriate color in the appearing **Color Dialog**. A red/green/blue value of 192,192,192 seems to look like silver. After picking a color, click on the small green button with the checkmark on the **Cancel or Save** toolbar.

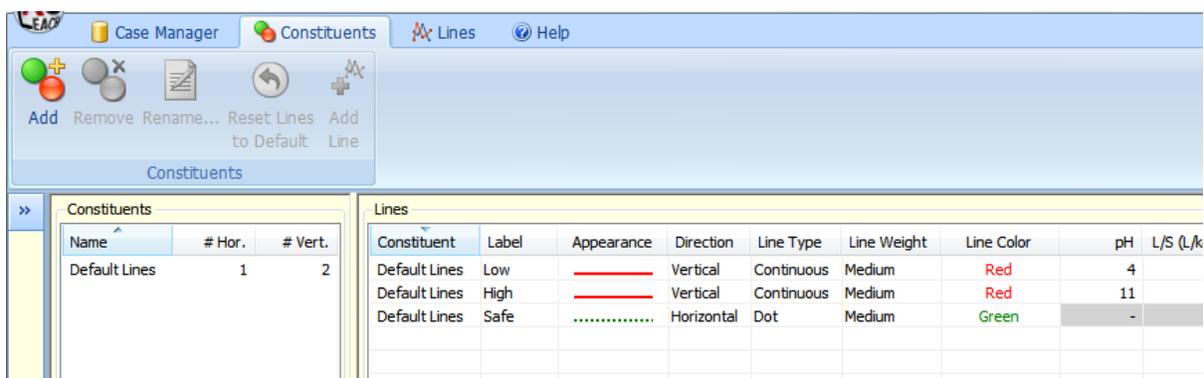
## Starting from scratch

If you want to create a list from scratch, press the **Create** button on the **Load Indicator Lines** tab group of ribbon tab **Case Manager**. An empty set of indicator lines is created with one “constituent” named **Default Lines**. This entry serves as a template for constituents that are added later. Every constituent that is added will initially get a copy of the lines that are part of this entry. Suppose we want to make a list of lines in which each constituent will have two vertical lines at pH values of 4 and 11, and one horizontal line with a variable concentration value.

In this case it is convenient to give the template these lines and add constituents later. Select the **Default Lines** entry and press button **Add Line**, tab group **Constituents**, ribbon tab **Constituents** trice. Three lines are created:



Edit the fields of the lines until it looks like this:



