LeachXS CBP Version 2.0 User's Guide

User Guide (rev. 0)



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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 show 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.

Select a LeachXS dat		ocume	ents → My Documents → LeachXS User Objects → D	ATABASES	✓ 4y Search DATABAS	SES P	#1 Select the
Organize 🔻 New	v folder				8==	• 🔟 🔞	new database
🛠 Favorites 💻 Desktop			Documents library DATABASES				p
Downloads			Name	Date modifier	Туре	Size	
🖳 Recent Places		E	Development CBP database Sept_2013.mdb	21-11-2013 15:37	Microsoft Access Database	5,460 KB	#2 Click "Open"
🔚 Libraries			Empty.mdb	21-11-2013 15:37	Microsoft Access Database	1,600 KB	Button
Documents			USEPA CCRs 12-2009 rev 1.mdb	21-11-2013 15:36	Microsoft Access Database	9,184 KB	
🌙 Music							7
Pictures							
Videos							
🛤 Computer		-					
	File <u>n</u> ame:	Devel	lopment CBP database Sept_2013.mdb		✓ MS Access 2005 D Open	atabase (*.mc 💌 Cancel	

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

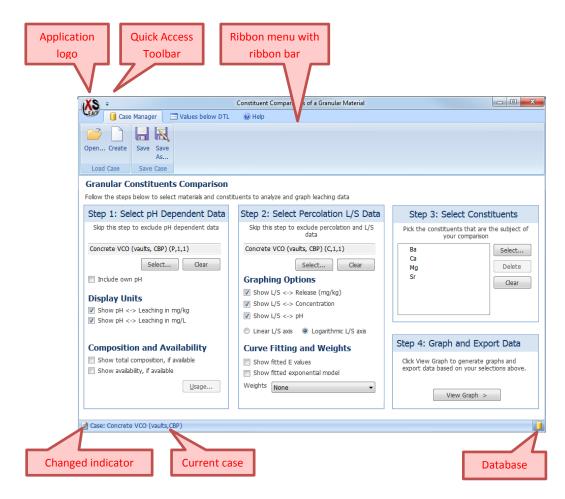
The default databases in LeachXS contain leaching test and material property data collected from a broad range of studies and projects. The user can compare their own data to selected data within these default databases by importing their data into the database. Microsoft Excel® workbooks used as the 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 1st sampling, etc.) while the second number indicates the replication of the test method (e.g., "2" for the 2nd 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

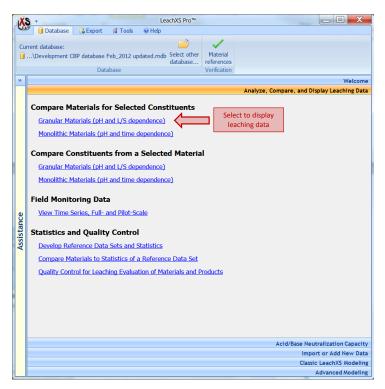
Compare field data as time series or scale-up series from field measurements. *This section is not described in this version of the guide.*

Statistics and Quality Control

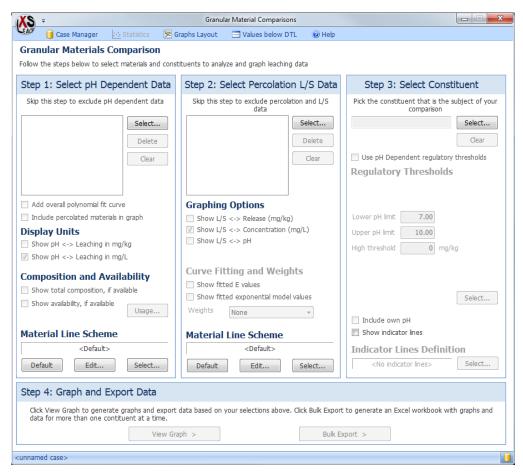
Analysis of material sets relative to statistical representations and quality control objectives. *This section is not described in this version of the guide*.

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.

XS =	Granular Material Comparisons				
🐨 📋 Case Manager 🔛 Statistics 🛛 🔀 G	raphs Layout 🛛 🖃 Values below DTL 🛛 🙆 Help				
Granular Materials Comparison					
Follow the steps below to select materials and const	ituents to analyze and graph leaching data				
Step 1: Select pH Dependent Data	Step 2: Select Percolation L/S Data	Step 3: Select Constituent			
Skip this step to exclude pH dependent data	Skip this step to exclude percolation and L/S data	Pick the constituent that is the subject of your comparison			
Select	Select	Select Clear			
Clear	Clear	Use pH Dependent regulatory thresholds			
		Regulatory Thresholds			
Add overall polynomial fit curve	Graphing Options				
Include percolated materials in graph	Show L/S <-> Release (mg/kg)	Lower pH limit 7.00			
Display Units	Show L/S <-> Concentration (mg/L)	Upper pH limit 10.00			
Show pH <-> Leaching in mg/kg	Show L/S <-> pH	High threshold 0 mg/kg			
Show pH <-> Leaching in mg/L					
Composition and Availability	Curve Fitting and Weights				
Show total composition, if available	Show fitted E values				
Show availability, if available	Show fitted exponential model values	Select			
Usage	Weights None -	Include own pH			
Material Line Scheme	Material Line Cohema	Show indicator lines			
<pre></pre>	Anterial Line Scheme				
		Indicator Lines Definition			
Default Edit Select	Default Edit Select	<no indicator="" lines=""> Select</no>			
Step 4: Graph and Export Data					
Click View Graph to generate graphs and export data based on your selections above. Click Bulk Export to generate an Excel workbook with graphs and data for more than one contituent at a time.					
View Gra	ph > Bulk E	kport >			
<unnamed case=""></unnamed>					
Sumaneu case>					

The **Sample Selector** will show up:

KS 😪 🗞 🕫		Sample S	Selector		
📔 Sample Manager 🔒	Samples 🛛 🖓 = Filteri	ing 🕜 Help			
Delete Clear Expand Collapse All All Group Sa	Show/Hide				
Available Samples					Selected Samples (4)
All Available Often Used Favorites					Name
Name Blast Furnace Slag BFS (CBP) (P, 1, 2 Coal Fly Ash FAF (CBP) (C, 1, 1) Coal Fly Ash FAF (CBP) (C, 1, 2) Coal Fly Ash FAF (CBP) (C, 1, 3) Coal Fly Ash FAF (CBP) (P, 1, 1) Coal Fly Ash FAF (CBP) (P, 1, 1) Coal Fly Ash FAF (CBP) (P, 1, 1) Coarete VCO (valuts, CBP) (C, 1, 2) Concrete VCO (valuts, CBP) (P, 1, 1) Concrete VCO (valuts, CBP) (C, 1, 2) Concrete VCO (valuts, CBP) (C, 1, 2) Concrete VCT (valuts, CBP) (C, 1, 2) Concrete VCT (valuts, CBP) (P, 1, 1) V Concrete VCT (valuts, CBP) (P, 1, 1) V Concrete VCT (valuts, CBP) (P, 1, 2) Mortar BGM rev1 (tank grout, CBP))	H Dependence Percolation Percolation PH Dependence PH Dependence Percolation PH Dependence	Test Subtype US-EPA Method 1313 US-EPA Method 1314 US-EPA Method 1314 US-EPA Method 1313 US-EPA Method 1313 US-EPA Method 1314 US-EPA Method 1314	•	C [4 items] A Concrete VCO (vaults, CBP) (P, 1, 1) Concrete VCO (vaults, CBP) (P, 1, 2) Concrete VCT (vaults, CBP) (P, 1, 1) Concrete VCT (vaults, CBP) (P, 1, 2)

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**.

Skp this step to exclude percolation and I/S Skp this step to exclude percolation and I/S Pick the construent that is the subject of your comparison Chick View Graph and energy	XS =	Granular Material Comparisons		
Follow the steps below to select materials and construents to analyze and graph leaching data Step 1: Select PH Dependent Data Step 2: Select Percolation L/S Data Step 3: Select Constituent Step 4: G Skip this step to exclude pH dependent data Skip this step to exclude percolation and L/S Pick the construent that is the subject of your comparison Select Chick View Graph and entered a graph leaching data Step 3: Select Constituent Chick View Graph and entered a graph leaching data Chick View Graph and entered a graph leaching data Select Dick to construent that is the subject of your comparison Chick View Graph and entered a graph leaching data Chick View Graph and entered a graph leaching data Select Dick View Graph and entered entered and entered and entered and entered	🚺 Case Manager 🔛 Statistics 😒	Graphs Layout 🔤 Values below DTL 🔞 Help	н	
Step 1: Select pH Dependent Data Step 2: Select Percolation L/S Data Step 3: Select Constituent Ske this step to exclude pH dependent data Ske this step to exclude percolation and US Pick the constituent that is the subject of your comparison Concrete VC0 (vauts, CBP) Select Delete Clear Pick the constituent that is the subject of your comparison Clear Concrete VC1 (vauts, CBP) Clear Delete Clear Use pH Dependent regulatory thresholds View Graph and deport dat based on your selections Add overal polynomial fit curve Show J/S <> Release (mg/kg) Show U/S <>> PH Delete Curve Fitting and Weights Show total composition and Availability Show fited exponential model values Select Select Buk Export Material Line Scheme Coefault> Default Edt Select Select Select				
Skp this step to exclude pit dependent data Skp this step to exclude percolation and U/s data Pick the construent that is the subject of your comparison Chick View Graph and export data Concrete VCD (vauts, CBP) Select Delete Char Concrete VCT (vauts, CBP) Char Delete Char Own Ph Concrete VCT (vauts, CBP) Show This -> Release (mg/kg) Display Units Show VJS <> Release (mg/kg) Show VJS <>> PH Lower pH limt 7.00 Upper pH limt Tool Show pH <> Leaching in mg/L Curve Fitting and Weights Show fited exponental model values Select Buck Export Show visit composition, fit available Show fited exponental model values Select Buck Export Material Line Scheme _obfault>	Follow the steps below to select materials and cor	istituents to analyze and graph leaching data		
data comparison concrete VC0 (vauts, CBP) Select Concrete VC0 (vauts, CBP) Delete Concrete VC1 (vauts, CBP) Delete Select Select Display Units Show VJ <<-> Release (mg/kg) Show VJ <>> Lashing in mg/kg Show VJ <<-> PH Show VJ <>> Lashing in mg/kg Show fited exponental model values Show VJ <<>> Lashing in mg/kg Show fited exponental model values Show votal composition, f available Select Material Line Sche	Step 1: Select pH Dependent Data	Step 2: Select Percolation L/S Data	Step 3: Select Constituent	Step 4a: Graph
Clear Own PH Clear Use pH Dependent regulatory thresholds Material Line Scheme Graphing Options Show tJ <-> Release (mg/kg) Step 4b: Eb Char Char Char Char Char Material Line Scheme Show tJ <-> Default Curve Filting Curve Filting Curve Filting Material Line Scheme Curve Filting Curve Filting Select Select Default Edt Select Curve Filting Select	Concrete VCO (vaults, CBP) Concrete VCO (vaults, CBP) Concrete VCO (vaults, CBP)	data Select	comparison Select	
A void void a population to date Craphing Opticities Include percentation in graph Show U/S <> Release (mg/kg) Display Units Show U/S <>> Release (mg/kg) Show pH <> Leaching in mg/kg Show U/S <>> Release (mg/kg) Show pH <> Leaching in mg/kg Show U/S <>> Release (mg/kg) Show pH <> Leaching in mg/kg Curve Fitting and Weights Show tail composition, f available Show tail composition, f available Show tail composition, f available Show tail composition, f available Show tail composition, f available Usage Material Line Scheme Opfault Opfault Edt Select Default	Clear	Clear		View Graph >
Include percolated materials in graph If show L/S <> Release (mg/kg) Lower pH limit 7.00 Upper pH limit 7.00 Upper pH limit 10.00 Upper pH l	Add overall polynomial fit curve	Graphing Options		Step 4b: Export
Composition and Availability Curve Fitting and Weights Buck Export Show total composition, if available Show fitted E values Buck Export Show availability, if available Usage Material Line Scheme Include own pH Material Line Scheme Adterial Line Scheme Include own pH Obfault> Obfault> Indicator lines Default Edt Select Select	Display Units Show pH <-> Leaching in mg/kg	 ✓ Show L/S <-> Release (mg/kg) ✓ Show L/S <-> Concentration (mg/L) 	Upper pH limit 10.00	Click Bulk Export to generate an Excel workbook with graphs and data for more than one contituent at a
Material Line Scheme Material Line Scheme Image: Scheme scheme <default> <default> Indicator Ines Default Edt Select <no indicator="" ines<="" td=""></no></default></default>	Show total composition, if available Show availability, if available	Show fitted E values Show fitted exponential model values		Eulk Export >
Default Edt Select Select Select	Material Line Scheme	Material Line Scheme	Show indicator lines	
Delour Lukin Jeleur Delour Lukin Jeleur	<default></default>	<default></default>	Indicator Lines Definition	
ad <unnamed case=""></unnamed>	Default Edit Select	Default Edit Select	<no indicator="" lines=""> Select</no>	

Displaying Selected Data

After selecting the data sets for comparison, the **Granular Materials Comparison** screen will show the date 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).

(XS =	Granular Material Comparisons						
🚺 Case Manager 🔛 Statistics 💌	Graphs Layout 🛛 🔄 Values below DTL 🛛 🔞 Help						
Granular Materials Comparison							
Follow the steps below to select materials and constituents to analyze and graph leaching data							
Step 1: Select pH Dependent Data	Step 2: Select Percolation L/S Data	Step 3: Select Constituent	Step 4a: Graph				
Skip this step to exclude pH dependent data Concrete VCO (vaults, CBP) Concrete VCO (vaults, CBP)	Skip this step to exclude percolation and L/S data Concrete VCO (vaults, CBP) Concrete VCO (vaults, CBP)	Pick the constituent that is the subject of your comparison Select	Click View Graph to generate graphs and export data based on your selections.				
Concrete VCT (vaults, CBP) (Delete Concrete VCT (vaults, CBP) (Clear	Concrete VCT (vaults, CBP) (Delete Concrete VCT (vaults, CBP) (Clear	Clear Use pH Dependent regulatory thresholds Regulatory Thresholds	View Graph >				
Add overall polynomial fit curve	Graphing Options	Lower pH limit 7.00	Step 4b: Export				
 Include percolated materials in graph Display Units Show pH <-> Leaching in mg/kg Show pH <-> Leaching in mg/L 	 ✓ Show L/S <-> Release (mg/kg) ✓ Show L/S <-> Concentration (mg/L) ─ Show L/S <-> pH 	Upper pH limit 10.00 High threshold 0 mg/kg	generate an Excel workbook with graphs and data for more than one contituent at a				
Composition and Availability Show total composition, if available Show availability, if available Usage	Curve Fitting and Weights Show fitted E values Show fitted exponential model values Weights None	Select	time. Bulk Export >				
Material Line Scheme	Material Line Scheme	Show indicator lines					
<default></default>	<default></default>	Indicator Lines Definition					
Default Edit Select	Default Edit Select	<no indicator="" lines=""> Select</no>					
Z <unnamed case=""></unnamed>							

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.

(XS =	Granular Material Comparisons		
🐨 📔 Case Manager 🔛 Statistics 🔀	Graphs Layout 🛛 🖃 Values below DTL 🛛 🔞 Help		
Granular Materials Comparison			
Follow the steps below to select materials and con	stituents to analyze and graph leaching data		
Step 1: Select pH Dependent Data	Step 2: Select Percolation L/S Data	Step 3: Select Constituent	Step 4a: Graph
Skip this step to exclude pH dependent data	Skip this step to exclude percolation and L/S data	Pick the constituent that is the subject of your comparison	Click View Graph to generate graphs and export data
Concrete VCO (vaults, CBP) (Concrete VCO (vaults, CBP) (Concrete VCT (vaults, CBP) (Delete	Concrete VCO (vaults, CBP) (Concrete VCO (vaults, CBP) (Concrete VCT (vaults, CBP) (Delete	Select	based on your selections.
Concrete VCT (vaults, CBP) (Concrete VCT (vaults, CBP) (Use pH Dependent regulatory thresholds	View Graph >
Own pH	۰ III ۲	Regulatory Thresholds	
Add overall polynomial fit curve	Graphing Options		Step 4b: Export
Include percolated materials in graph	Show L/S <-> Release (mg/kg)	Lower pH limit 7.00	Click Bulk Export to generate an Excel
Display Units	✓ Show L/S <-> Concentration (mg/L) ✓ Show L/S <-> pH	Upper pH limit 10.00	workbook with graphs and data for
Show pH <-> Leaching in mg/kg	Show Lys <-> pH	High threshold 0 mg/kg	more than one
Show pH <-> Leaching in mg/L	Curve Fitting and Weights		time.
Composition and Availability	Show fitted E values		Bulk Export >
Show total composition, if available	Show fitted exponential model values	Select	
Show availability, if available	Weights None -		
Natarial Line Colorea		Include own pH Show indicator lines	
Material Line Scheme	Material Line Scheme		
<default></default>	<default></default>	Indicator Lines Definition	
Default Edit Select	Default Edit Select	<no indicator="" lines=""> Select</no>	

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

XS =	Granular Material Comparisons		
🐨 📔 Case Manager 🔛 Statistics 🔀	Graphs Layout 🛛 🖃 Values below DTL 🛛 🔞 Help		
Granular Materials Comparison			
Follow the steps below to select materials and con	stituents to analyze and graph leaching data		
Step 1: Select pH Dependent Data	Step 2: Select Percolation L/S Data	Step 3: Select Constituent	Step 4a: Graph
Skip this step to exclude pH dependent data	Skip this step to exclude percolation and L/S data	Pick the constituent that is the subject of your comparison	Click View Graph to generate graphs
Concrete VCO (vaults, CBP) (Concrete VCO (vaults, CBP) (Concrete VCT (vaults, CBP) (Delete	Concrete VCO (vaults, CBP) Concrete VCO (vaults, CBP) Concrete VCT (vaults, CBP)	Select	and export data based on your selections.
Concrete VCT (vaults, CBP) (Concrete VCT (vaults, CBP) (Use pH Dependent regulatory thresholds Regulatory Thresholds	View Graph >
Add overall polynomial fit curve	(III)		Step 4b: Export
Add overall polynomial fic curve Include percolated materials in graph	Graphing Options Show L/S <-> Release (mg/kg)	Lower pH limit 7.00	Click Bulk Export to
Show pH <-> Leaching in mg/kg Show pH <-> Leaching in mg/kg	✓ Show L/S <-> Kelease (mg/kg) ✓ Show L/S <-> Concentration (mg/L) ✓ Show L/S <-> pH	Upper pH limit 10.00 High threshold 0 mg/kg	generate an Excel workbook with graphs and data for more than one contituent at a time.
Composition and Availability Show total composition, if available Show availability, if available Usage	Curve Fitting and Weights Show fitted E values Show fitted exponential model values Weights None	Select	<u>B</u> ulk Export >
Material Line Scheme	Material Line Scheme	Show indicator lines	
<default></default>	<default></default>	Indicator Lines Definition	
Default Edit Select	Default Edit Select	<no indicator="" lines=""> Select</no>	
✓ <unnamed case=""></unnamed>			

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

Constituen	t Selector				
Selection @ Help					
Delete Clear Edit					
Available Constituents	Selected Constituent				
All Often Used Favorites	Name				
Name	Inorganic [1 item] 🔷 🔺				
Inorganic [77 items] - 🔺 🛓	Ca				
Ag					
Al					
As					
Au					
В					
Ba					
Be Bi					
Br					
Ca					
Cd					
Ce					
a					
CNT					
Select by Typing (Press Alt-T)					

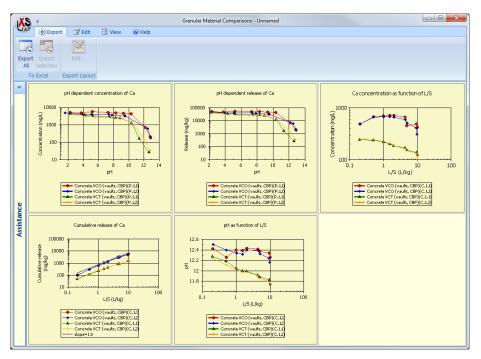
For a complete description of the **Constituent Selector**, see chapter "The Constituent Selector" on page 128.

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.