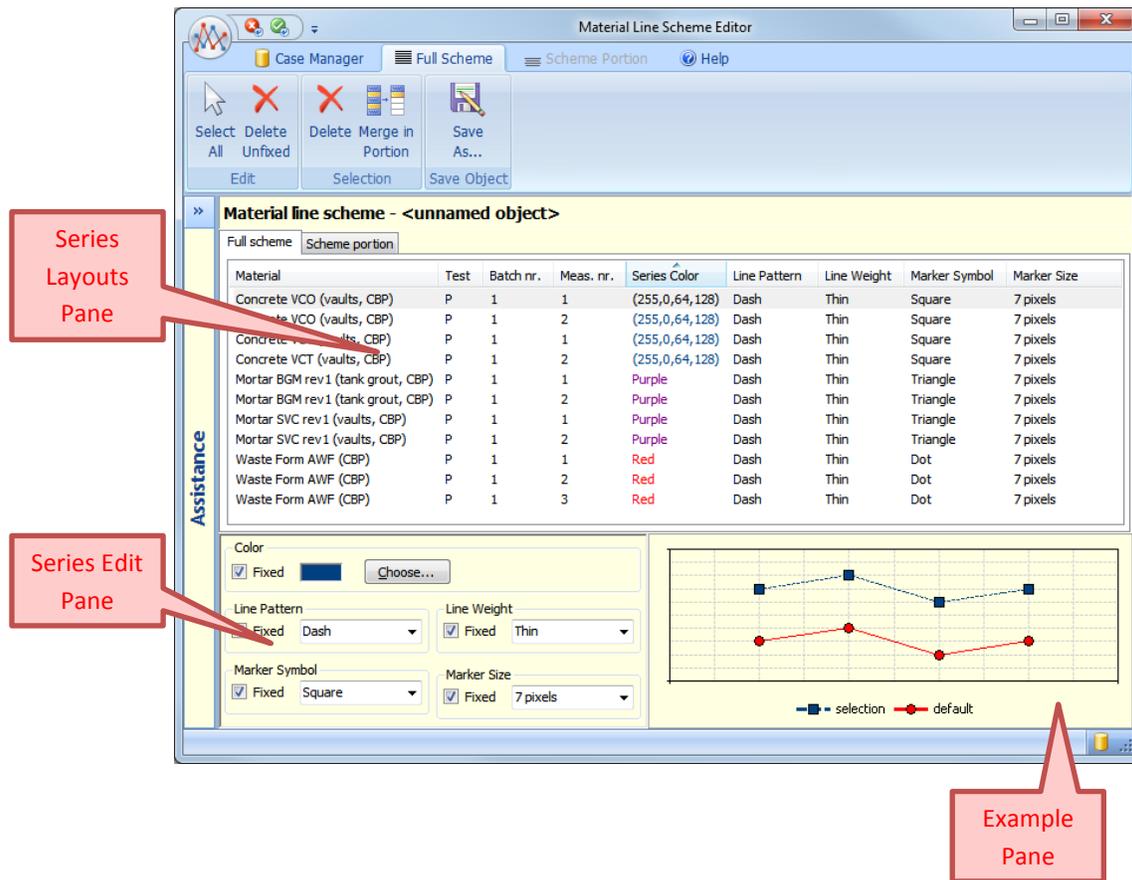
If you add constituents, every constituent will get this set of lines. Add extra constituents with the **Constituent Selector** by pressing the **Add** button on tab group **Constituents** of ribbon tab **Constituents**. All you have to do is filling in concentrations for every horizontal line.

You can make your set permanent by pressing button **Save As...** on tab group **Save Case** of ribbon tab **Case Manager**.

## The Material Line Scheme Editor

If your graph contains multiple data series, LeachXS uses a default line, color and marker scheme to format the series. The default scheme minimizes the chance that two data series have the same layout. If you are not happy with the default scheme, you can use the **Material Line Scheme Editor** to fully control the layout of data series.

A series layout is bound to a sample. If a scheme is defined in a comparison graph, all sample series in the graph that have a layout defined in the scheme will be drawn according to their layout. All samples that are not included in the scheme will get a layout according to the default scheme.



The **Series Layout Pane** contains two tab pages. The **Full scheme** tab contains the current series layout details. You can use the **Scheme portion** tab to edit a subset of the current scheme and merge it later to the full scheme.

The **Series Edit Pane** contains all the editable aspects of the selected series layouts from the **Series Layouts Pane**.

The **Example Pane** shows an impression of how a selected layout will look like. If there are more layouts selected, the one that you selected first will be shown.

## Series Layouts Pane

Use this pane to make a selection of layouts to be edited. Apart from selecting one or more layouts, you can filter, group and sort the layouts by right-clicking a column and choosing the desired option. Using these options, you might find it easier to select the layouts you want to edit.

If you want to add layouts for other samples, go to the Scheme portion tab and press button **Load Materials** on ribbon tab **Scheme Portion**. You can edit the layouts and then transfer them to the full scheme by selecting them and pressing button **To Full Scheme** on the same ribbon tab.

## Editing Layouts

You can edit layouts by selecting one or more layouts in the **Series Layouts Pane** and using the controls on the **Series Edit Pane** to edit them. If you have selected more than one layout, changes you make will apply to all selected layouts. The layout aspects you can change are:

- line and marker color
- marker symbol
- marker size
- line pattern
- line weight

*Note that you cannot change line and marker color separately: they will always have the same color.*

## Saving and Loading Layouts

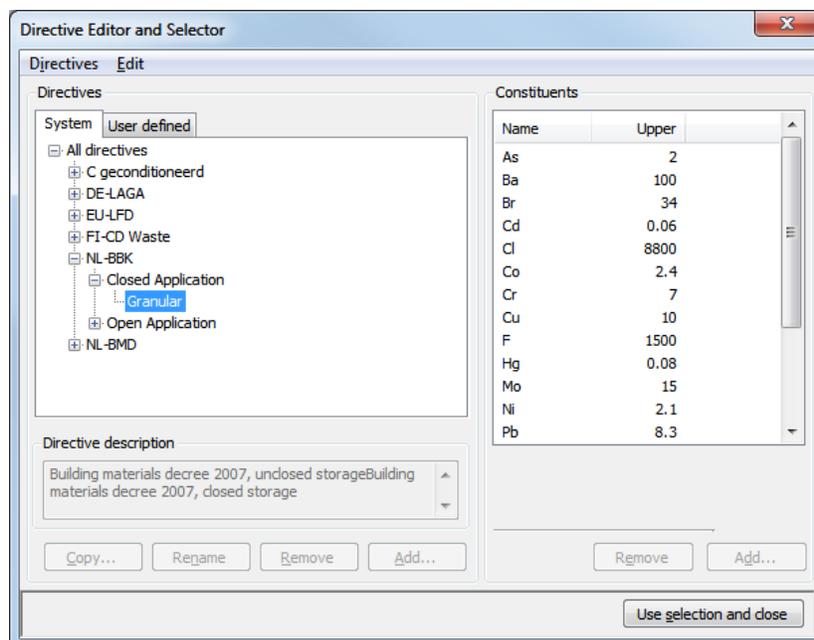
You can save schemes to disk and load them for use in e.g. another comparison case. Use the **Save**, **Save As...** and **Open** buttons on the **Case Manager** ribbon tab to save and load schemes. The **Case Manager** will show up to assist you in locating a previously saved scheme or creating a place to save it. See “LeachXS Cases and Case Management” on page 100 for more information.

If you have started the editor from a comparison module, you can save the scheme by pressing the small green button in the top left portion of the editor window: the changes in the scheme are made permanent and control is returned to the comparison module.

## Directive selection dialog

In many instances users want to compare test data with regulatory criteria or limit values. To facilitate such comparison a library of regulatory limit values is provided from which a selection can be made. The regulations contain separate values for granular and monolithic materials and thus specific regulations can only be called in connection with the appropriate test data.

Besides picking an existing, built-in directive, you can create and edit your own directives. A directive has one or more material categories and material categories have limits for granular and monolithic constituents. Besides an upper limit, user defined directives can have a lower limit. The lower limits are only used in graphs containing directive information, boxing your data between a low and high pH values and the upper and lower limits.



The pane on the left, the **Directives** pane, shows information on the built-in directives (**System** tab) and the directives you created (**User defined** tab). There are buttons to **Add**, **Remove** and **Rename** user defined directives and to **Copy** an existing directive as a user defined one, giving you a jump start in creating a homemade directive. You can add or modify a description of a user defined directive in the **Directive description** pane.

The **Constituents** pane on the right, which becomes visible if you select a granular or monolithic section of a directive, shows all defined constituents with their limits. You can **Remove** a selected constituent or add new ones by clicking the **Add** button. “The Constituent Selector” on page 128 will appear, helping you in selecting constituents. When a constituent is selected in the **Constituents** pane, you can edit the limits in the fields below the constituent list.

## Creating and Editing Lists

Many tools make use of small editors that help you to create lists of values.

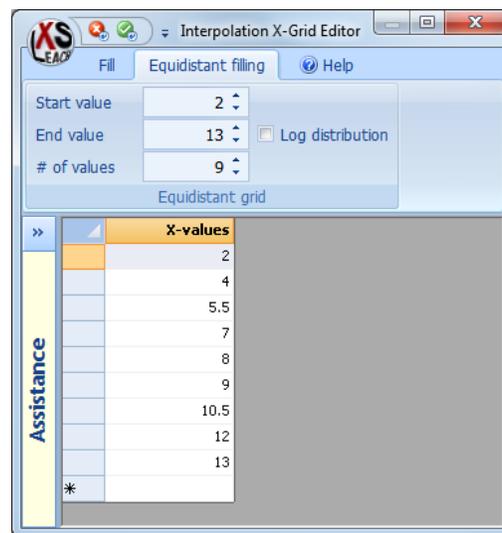
If you want to create statistical data sets from existing samples, the sample series all need to be brought to a common set of x-values in order to be properly evaluated. The **Interpolation Grid Editor** helps you to define such a set.