🗙 🗧 Granular Material Comparisons							
🚺 Case Manager 🔛 Statistics 🔀	Graphs Layout 🛛 🖃 Values below DTL 🛛 🔞 Help						
Granular Materials Comparison							
Follow the steps below to select materials and constituents to analyze and graph leaching data							
Step 1: Select pH Dependent Data	Step 2: Select Percolation L/S Data	Step 3: Select Constituent	Step 4a: Graph				
Skip this step to exclude pH dependent data	Skip this step to exclude percolation and L/S data	Pick the constituent that is the subject of your comparison	Click View Graph to generate graphs				
Concrete VCO (vaults, CBP) (Concrete VCO (vaults, CBP) (Concrete VCT (vaults, CBP) (Delete	Concrete VCO (vaults, CBP) Concrete VCO (vaults, CBP) Concrete VCT (vaults, CBP)	Ca Select Clear	and export data based on your selections.				
Concrete VCT (vaults, CBP) (Concrete VCT (vaults, CBP) (Use pH Dependent regulatory thresholds Regulatory Thresholds	View Graph >				
۲۰۰۰ Own pH	4 111	<no selected="" thresholds=""></no>	Step 4b: Export				
Add overall polynomial fit curve	Graphing Options						
Include percolated materials in graph	Show L/S <-> Release (mg/kg)	Lower pH limit 7.00	Click Bulk Export to generate an Excel				
Display Units Show pH <-> Leaching in mg/kg Show pH <-> Leaching in mg/L	 ✓ Show L/S <-> Concentration (mg/L) ✓ Show L/S <-> pH 	Upper pH limit 10.00 High threshold 0 mg/kg	workbook with graphs and data for more than one contituent at a time.				
Composition and Availability	Curve Fitting and Weights						
Show total composition, if available	Show fitted E values Show fitted exponential model values	Select	<u>B</u> ulk Export >				
Show availability, if available	Weights None	Include own pH					
Material Line Scheme	Material Line Scheme	Show indicator lines					
<default></default>	<default></default>	Indicator Lines Definition					
Default Edit Select	Default Edit Select	<no indicator="" lines=""> Select</no>					
✓ <unnamed case=""></unnamed>							

The following is an example display of selected data:

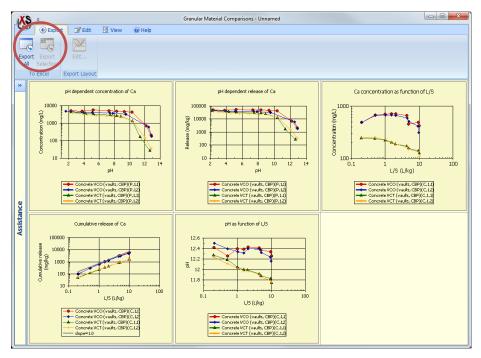


This graph window is detached from the **Granular Materials Comparison** window. This means that you can make another comparison, show its graphs and compare that window with the one above.

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.

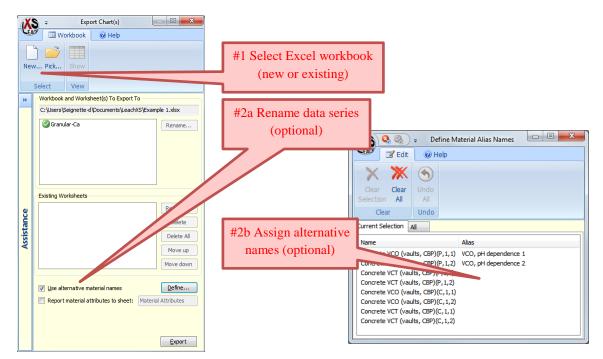


To export an individual pane in the output window, click within the white area to highlight it and then select **Export Selection**. To export the all charts, select **Export All**. Follow the instructions on the resultant **Export Charts** screen shown below.

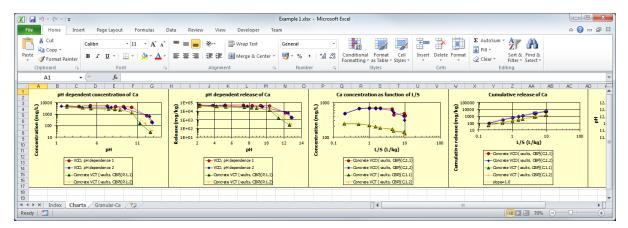
X	Export Chart(s)	? ×
G	Workbook 🛛 🛞 Help	
) 📄 🔳	
Ne	N Pick Show	
	Select View	
»	Workbook and Worksheet(s) To Export To	
-	C:\Users\Andy Garrabrants\Desktop\LXS-GM-Test.>	dev
	@Granular-Ca	Rename
	Existing Worksheets	
		Rename
Assistance		
E I		Delete
sis		Delete All
¥		Move up
		Move down
		Move down
		Define
	Use alternative material names	
	Report material attributes to sheet: Material	Attributes
		Export

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.

XS =	Granular Material Comparisons				
🚺 Case Manager 🔛 Statistics 💌	Graphs Layout 🛛 🖃 Values below DTL 🛛 🔞 Help				
Granular Materials Comparison					
Follow the steps below to select materials and con	stituents to analyze and graph leaching data				
Step 1: Select pH Dependent Data	Step 2: Select Percolation L/S Data	Step 3: Select Constituent	Step 4a: Graph		
Skip this step to exclude pH dependent data	Skip this step to exclude percolation and L/S data	Pick the constituent that is the subject of your comparison	Click View Graph to generate graphs		
Concrete VCO (vaults, CBP)	Concrete VCO (vaults, CBP) (Select	Ca Select	and export data based on your		
Concrete VCO (vaults, CBP) (Delete	Concrete VCO (vaults, CBP) (Clear	selections.		
Concrete VCT (vaults, CBP) (Concrete VCT (vaults, CBP) (Concrete VCT (vaults, CBP) (
Clear	Clear	Use pH Dependent regulatory thresholds	View Graph >		
		Regulatory Thresholds			
< Ⅲ ► Own pH	۰ III ا	<no selected="" thresholds=""></no>			
Add overall polynomial fit curve	Graphing Options		Step 4b: Export		
Include percolated materials in graph	Show L/S <-> Release (mg/kg)	Lower pH limit 7.00	Click Bulk Export to generate an Excel		
Display Units	Show L/S <-> Concentration (mg/L)	Upper pH limit 10.00	workbook with		
Show pH <-> Leaching in mg/kg	♥ Show L/S <-> pH	High threshold 0 mg/kg	graphs and data for more than one		
Show pH <-> Leaching in mg/L			contituent at a time.		
Composition and Availability	Curve Fitting and Weights				
Show total composition, if available	Show fitted E values		<u>B</u> ulk Export >		
Show availability, if available	Show fitted exponential model values	Select			
<u>U</u> sage	Weights None -	Include own pH			
Material Line Scheme	Material Line Scheme	Show indicator lines			
<pre></pre>	<pre>> </pre>	Indicator Lines Definition			
Default Edit Select	Default Edit Select	<no indicator="" lines=""> Select</no>			
Select Select	Eur Select]		
🖉 <unnamed case=""></unnamed>					

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

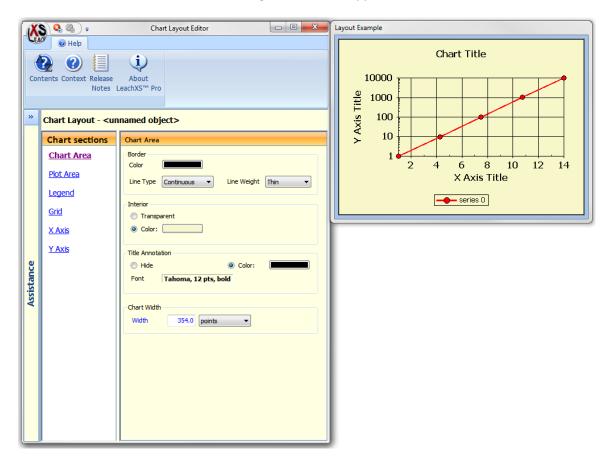
The **Graphs Layout** tab contains options to control how chart elements will appear. You can control the layout of every type of graph, save layouts for later use and change default settings for every graph type.

XS	Ŧ				Granular Material Comparisons
LEACH	间 Case Manager	: Statistics	🔀 Grap	hs Layout	🔤 Values below DTL 🛛 🔞 Help
			X		
Graph	pH-Concentration	Defaul Layou	t Edit	Set as Defa Layout	fault Default From Other Set as Default
		Selected graph			All graphs

The left side of the tab page shows a box containing the type of graph to edit. Click on the downpointing 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:

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

Add overall polynomial fit curve	A least-squares polynomial is drawn through the data
	points.
Include percolated materials in graph	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:

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

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.

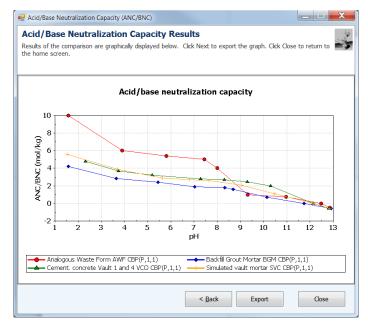
X	÷			LeachXS Pro™		
CEA	🖉 间 Database	🔒 Export 🛛 🧌	Tools 🛛 🔞 H	Help		
	rent database: \Development C	CBP database Feb_2	2012 updated	d.mdb Select other database	Material references	
		Database	9		Verification	
»						Welcome
						Analyze, Compare, and Display Leaching Data
						Acid/Base Neutralization Capacity
	Compare Ac	id/Base Neutrali	zation Capa	cities		
	Run the AN	C/BNC Calculator				
υ						
Assistance						
sta						
ssi						
						Import or Add New Data
						Classic LeachXS Modeling
						Advanced Modeling

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).

Material Selection Click Select to choose the materials you want to include it	in the comparison or calculations. Cl	ick Next to continue.
Selected Materials		
Analogous Waste Form AWF CBP (P,1,1) Backfil Grout Mortar BGM CBP (P,1,1) Cement. concrete Vault 1 and 4 VCO CBP (P,1, Simulated vault mortar SVC CBP (P,1,1)	Select Clear	
	< Back Next >	Cancel

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).

X	= Export Chart(s)	? X
LEA	Workbook 🛛 🞯 Help	
Ne	Pick Show	
	Select View	
»	Workbook and Worksheet(s) To Export To	
	C:\Users\\Documents\My Dropbox\ANCCap-ANCV	Vizard.xlsx
	Scenario Scenario	Rename
	Existing Worksheets	
a		Rename
Assistance		Delete
sis		Delete All
¥		Move up
		Move down
	Use alternative material names	Define
	Report material attributes to sheet: Material A	Attributes
		<u>E</u> xport

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.

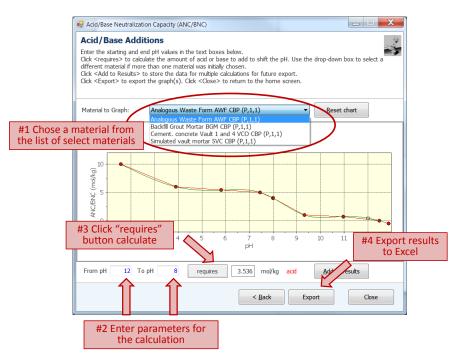
X	S ∓ LeachXS Pro™		
6	🖉 📑 Database 🛛 💫 Export 🛛 🧌 Tools 🛛 🞯 Help		
	rrent database: \Development CBP database Feb_2012 updated.mdb Select other database Database	Material references Verification	Welcome
			Analyze, Compare, and Display Leaching Data
			Acid/Base Neutralization Capacity
Assistance	Compare Acid/Base Neutralization Capacities Run the ANC/BNC Calculator		
			Import or Add New Data
			Classic LeachXS Modeling
			Advanced Modeling

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 dropdown 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.



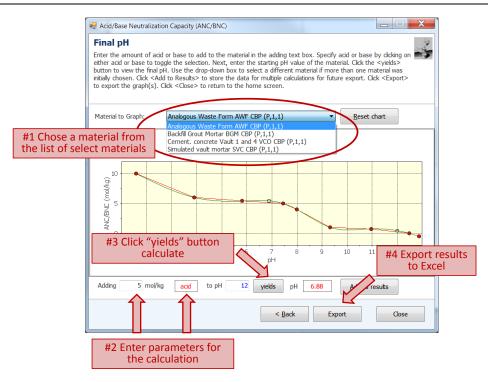
The resulting titration curve and the numerical data for this calculator may be exported to a Microsoft Excel[®] workbook using the Export Charts window accessed by clicking the Export button.