With the **Interpolation Grid Manager**, you can make predefined lists of interpolation values.

With the **List Generator**, you can generate a list of equidistant values or values whose distances increase with a constant factor.

### Interpolation Grid Editor

With the **Interpolation Grid Editor** you can create or modify an interpolation grid.

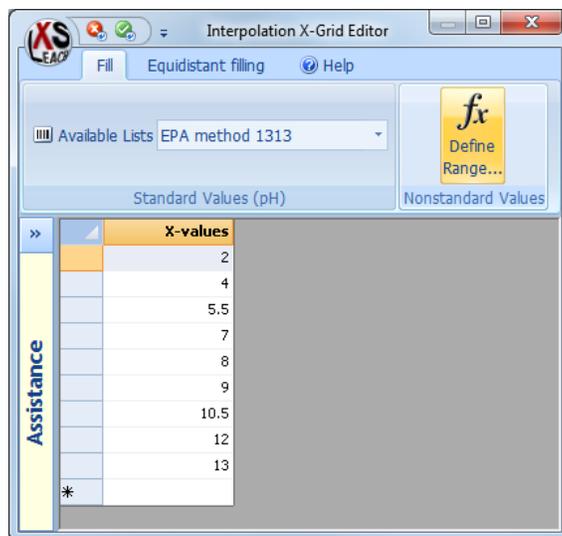


You can add a value by typing it in the row starting with an asterisk. Delete a value by selecting the row to be deleted and press the **Delete** button of your keyboard. To edit a value, double-click it and type the new value.

After you have edited or added values, the values can be sorted in ascending or descending order by clicking the column header.

If you want to create an equidistant list of values, you can use the options on the **Equidistant filling** ribbon tab. Define a start and end value, the number of values and the list is filled with equidistant values. If you check the **Log distribution** box, a logarithmic (base 10) distribution is used, the powers being uniformly distributed.

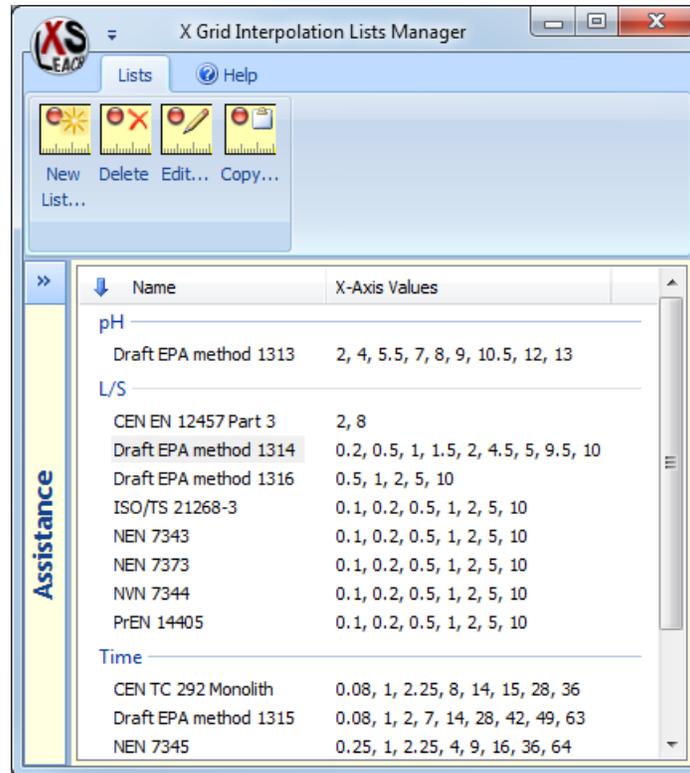
You can also use functions from the **Fill** ribbon tab to select a list of predefined values or generate a list of non-equidistant values.



Choose a defined list from the choices in **Available List**, or press **Define Range...** to fully control how the list is built up. See “Interpolation Grid Manager” on page 146 for managing the available lists or “List Generator” on page 147 for creating a non-standard list of values.

## Interpolation Grid Manager

When you want to create reference data sets from statistical values, the first step to take is aligning the pH, L/S or time values of your source data to a uniform set of values by means of interpolating the original data. You can choose to manually define a set of values, but LeachXS offers a number of predefined lists that are used commonly. The **Interpolation Grid Manager** can be used to add or modify these predefined lists. It can be called from the main LeachXS window on tab page **Tools**, button **X-Grid Interpolation Manager**.



This editor shows you all predefined list, grouped by entity.

Add a new predefined list by selecting the group name of the desired entity and press the **New List...** button. The **Interpolation Grid Editor** will show up, allowing you to type in the values you want in the list.

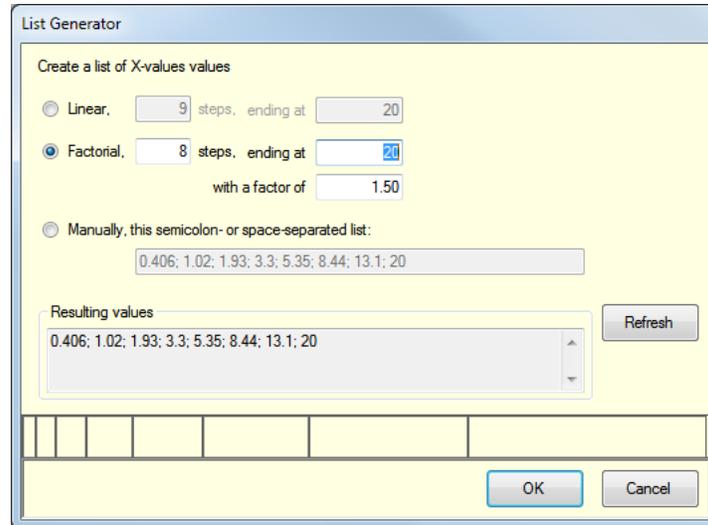
If you want to delete a predefined list, select it and press the Delete button.

If you want to change the name of a list, select the list and hit the **F2** button. If you want to edit the contents of an existing list, selected and press the **Edit...** button. the **Interpolation Grid Editor** will show up.

All your changes will be saved automatically if you close the editor.

## List Generator

The List Generator can generate a series of values.



To create a list of equidistant values, check the **Linear** radio button and fill in the number of steps to create and the last value.

To create a list of values, whose distances increase with a constant factor, check the **Factorial** button and fill in the desired number of steps, the end value and the factor by which successive distances increase.

You can also type the list of values by hand. Check the **Manually** radio button and type the values, separated by semicolons.

The bottom pane gives you an impression of how successive distances relate to each other.

## Technical Topics

---

### File locations

This section gives an overview where LeachXS stores or expects files. The following symbolic names are used for file locations:

Location name	Physical location
<i>[Install location]</i>	C:\Program Files (x86)\LeachXS Lite This location is the default location where LeachXS is installed. You might have chosen a different location during the installation process of LeachXS.
<i>[Application data]</i>	C:\Users\ <username>\AppData\Roaming\LeachXS Lite</username>
<i>[Local Application data]</i>	C:\Users\ <username>\AppData\Local\ECN_TSC</username>
<i>[User data]</i>	C:\Users\ <username>\Documents\LeachXS User Objects</username>
<i>[Template location]</i>	C:\Users\ <username>\AppData\Roaming\Microsoft\Templates</username>

The phrase <username> denotes the name you use to log on to your computer.

### Software Modules

All software modules are installed in *[Install location]*.