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).

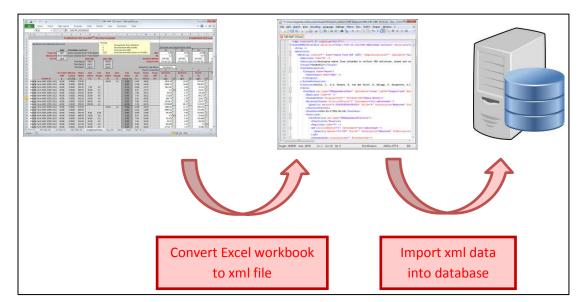
In LeachXS, the "natural pH" (sometimes called the "own pH" for brevity) is defined as the pH response at a liquid-to-solid ratio of 10 L/kg when no acid or base is added.



The 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)

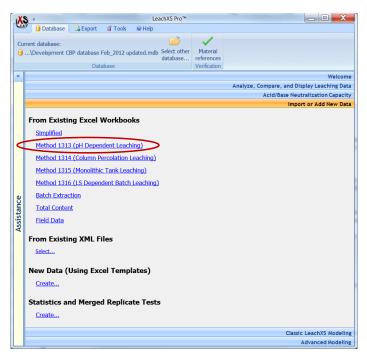
Accesses blank Microsoft Excel[®] data templates for data entry from within the LeachXS program.

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

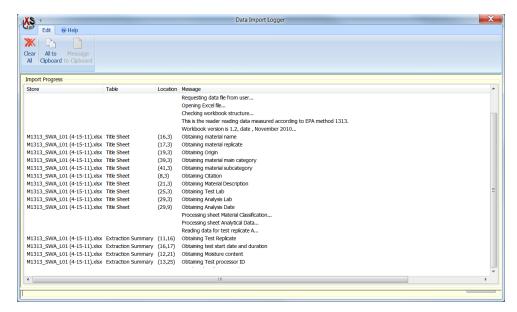
Importing Data from a LEAF Template into a LeachXS Database

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

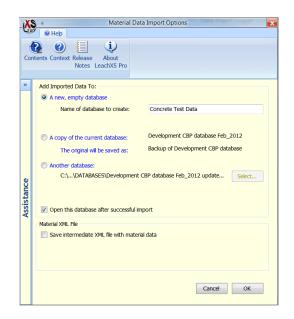
Creates a new database and activates a dialog box for naming the database to be created

• A copy of the current database

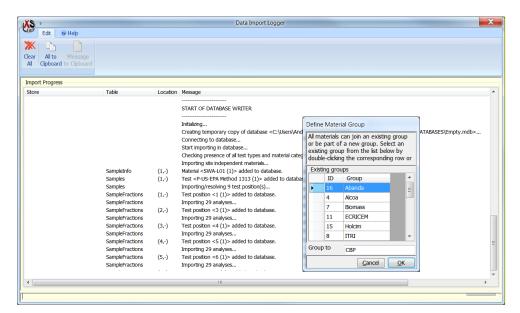
Saves a backup of the current database (e.g., the database displayed) and adds the new data to the current database.

• Another database

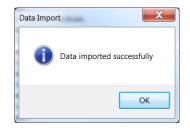
Activates a browser window to locate an existing database, saves a backup of the selected database and adds the new data to the selected database.



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.

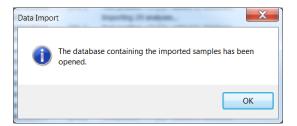


If fields (e.g., laboratory names, material source groups, etc.) in the data template do not match the categories native to LeachXS, a pop-up window (e.g., see the **Define Material Group** window above) will allow the user to "map" the field to an accepted LeachXS category). Upon a successful import,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

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Method 1316 Template v2.xltx	200KB	MS Excel-sj	21-1	
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• 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:

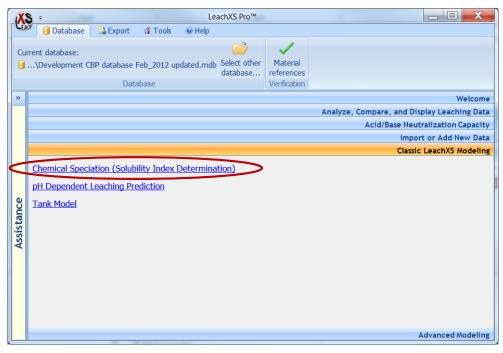
- Chemical Speciation Modeling
- pH Dependence Prediction Modeling

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.



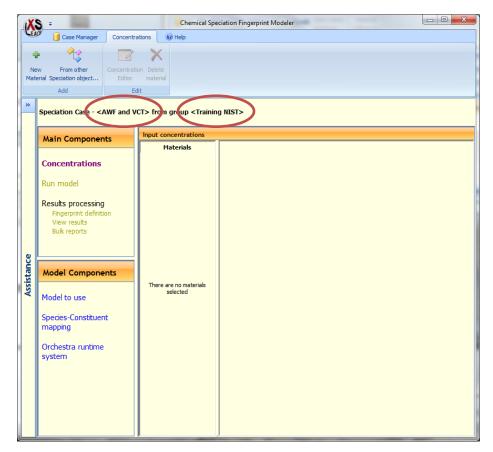
Select the **Open** icon from ribbon menu of the **Case Manager** tab on the top bar menu.

	Case Manager Con Con As Coad Case	Chemical Speciation Fingerprint Modeler	X
>>	Speciation Case - <unnan< th=""><th>red object></th><th></th></unnan<>	red object>	
	Main Componen	Materials	_
	Concentrations		
	Run model		
9	Results processing Fingerprint definition View results		
Assistance	Model Compone		
Ass	Model to use	There are no materials selected	
	Species-Constituent mapping		
	Orchestra runtime system		
	J	لي	

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).

X	S 😇 =		Speciation Case Manager
Ľ.	Map store 🛛 😽 Zīp store 💷 Group	📑 Case	Welp
Ne	w Depen Report Copy Cut P	aste Delete	Rename Protected
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»	Speciation Case: select case to open		
	Stores and Groups	Cases of gro	oup Training NIST
1	All stores System Map store	👃 Name	Created Last Modified
	Map Store (\LeachXS User Objects)	AWF an	nd VCT 6-4-2012 17:50 6-4-2012 17:50
Assistance	CaSilicate CBP Materials CBP reference April2010 CD reference April2010 Conrete EAF Loncnar EAF Loncnar EAF Loncnar Mining waste Si bring april A General Mining waste Si bring april A General Mining waste Si bring april A General Training NIST		
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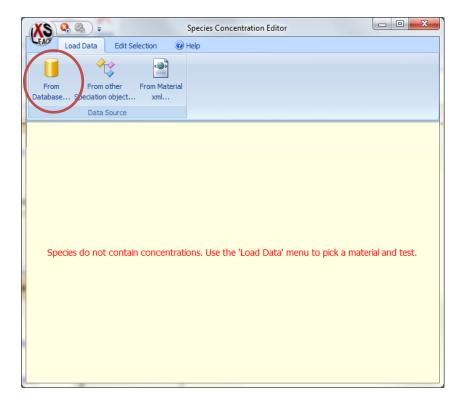
Double click on newly created case name (AWF and VCT) to start the Chemical Speciation Fingerprint Modeler window.



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.

IX.	S. ≠	Constant and		Chemical Spe	ciation Fingerprint Modeler	- 0 X
LEA	🖉 📋 Case Manager	Concentra	ations	Help		
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Ne	erial Speciation object	Concentrati Editor	on Delete material			
Mat	Add	Editor				
»						
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	mann componer			terials		
	Concentrations		<undefin< th=""><th>ed><1></th><th></th><th></th></undefin<>	ed><1>		
	Run model					
	Results processing Fingerprint definit					
	View results Bulk reports					
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8						
Assistance	Model Compone	ents				
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	Model to use					
	Species-Constituer mapping	nt				
	Orchestra runtime system	•				
					<u> </u>	

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.

Load Da	ata Edit	Selection	Help						
Reset to Undo Resured Edits Conce	Set as Not Measured		ste						
				ns are ord					
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-09
Br-	1.09E-07	1.09E-07	1.09E-07	1.09E-07	1.09E-07	1.09E-07	1.09E-07	1.09E-07	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	2.54E-10	2.54E-10	2.54E-10	2.54E-10	2.54E-10	2.54E-10
CI-	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	1.86E-07	1.86E-07	1.86E-07	1.86E-07	1.86E-07	1.86E-07	1.86E-07	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
НЗВОЗ	0.000273	0.000164	0.000108	5.64E-05	4.31E-05	1.28E-05	2.05E-05	6.03E-05	6.18E-05
110000			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.

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t Ak	Case Manager C	oncentrations	🕜 Help						
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	Add	Edit							
T	^								
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Ì	Main Components	Input o	concentrations in	mol/L, fractions o	rdered by p	н			
			Materials	Ilement	1.58	3.90	5.81	7.45	7.
	Concentrations		Form AWF	Ag+	-	-	-	-	
I	Concentrations	(CBP)	(A,P,A)	Al+3	0.038	0.001	1.35E-05	6.61E-07	1.48E
I				Ba+2	1.2E-05	1E-05	9.17E-06	9.56E-06	1.23E
I	Run model			Br-	1.09E-07	1.09E-07	1.09E-07	1.09E-07	1.09E
I				Ca+2	0.13	0.11	0.096	0.083	0.0
I	Results processing			Cd+2	9.4E-08	2E-08	2.54E-10	2.54E-10	2.54E
I	Fingerprint definition			CI-	9.15E-08	9.15E-08	9.15E-08	9.15E-08	9.15E
I	View results			CrO4-2	1.83E-05	7.62E-07	9.62E-09	9.62E-09	9.62E
	Bulk reports			Cu+2	3E-05	2.2E-06	1.65E-07	1.7E-07	1.2E
				DOC	1.67E-08	0.000335	0.000333	0.000348	0.0003
				F-	1.86E-07	1.86E-07	1.86E-07	1.86E-07	1.86E
K		=1		Fe+3	0.003	8.5E-06	1.37E-06	1.72E-07	2.89E
I	Model Components			H2CO3	-	-	-	-	
I	model components			H3AsO4	1.5E-05	3.57E-07	2.73E-07	1.12E-06	1.41E
I				H3BO3	0.000273		0.000108	5.64E-05	4.31E
I	Model to use			H4SiO4	0.072	0.001	0.00069	0.000546	0.00
I				Hg+2	-	-	-	-	
I	Species-Constituent			I-	-	-	-	-	
	mapping			K+	0.009	0.007	0.006	0.006	0.0
	mapping			Li+	0.000182	0.000169	0.000161		0.000
	Out of the second se			Mg+2	0.051	0.043	0.036	0.029	0.0
	Orchestra runtime			Mn+2	0.000899		0.000266	9.49E-05	3.74E
	system			MoO4-2		3.13E-07	1.34E-06	1.81E-06	1.87E
				•	III				•

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.