### License

Your license is encrypted in file: *[Application data]\About.lxs*. If, for some reason, you want to change your license, remove this file. The next time you start LeachXS you will be prompted for a username and license key.

### Window states

LeachXS remembers the state of all windows. The main state parameters are window size and position, minimized/maximized or normal size and on what screen the window is displayed, if you use more than one screen. Some windows and dialogs remember the last state of checkboxes, combo boxes, radio buttons and other user interface controls as well. The states are stored in:

*[Local Application data]\LeachXS\_Lite.exe\_Url\_<key>\<version>\user.config*,

where <key> is a unique series of characters and <version> is the version of LeachXS you are using.

### Most Recently Used cases

Every module that is capable of editing, loading, creating and saving cases keeps track of the cases that have been used. The 10 most recently used ones are remembered and stored in:

*[Application data]\MruLists<casetype>.mru*, where <casetype> is an indication of the type of case.

## Databases

The default location of all LeachXS databases with samples is *[User data]\DATABASES*. All databases that are shipped with the installation procedure of LeachXS are stored here. LeachXS presents the content of this location by default if you want to select a database. However, you are free to store a database anywhere you like.

## Software License

Your software license is encrypted in the following file: *[Application data]\About.lxs*. If you need to switch from license, remove this file. LeachXS will prompt for a username and license key next time you start it.

## Pre-installed examples

When LeachXS is installed, example cases are installed as template for new cases, giving you a head start. All these examples are in folder *[Application data]\FactoryDefaults*. Cases for a specific type of examples all have their own subfolder.

*Note that pre-installed examples are read only. You cannot overwrite them. Don't save your own cases in the folder with pre-installed examples.*

## User Cases

All cases you make yourself are stored by default in a separate folder: *[User data]*. Cases of a specific type all have their own subfolder. You can make alternative locations for cases. These locations are called **Map Stores**. You can create them in the Object Manager. See "LeachXS Cases and Case Management" on page 100.

## Templates for lab data input

LeachXS installs data templates that you can use in Microsoft Excel® for entering data on leaching tests. Among them are data templates for EPA methods 1313, 1314, 1315 and 1316. You'll find them in folder *[Template location]*. This location is the same as where Microsoft Excel® assumes that user templates are located.

## CSTR calculation

The CSTR fitting is done by performing a weighted linear regression of the natural logarithms of the concentration values. The result of the weighted linear regression is a slope (*A*) and offset (*B*).

The following function is minimized:

$$\chi^2(A, B) = \sum_{i=1}^N \left( \frac{Y_i - A - BX_i}{Sig_i} \right)^2$$

Where:

$N$	Number of points.
$i$	Index of point (between 1 and $N$ ).
$X_i$	$i^{\text{th}}$ L/S value.
$Y_i$	$\ln(C_i)$ .
$C_i$	Concentration of $i^{\text{th}}$ point.
$Sig_i$	Estimated uncertainty of $Y_i$ .

The CSTR curve value in point  $X_i$  can be obtained from:

$$CSTR_i = e^A \cdot e^{-BX_i}$$

### Weights

No weighting:

$$Sig_i = 1 \text{ for } i \text{ between } 1 \text{ and } N.$$

Standard weighting:

$$Sig_i = 0.05 * Y_i$$

Favor low/midrange/high L/S values:

First, create 3  $XW$  values:

$$XW_1 = \ln(X_1)$$

$$XW_3 = \ln(X_N)$$

$$XW_2 = 0.5 * (XW_1 + XW_3)$$

Now, create 3  $YW$  values, depending on the range to favor:

Favor low L/S values:

$$YW_1 = 1, YW_2 = \text{SQRT}(10), YW_3 = 10.$$

Favor midrange L/S values:

$$YW_1 = 10, YW_2 = 1, YW_3 = 10.$$

Favor high L/S values:

$$YW_1 = 10, YW_2 = \text{SQRT}(10), YW_3 = 1.$$

Then, a polynomial of degree 2 is fitted through the three points  $(XW_i, YW_i)$ .

The uncertainties are constructed by:

$$Sig_i = \text{Polynomial}(\ln(X_i))$$