V	6 0		enemieur opeeludion	Fingerprint Modele	•				
EA	🖉 🧻 Case Manager	Concent	trations 🕜 Help						
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	· 🕹								
Ne			tration Delete						
lat	erial Speciation object	Edit	or material						
	Add		Edit						
	Speciation Case - <unn< td=""><td>amed o</td><td>bject> (changed)</td><td></td><td></td><td></td><td></td><td></td><td></td></unn<>	amed o	bject> (changed)						
	Main Components		Input concentrations in	mol/L, fractions o	rdered by p	Н			
			Materials	👃 Element	2.29	4.22	5.28	7.45	8
	Constantions		Waste Form AWF	Ag+	-	-	-	-	
	Concentrations		(CBP) (A,P,A)	Al+3	0.023	0.000345	3.78E-06	1.08E-05	1.29E
			Concrete VCT (vaults, CBP) (A,P,A)	Ba+2	2.65E-05	2.42E-05	2.12E-05	1.32E-05	1.03E
	Run model		(Vaules, CBP) (A,P,A)	Br-	1.09E-07	1.09E-07	1.09E-07	1.09E-07	1.09E
				Ca+2	0.11	0.093	0.082	0.072	0.0
	Results processing			Cd+2	4.27E-08	5.34E-09	7.09E-09	5.07E-10	5.07E
	Fingerprint definition			d-	9.15E-08	9.15E-08	9.15E-08	9.15E-08	9.15E
	View results			CrO4-2	9.77E-06	9.45E-08	4.84E-08	9.03E-08	1.18E
	Bulk reports			Cu+2	9.89E-06	8.88E-07	1.92E-07	1.98E-07	1.9E
				DOC	0.000558	0.000408	0.000422	0.000458	0.000
				F-	0.001	0.000819	0.000649	0.000667	0.0006
				Fe+3	0.003	0.001	0.00046	9.81E-07	5.19E
				H2CO3	-	-	-	-	
	Model Components	5		H3AsO4	5.88E-06	1.02E-06	2.57E-07	1.3E-07	4.33E
				H3BO3	0.000106	7.22E-05	5.74E-05	3.75E-05	2.56E
	Model to use			H4SiO4	0.057	0.002	0.000942	0.00077	0.000
	Proder to use			Hg+2	-	-	-	-	
	Consider Constitution			I-	-	-	-	-	
	Species-Constituent			К+	0.003	0.003	0.002	0.002	0.0
	mapping			Li+	0.000128	0.00011	9.68E-05	8.79E-05	8.3E
				Mg+2	0.026	0.020	0.017	0.014	0.0
	Orchestra runtime			Mn+2	0.000411	0.000265	0.000202	8.22E-05	9.21E
	system			MoO4-2		3.15E-07	2.89E-07	4.46E-07	4.52E
				•					F.

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.

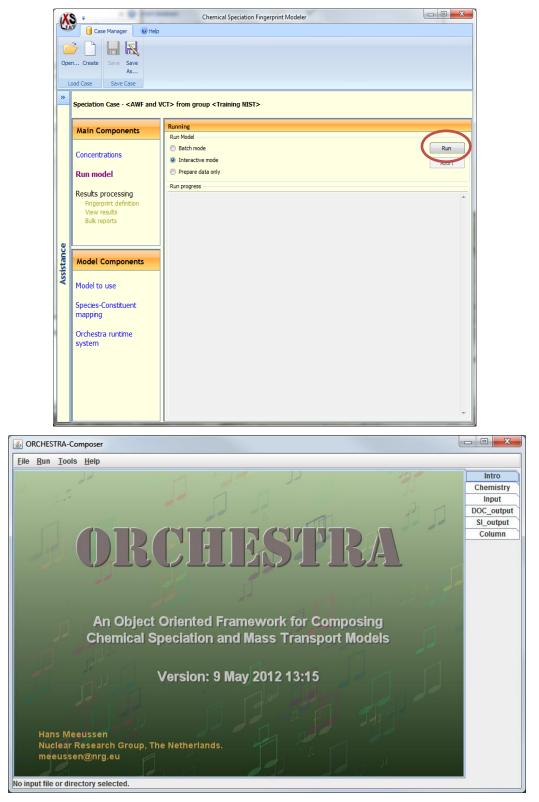
Hit **Run model** to start the model run.

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

X	S =	Chemical Speciation Fingerprint Modeler	
LEA	🦉 📋 Case Manager 🛛 🔞 Help		
Ope	n Create Save Save		
	As		
L	oad Case Save Case		
»	Speciation Case - <awf \<="" and="" th=""><th>ICT> from group <training nist=""></training></th><th></th></awf>	ICT> from group <training nist=""></training>	
	Main Components	Running	
	Main Components	Run Model	
	Concentrations	Batch mode	Run
	Concentrations	Interactive mode	Abort
	Run model	Prepare data only	
	Deguite processing	Run progress	
	Results processing Fingerprint definition		^
	View results		
	Bulk reports		
l S			
Assistance	Model Components		
Ass	Model to use		
	inder to use		
	Species-Constituent		
	mapping		
	Orchestra runtime		
	system		
			-

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.



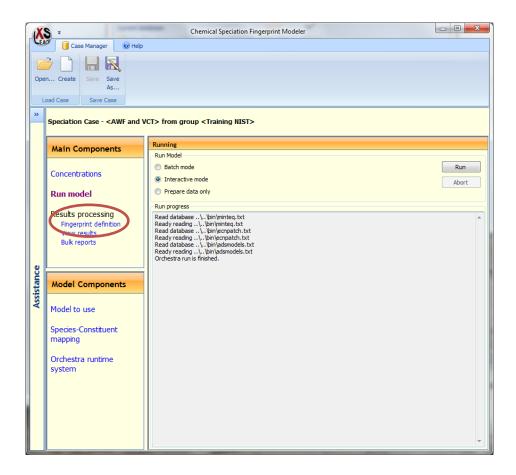
To start Orchestra by hitting Run (top left) twice (safety to avoid accidental starting of the model)

🔹 Orchestra Message Logger	x
Expanding phases	
(Expander) Including file: uiobjects.txt	
(Expander) Including file:\\bin\objects2008.txt	
(Expander) Including file: minerals.txt	
Expanding entities 1.172 s	
Reading variables 4.206 s	
Parsing expressions of chemistry1.inp	
Optimizing expressions of chemistry1.inp	
1.705 sec.	
40491 variables, 178400 expressions, 38 equations.	
Switching on: FA_don.logact: 0.0	
Switching on: FA1.unknown: 0.1	
Switching on: FA2.unknown: 0.1	
chemistry1.inp: Improving start estimations:.	
OK!	
Total Calculation Time: 5.67 sec.	-

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.

Exit confi	irmation
?	This will exit the Orchestra Composer. Is that OK?
	Yes No

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.

X	S =	Chemical Speciation Fingerprint Modeler	X
CE/	🖉 📋 Case Manager 🛛 🍀 Speci	ation Fingerprint @ Help	
Loa	Speciation object As	erprint dtor Grouping Edit	
»	Speciation Case - <awf and="" th="" v<=""><th>/CT> from group <training nist=""></training></th><th></th></awf>	/CT> from group <training nist=""></training>	
	Main Components	Fingerprint definition	
	Concentrations		
	Run model		
	Results processing Fingerprint definition View results		
	Bulk reports		
Assistance	Model Components		
As	Model to use	No fingerprint defined	
	Species-Constituent mapping		
	Orchestra runtime system		

In opening the Fingerprint editor switch to Al+3.

	View 🕜 Help							
X 💥 🚺								
elete Clear	lo By							
	iping Species							
Selection	Grouping							
vailable species	Analogous Waste Form AWF CBP (A,P,A)		VCT CDD	(4.0.4)				
Species	Analogous Waste Form AWF CBF (A,F,A)	ement. concrete Vault 2	VCT CBP	(A,P,A)				
Ag+	Fi	ractions or positions are	ordered b	у рН				
Ag+ Al+3	Mineral	Combined	Hit rate	Fit rate	1.58	3.90	5.81	7.45
Ba+2	AA_2CaO_Al2O3_8H2O[s]	000	000	000	-9.96	-5.01	-2.99	
Br-	AA_2CaO_Al2O3_5iO2_8H2O[s]	038	022	055				
Ca+2	AA_3CaO_Al2O3[Ca[OH]2]0_5_[CaCO3]0_5_	11_5H2O[s] 000	000	000				
Cd+2	AA_3CaO_Al2O3_6H2O[s]	000	000	000				
Cl- ≡ Co+2	AA_3CaO_Al2O3_CaCO3_11H2O[s]	000	000	000				
CrO4-2	AA_3CaO_Al2O3_Ca5O4_12H2O[s]	053	022	084				
Cu+2	AA_4CaO_Al2O3_13H2O[s]	006	011	000				
F-	AA_AI[OH]3[am]	000	000	000				
Fe+3	AA_CO3-hydrotalcite	010		009				
H2CO3	AA_CaO_Al2O3_10H2O[s]	025	022	028				
H3AsO4	AA_Ettringite	006	011	000		-0.05		
H3BO3 H4SiO4		006	011	000		2,84		
Ha+2	AA_OH-hydrotalcite[cr]	000	000	000				
I-	AA_Tricarboaluminate	000	000	000				
К+	Al203	000	000	000				
Li+	Al4[0H]10504	000	000	000				
Mg+2	AlAsO4:2H2O	000	000	000				
Mn+2 MoO4-2 +	Alohso4	000	011	000	-0.12			
		000	000	000	-5.31			
elected minerals	Alsb	000	000	000		-107.63		
	Al[OH]3[a]	006	011	000		0.22		
Mineral	Albite[low]	000	000	000				
	AlumK	000	000	000	1.34			
		006	011	000	0.03			
	Analbite	000	000	000				
	Analcime	000	000	000				
	Annite	000	000	000				
	Anorthite	000	000	000				
	E Boehmite	000	000	000				
	C2AH8_ECN	000	000	000				
	Ca-Nontronite	000	000	000				
	CaAH10_ECN	000	000	000				

Change the range of SI values in View.

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

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Minerals		/iew	Ø Help												
ersaturation va	lue	-1.0	A Over/undersaturation * Fit weight 1												
ersaturation val	Je	1.00	A Within limits * Hit weight 1												
Saturation Ir	ndexe	s	Saturation Coloring Figure of Merit weights												
ailable species			ous Waste Form AWF CBP (A,P,A) Cement. conc	rete Veult 2	VCT CDD	(4.0.4)									
Species ^		Analogo	Certent. conc	rete vauit z	VCT CBP	(A,P,A)									
Ag+					Fra	actions or	position	s are ord	ered by p	н					
Al+3			Mineral	Combined	Hit rate	Fit rate	1.58	3.90	5.81	7.45	7.99	9.32	10.96	12.48	12.87
Ba+2		A4	4_2CaO_Al2O3_8H2O[s]	021	022	020							-0.95	-0.61	
Br-		A4	A_2CaO_Al2O3_5iO2_8H2O[s]	066	044	087				-0.99	-0.62		0.18	0.06	
Ca+2		A4	A_3CaO_Al2O3[Ca[OH]2]0_5_[CaCO3]0_5_11_5H2O[s]	039	022	056							-0.51	-0.35	
Cd+2 Cl- ≡		E A4	A_3CaO_Al2O3_6H2O[s]	021	022	020							-0.97	-0.59	
Co+2		📄 A4	A_3CaO_Al2O3_CaCO3_11H2O[s]	014	022	006							-0.91	-0.97	
Cr04-2		A4	A_3CaO_Al2O3_Ca5O4_12H2O[s]	058	022	095							0.07	-0.02	
Cu+2		📄 A4	A_4CaO_Al2O3_13H2O[s]	045	022	068							-0.44	-0.04	
F-		E A4	A_AI[OH]3[am]	000	000	000									
Fe+3		A4	A_CO3-hydrotalcite	050	044	057				-0.70	-0.22	-0.32	-0.34		
H2CO3			A_CaO_Al2O3_10H2O[s]	058	067	050			0.35	-0.31	-0.06		0.02	0.30	-0.81
H3AsO4 H3BO3			A_Ettringite	026	022	029		-0.05							0.74
H4SiO4			A Gibbsite	042	022	061				0.46	0.29				
Hg+2			– A_OH-hydrotalcite[cr]	028	022	034			-0.41	0.84					
I-			A Tricarboaluminate	012	011	014							-0.61		
K+			203	000	000	000									
Li+			4[OH]105O4	006	011	000			0.70						
Mg+2 Mn+2			As04:2H20	000	000	000									
MoO4-2 +			0H504	048	022	074	-0.12	0.35							
			P04	000	000	000									
	-		Sb	000	000	000									
ected minerals	71		[OH]3[a]	044	022	065		0.22	0.44						
Mineral			bite[low]	006	011	000		-1.19	-0.89						
			umK	016	011	021			-0.42						
			unite	011	022	000	0.03		0.69						
			nalbite	000	000	000	-1.82		-1.07						
			nalcime	028	033	023			-0.61	-0.90	-0.79				
			nnite	020	000	020			-8.64	-11.57	-11.19				
			northite	000	000	000									
			pehmite	000	000	000									
			2AH8 ECN	000	000	000									
			a-Nontronite	000	000	000			-0.94						
			a-Noncronice aAH10_ECN	006	000	000			-14.14						
		Cr	-Ettringite	056	078	035			-0.94	-0.49	-0.23	0.05	0.96	0.52	-0.76

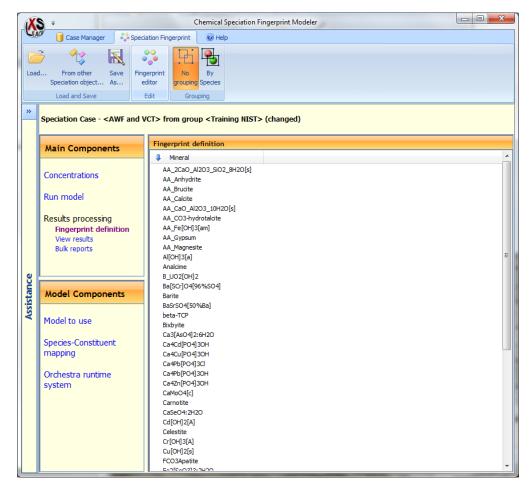
Based on the SI units selections of minerals can be made by going through all elements and all possible mineral phases. This does require some knowledge of possible mineral phases, as some phases are kinetically very slow and thus do not take part in the equilibrium based modeling. Other phases are only 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.

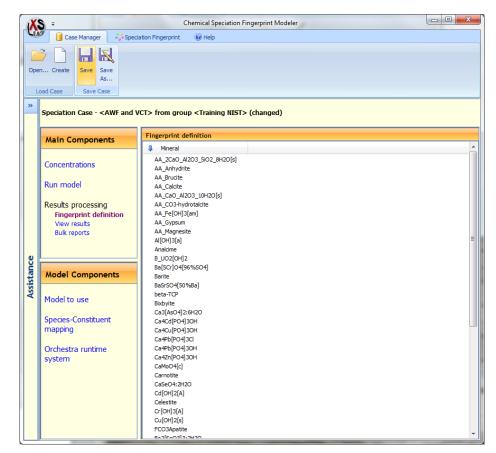
LeachXS CBP Version 2.0 User's Guide (rev. 0)

KS 🔍 🖏 🕫			43 -	Mineral Se	lector by S	Saturation	Indexes		-					R. A. 1	
Minerals	View	@ Help													
ndersaturation value	-1.	0 A Over/undersaturation * Fit weight 1													
versaturation value	1.0	00 A Within limits * Hit weight 1													
Saturation Inde	xes	Saturation Coloring Figure of Merit weights													
vailable species	Anal	ogous Waste Form AWF CBP (A,P,A) Cement. cond	rete Vault 2	VCT CBP	(A,P,A)										
Species ^					ctions or	position	s are ord	ered by n	чн						
Ag+		Mineral	Combined			1.58	3.90	5.81	7.45	7.99	9.32	10.96	12.48	12.87	
Al+3		AA_2CaO_Al2O3_8H2O[s]	021	022	020	-9.96	-5.01	-2.99	-2.67	-2.22	-2.63	-0.95	-0.61	-1.77	
Ba+2 Br-		AA_2CaO_AI2O3_6120[s]	021	022	020				-0.99	-0.62		-0.95	-0.61	-1.02	
Ca+2															
Cd+2		AA_3CaO_Al2O3[Ca[OH]2]0_5_[CaCO3]0_5_11_5H2O[s]	039	022	056							-0.51	-0.35	-1.53	
CI- ≡		AA_3CaO_Al2O3_6H2O[s]	021	022	020							-0.97	-0.59	-1.78	
Co+2		AA_3CaO_Al2O3_CaCO3_11H2O[s]	014	022	006							-0.91	-0.97	-2.12	
CrO4-2		AA_3CaO_Al2O3_Ca5O4_12H2O[s]	058	022	095							0.07	-0.02	-1.17	
Cu+2		AA_4CaO_Al2O3_13H2O[s]	045	022	068							-0.44	-0.04	-1.25	
F-		AA_A[[OH]3[am]	000	000	000									-4.34	
Fe+3 H2CO3	V	AA_CO3-hydrotalcite	050	044	057				-0.70	-0.22	-0.32	-0.34		-1.51	
H3AsO4	V	AA_CaO_Al2O3_10H2O[s]	058	067	050			0.35	-0.31	-0.06		0.02	0.30	-0.81	
H3BO3		AA_Ettringite	026	022	029		-0.05							0.74	
H4SiO4		AA_Gibbsite	042	022	061				0.46	0.29				-2.86	
Hg+2		AA_OH-hydrotalcite[cr]	028	022	034			-0.41	0.84					1.26	
I-		AA Tricarboaluminate	012	011	014							-0.61		-2.17	
K+			000	000	000									-8.09	
Li+		Al4[OH]10504	006	011	000			0.70						-6.78	
Mg+2		AlAs04:2H20	000	000	000			-2.66						-12.60	
Mn+2															
MoO4-2 👻		Alohso4	048	022	074	-0.12	0.35							-11.34	
< _ >		AIPO4	000	000	000									-13.82	
Selected minerals		AlSb	000	000	000									-114.44	
		Al[OH]3[a]	044	022	065		0.22	0.44						-5.48	
Mineral		Albite[low]	006	011	000			-0.89						-2.98	
AA_2CaO_Al2C		AlumK	016	011	021			-0.42						-7.02	
AA_CaO_Al2O3		Alunite	011	022	000	0.03		0.69						-5.68	
AA_CO3-hydro		Analbite	000	000	000									-3.16	
Al[OH]3[a] Analcime		Analcime	028	033	023			-0.61	-0.90	-0.79				-2.25	
Laumontite		Annite	000	000	000									-12.63	
counterrote		Anorthite	000	000	000									-3.48	
		Boehmite	000	000	000									-4.68	
		C2AH8 ECN	000	000	000									-8.83	
		Ca-Nontronite	006	011	000			-0.94						-5.65	
			000	000	000									-15.30	
		CaAH10_ECN						-14.14					-14.19		
<		Cr-Ettringite	056	078	035			-0.94	-0.49	-0.23	0.05	0.96	0.52	-0.76	

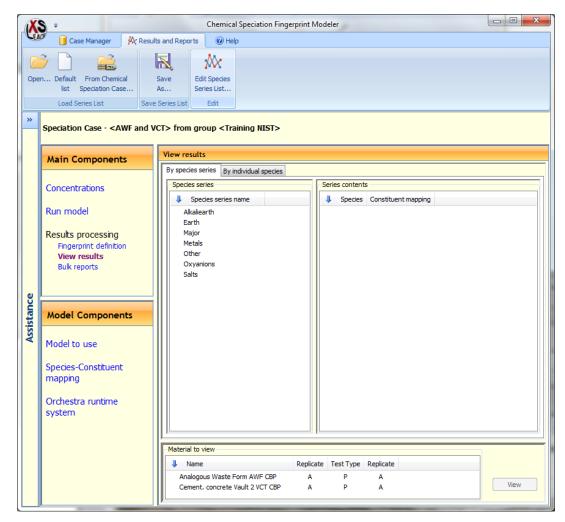
Confirm selections by hitting the green button in the top left of the pane.



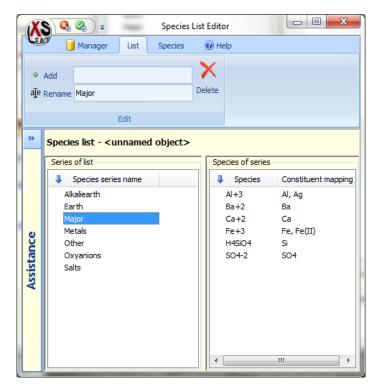
This forms the **Fingerprint definition** for the subsequent modeling of pH dependence test data. In the top button bar, hit **Case manager** and then hit **Save** to retain the selection.



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

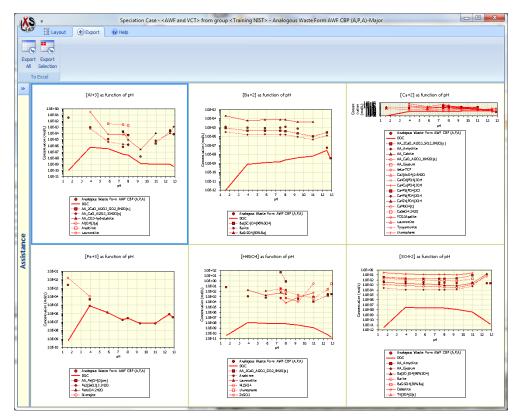


Under Species series element selections can be made with the Edit Species list editor.



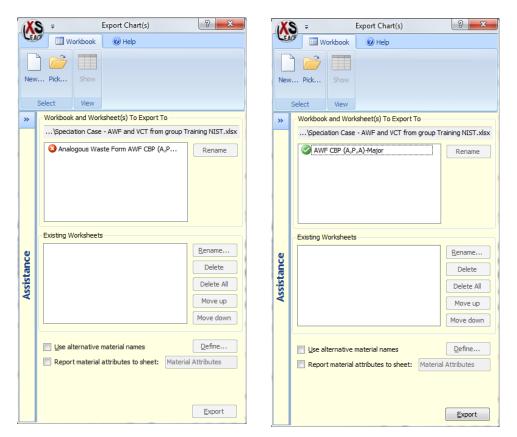
With Add one can add a new Substances list. It is only possible to view substances that have been mapped in the model. To view additional substances, the list of substances must be expanded first in the model.

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.

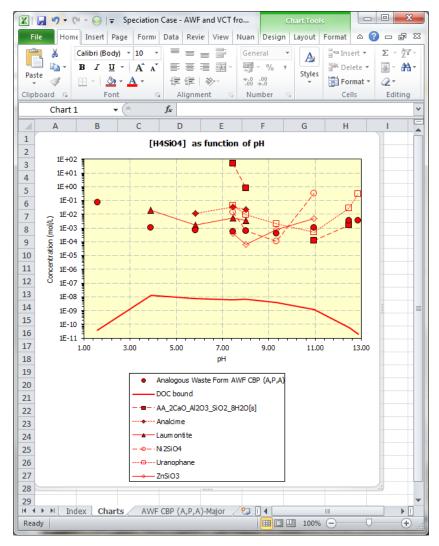
Hit **Export selection** of **Export all**. The first will export a selection of graphs. The latter will export all species in the list.



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

X		? <mark>X</mark>
VE/	Workbook 🛛 🛞 Help	
New	Pidk Show	
	Select View	
»	Workbook and Worksheet(s) To Export To	
	\Speciation Case - AWF and VCT from group T	raining NIST.xlsx
	AWF CBP (A,P,A)-Major	Rename
	Existing Worksheets	
e	Index Charts	Rename
a l	AWF CBP (A,P,A)-Major	Delete
Assistance		Delete All
-SA		Move up
		Move down
	[
	Use alternative material names	Define
	Report material attributes to sheet: Materia	al Attributes
		Export

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



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

X	S =	Chemical Speciation Fingerprint Modeler	- 0 X
CEA	🖉 📋 Case Manager 🛛 🖗 Res	ults and Reports 🛛 🛞 Help	
	n Default From Chemical	Save Edit Species	
Ope	list Speciation Case	As Series List	
	Load Series List Sa	re Series List Edit	
»	Speciation Case - <awf and<="" th=""><th>VCT> from group <training nist=""></training></th><th></th></awf>	VCT> from group <training nist=""></training>	
	Main Components	Bulk reports	
		By species series By individual species	
	Concentrations	Species series	
	Run model	All Species Lists	
	Kun model		
	Results processing		
	Fingerprint definition View results		
	Bulk reports		
8			
Assistance	Model Components		
As	Model to use		
	Species-Constituent		
	mapping		
	Orchestra runtime		
	system		
		Material to view	
		Name Replicate Test Type Replicate	
		Analogous Waste Form AWF CBP A P A	Report
		Cement, concrete Vault 2 VCT CBP A P A	Report

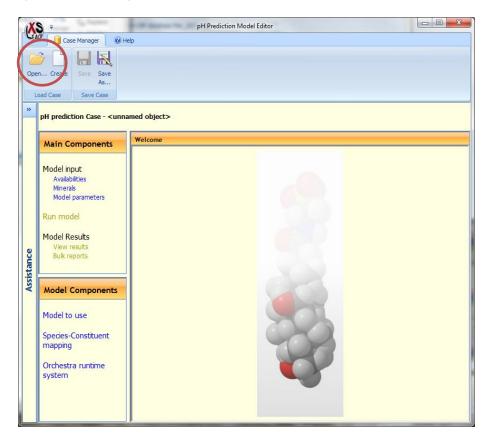
The speciation fingerprint is used in the subsequent pH dependence test modeling.

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.

X	S ∓ LeachXS Pro™		
LE.	🥙 📋 Database 🔛 Export 🖓 Tools 💿 Help		
Cur	rent database:	\checkmark	
	D:\\Development CBP database Mar_2012.mdb Select other database	Material references	
	Database	Verification	
»			Welcome
		Analyz	ze, Compare, and Display Leaching Data
			Acid/Base Neutralization Capacity
			Import or Add New Data
ø			Basic Modeling
Assistance	Chemical Speciation (Solubility Index Determination)		
ist	pH Dependent Leaching Prediction		
Ass	Cementitious Barriers Tank Model		
			Advanced Modeling

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.

X	S =		pH Prediction Mo	del Editor
CE/	🖉 📋 Case Manager 🛛 🛄 A	vailabilities 🛛 🛞	Help	
	From From other abase Case Load Edt			-
	Main Components	Availabilities	group < training wis	
				Dummy (A,A,A)
	Model input Availabilities Minerals Model parameters	Ag+ Al+3 Ba+2	Availability (mg/kg) - - -	
	Run model	Br- Ca+2 Cd+2 Cl-	-	
Assistance	Model Results View results Bulk reports	Co+2 CrO4-2 Cu+2 DOC	- - -	E
Assist	Model Components	F- Fe+3 H2CO3	-	
	Model to use	H3AsO4 H3BO3 H4SiO4 K+	- - -	
	Species-Constituent mapping	Li+ Mg+2 Mn+2	-	
	Orchestra runtime system	MoO4-2 Na+ Ni+2	-	
		Pb+2 PO4-3 Sb[OH]6-	-	

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.

EA	🖉 🚺 Case Manager 🛛 🛃 A	vailabilities 🛛 🔞	Help							
1										
F	rom From other Availability									
ata	base Case Editor									
	Load Edit									
٦	λ									
	pH prediction Case - <aw< th=""><th>F and VCT> from</th><th>group <training n<="" th=""><th>IST> (changed)</th><th></th></training></th></aw<>	F and VCT> from	group <training n<="" th=""><th>IST> (changed)</th><th></th></training>	IST> (changed)						
	Main Components	nts Availabilities								
		Analogous Waste Form AWF CBP (A,A,A)								
	Madalianut	👃 Element	Availability (mg/kg)							
	Model input Availabilities	Ag+	-							
	Availabilities	Al+3	1.04E+04							
	Minerais Model parameters	Ba+2	16.8							
	Model parameters	Br-	0.087							
	Run model	Ca+2	5.13E+04							
	Kun model	Cd+2	0.11							
		Cl-	3.22E+03							
	Model Results	Co+2	4.27							
	View results	CrO4-2	9.49							
	Bulk reports	Cu+2	19.0							
		DOC	140.7							
		F-	0.035							
	Model Components	Fe+3	1.41E+03							
	model components	H2CO3	-							
1		H3AsO4	11.3							
	Model to use	H3BO3	29.5							
		H4SiO4	2.02E+04							
	Species-Constituent	K+ Li+	3.71E+03 12.6							
	mapping	Mg+2	1.24E+04							
		Mg+2 Mn+2	493.9							
I	Orchestra runtime	Mi04-2	2.56							
	system	Na+	3.09E+03							
1	-,	Ni+2	3.03							
		Pb+2	3.06							
		PO4-3	0.12							

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 Predicton cases. If you have saved pH Predicton 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:

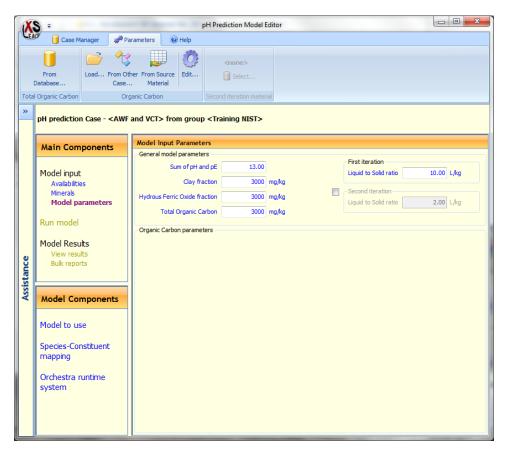


This option gives the possibility to edit the mineral selection. Let's accept the selection by clicking No. The mineral sets can be shown in alphabetical order and by Species (See below).

X	S =	pH Prediction Model Editor	
CE/	🦉 📋 Case Manager 🛛 🔺 M	inerals @ Help	
	d From Speciation From Other	Save Edit As Mineral Grouping	
»	pH prediction Case - <awf< th=""><th>and VCT> from group <training nist=""> (changed)</training></th><th></th></awf<>	and VCT> from group <training nist=""> (changed)</training>	
	Main Components	Minerals	
Assistance	Model input Availabilities Minerals Model parameters Run model Model Results View results Bulk reports	Image: Mineral AA_2CaO_Al203_SIO2_8H2O[s] AA_Anhydrite AA_Anhydrite AA_Anhydrite AA_Brucite AA_Caoldte AA_Caoldte AA_Cao_Al203_10H2O[s] AA_ACO3+hydrotaldte AA_CO3-hydrotaldte AA_Co3-hydrotaldte AA_Fe[OH]3[am] AA_Gypsum AA_Magnesite AI[OH]3[a] Analdme B_UO2[OH]2 Ba[SCr]04[96%SO4] E	111
Ass	Model Components	Barite BaSrSO4[50%Ba]	
	Model to use Species-Constituent	beta-TCP Bixbyite Ca3[AsO4]2:6H2O Ca4Cd[PO4]3OH Ca4Cu[PO4]3OH	
	mapping	Ca#b[P04]3Cl Ca#b[P04]3CH c=v7=0043cH	
	Orchestra runtime system	Ca42n[PO4]30H CaMo04[c] Carnotite Ca5e04:2420	
		Cd[OH]2[A] Celestite Cr[OH]3[A]	-

X	S =	pH Prediction Model Editor	х
CEA	🖉 📋 Case Manager 🛛 🔺 M	inerals @ Help	
Load	d From Speciation From Other	Save Edt As Mineral Grouping	
»	pH prediction Case - <awf< th=""><th>and VCT> from group <training nist=""> (changed)</training></th><th></th></awf<>	and VCT> from group <training nist=""> (changed)</training>	
	Main Components	Minerals	
	main components	Mineral	*
	Model input Availabilities Minerals Model parameters Run model	AI+3 AA_2CaO_Al2O3_SIO2_BH2O[s] AA_CaO_Al2O3_10H2O[s] AA_CO3+lydrotalcite AI[OH]3[a] Analcime Laumotite	H
Assistance	Model Results View results Bulk reports	Ba+2 Ba[SCr]O4[96%SO4] Barite BaSrSO4[50%Ba] Ca+2	
Assi	Model Components	AA_2CaO_Al2O3_SIO2_8H2O[s] AA_Anhydrite	
	Model to use Species-Constituent mapping Orchestra runtime system	AA_Cakite AA_CaO_Al203_10H20[s] AA_Goypsum beta-TCP Ca3[AsO4]2:6H2O Ca4Cd[PO4]3OH Ca4Cd[PO4]3OH Ca4Pb[PO4]3OH Ca4Pb[PO4]3OH	
		Ca42n[PO4]30H CaMo04[c] Ca5e04:2H20	-

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)

X	3 ÷	-		pH P	rediction Model I	Editor				
EA	🖉 🧻 Case Manager	Pa 🇬	arameters	Help						
	From Database Organic Carbon	Case	her From Sour . Material ganic Carbon		<none></none>	ial				
>	pH prediction Case	<awf< th=""><th>and VCT> f</th><th>rom group <t< th=""><th>raining NIST> (</th><th>(changed)</th><th></th><th></th><th></th><th></th></t<></th></awf<>	and VCT> f	rom group <t< th=""><th>raining NIST> (</th><th>(changed)</th><th></th><th></th><th></th><th></th></t<>	raining NIST> ((changed)				
	Main Componer		Model Inpu	ut Parameters						
	Main Components Model input Avaiabilities Minerals Model parameters Run model			del parameters Sum of pH and pE			First itera		10.00 L/	kg
			Hydrous Fe	Clay fraction erric Oxide fraction		mg/kg mg/kg	Second ite		2.02	
			Tot	tal Organic Carbor	3000	mg/kg	Liquid to S	olid ratio	2.00 L/	kg
	Kun model		Organic Ca	rbon parameters						
	Model Results		🌲 p	H Total (mg/kg)	Dissolved (mg/L)	Humic Acid (mg/L)	Fulvic Acid (mg/L)	Other (mg/L)	Solid (mg/kg)	Humic A
	View results Bulk reports		3. 5.	58 3000 90 3000 81 3000	0.0002 4.017 3.997	-	-	0.0002 4.017 3.997	3000 2960 2960	
	Model Compone	ents	7.		4.17 4.259	-	-	4.17 4.259	2958 2957	
			9.	32 3000 96 3000	4.428 5.273		-	4.428 5.273	2956 2947	
	Model to use		12. 12.	48 3000	12.42 14.07	-	-	12.42 14.07	2876 2859	
	Species-Constituer mapping	nt								
	Orchestra runtime system	•								
			•			1				,

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.

X) 😣	-			Ph	ase Editor	Sec. Contra				
LEA		Phase List Manager	🗹 Edit 🔍	View 🕜 Help							
Oper	/ U	Save As									
Ор	en l	Save									
»											
	4				Or	ganic Carbo	n				
			Total			Dissolved		Solid			
	pН	Total (mg/kg)	Dissolved (mg/L)	Solid (mg/kg)	Humic Acid (mg/L)	Fulvic Acid (mg/L)	Other (mg/L)	Humic Acid (mg/kg)	Fulvic Acid (mg/kg)	Other (mg/kg)	
	1.577	3000 🛄	0.0002	3000	-		0.0002	-	-	300	
Assistance	3.901	3000	4.017	2960	-	-	4.017	-	-	296	
a l	5.808	3000	3.997	2960	-	-	3.997	-	-	296	
sis	7.445	3000	4.17	2958	-	-	4.17	-	-	295	
	7.994	3000	4.259	2957	-	-	4.259	-	-	295	
	9.316	3000	4.428	2956	-	-	4.428	-	-	295	
	L 0.95 9	3000	5.273	2947	-	-	5.273	-	-	294	
	12.476	3000	12.42	2876	-	-	12.42	-	-	28	
	12.86	3000	14.07	2859	-	-	14.07	-	-	285	
	•									•	

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

X	S 🤒	%) ,			Ph	ase Editor	100-0100-00	-			
CE/	Ø 📋	Phase List Manage	r 📝 Edit 🖸	🖁 View 🛛 🔞 Help							
	W Hide phs graph Graphs		ute								
»											
					Or	ganic Carbo	n				
			Total			Dissolved		Solid			
	рН	Total (%)	Dissolved (%)	Solid (%)	Humic Acid (%)	Fulvic Acid (%)	Other (%)	Humic Acid (%)	Fulvic Acid (%)	Other (%)	
	1.577	100	6.667E-05	100	20	-	80	-	-	10	
Ĭ	3.901	100	1.339	98.66	20	-	80	-	-	10	
Assistance	5.808	100	1.332	98.67	20	-	100	-	-	10	
sis	7.445	100	1.39	98.61	-	-	100	-	-	10	
Ι×	7.994	100	1.42	98.58	-	-	100	-	-	10	
	9.316	100	1.476	98.52	-	-	100	-	-	10	
	10.95	100	1.758	98.24	-	-	100	-	-	10	
	12.476	100	4.14	95.86	-	-	100	-	-	10	
	12.86	100	4.69	95.31	-	-	100	-	-	10	
	•					m				•	

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.

X	S =			pH Pr	ediction Model 8	ditor				
EA	🖉 📋 Case Manager	🥔 Par	ameters	Help						
		Case	er From Source Material anic Carbon		<none></none>	ial				
»	pH prediction Case - <	AWF a	and VCT> fro	om group <tr< td=""><td>aining NIST> (</td><td>(changed)</td><td></td><td></td><td></td><td></td></tr<>	aining NIST> ((changed)				
	Main Components		Model Input	Parameters						
	Main Components		General model parameters Sum of pH and pE 13.00					First iteration		
	Model input Availabilities Minerals Model parameters Run model			Clay fraction	3000	mg/kg	Liquid to	Solid ratio	10.00 L/	kg
				ic Oxide fraction Organic Carbon		mg/kg mg/kg	Liquid to		2.00 L/	kg
				on parameters -						
	Model Results View results			Total (mg/kg)	Dissolved (mg/L)	Humic Acid (mg/L)	Fulvic Acid (mg/L)	Other (mg/L)	Solid (mg/kg)	Humic
.			1.58	3000	0.0002	4E-05	-	0.00016	3000	
	Bulk reports		3.90	3000	4.017	0.8034	-	3.214	2960	
			5.81		3.997	0.7994	-	3.198	2960	
			7.45		4.17	0.834	-	3.336	2958	
ž I	Model Component		7.99		4.259	0.8518	-	3.407	2957	
	moder component		9.32		4.428	0.8856	-	3.542	2956	
			10.96		5.273	1.055	-	4.218	2947 2876	
	Model to use		12.48 12.87		12.42 14.07	2.484 2.814	-	9.936 11.26	2876	
	Species-Constituent mapping									
	Orchestra runtime system									

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).

X	S =	-	pH P	rediction Model 8	ditor				
LEA	🥙 📋 Case Manager 🛛 🐗 Pa	rameters 🛛 🥝) Help						
	From Database			nalogous Waste Select	Form AWF CBP (A	N.C.A)			
Total	Organic Carbon Org	ganic Carbon		Second it	eration material				
»	pH prediction Case - <awf< th=""><th></th><th></th><th>raining NIST> (</th><th>(changed)</th><th></th><th></th><th></th><th></th></awf<>			raining NIST> ((changed)				
	Main Components	Model Input							
	Model input Availabilities Minerals		m of pH and pE Clay fraction	3000	mg/kg	First itera Liquid to S	Solid ratio	10.00 L/	¢g
	Model parameters	Hydrous Ferri	Oxide fraction	3000	mg/kg	Liquid to S		0.21 L/	ка
	Run model		Organic Carbon	3000	mg/kg	Erquio co c		0.21	
		Organic Carbo		1	1				
	Model Results		Total (mg/kg)		Humic Acid (mg/L)	Fulvic Acid (mg/L)			Humic Ac
Assistance	View results Bulk reports	1.58 3.90 5.81		0.0002 4.017 3.997	4E-05 0.8034 0.7994	-	0.00016 3.214 3.198	3000 2960 2960	
sis		7.45	3000 3000	4.17 4.259	0.834 0.8518		3.336 3.407	2958 2957	
×	Model Components	9.32		4.428	0.8856	-	3.542	2956	
		10.96	3000	5.273	1.055	-	4.218	2947	
	Model to use	12.48	3000		2.484	-	9,936	2876	
		12.87	3000	14.07	2.814	-	11.26	2859	
Q	Species-Constituent mapping								
	Orchestra runtime system								
		•		11					F.

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**.

X	S =		pH Prediction Model Editor
EA	🖉 📋 Case Manager 🛛 👬 S	pecies Mapping	@ Help
2	🗲 🗋 🔧 🔣		
oad	d Default From other Save	Species	No Mapped -
	case As	Mapping Editor g	rouping Unmapped
	Load and Save	Edit	Species grouping
,			
4	pH prediction Case - <aw< th=""><th>and VCT> from</th><th>a group <training nist=""> (changed)</training></th></aw<>	and VCT> from	a group <training nist=""> (changed)</training>
	Hais Comments	Species-Const	ituent Mapping
	Main Components	Species	Constituent mapping
	Model input Availabilities Minerals	Ag+ Al+3 Ba+2	Ag Al Ba
	Minerais Model parameters	Br- Ca+2 Cd+2	Br Ca Cd
	Run model Model Results	Cl- Co+2 CrO4-2	ପ ୦୦ ୦, ୦, ୯୩୩), ୦, ୯୩)
	View results Bulk reports	Cu+2 DOC F-	Cu Cu DOC F
		Fe+3	F Fe, Fe(II)
		H2CO3	C032-
2	Model Components	H3AsO4	As
	· · ·	H3BO3	В
	Madalas	H4SiO4	Si
	Model to use	К+	к
		Li+	Li
	Species-Constituent	Mg+2	Mg
	mapping	Mn+2	Mn, Mn(II)
		MoO4-2	Mo
	Orchestra runtime	Na+	Na
	system	Ni+2 Pb+2	Ni Pb
			Pb PO4
		PO4-3 Sb[OH]6-	PO4 Sb
		SECHI6- SeC4-2	SD Se

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

	ie Manager 🔅 Edit 🖸 View 🎯 Help		
Open Create	Save Save As		
Load Case	Save Case		
	ng - <unnamed object=""></unnamed>		
pecies mappi	g - Cumaned object>		
Species		Available	
Species	Constituent mapping	A Inorganic O	rgani
Mapped		Anne International	
Ag+	Ag	Ac	-
Al+3	Al	AC	
Ba+2	Ва	AI	Ξ
Br-	Br	Am	1
Ca+2	Ca	Ar	
Cd+2	Cd	As	
CI-	Cl	At	
Co+2	Co	Au	
CrO4-2	Cr, Cr(III), Cr(VI)	В	
Cu+2	Cu	Ba	
DOC	DOC	⊞ Be Bh	
F-	F	Bi	
Fe+3	Fe, Fe(II)	Bk	
H2CO3	CO32-	Br	
H3AsO4	As	С	
H3BO3	В	Ca	
H4SiO4	Si	CaCO3	
K+	к	Cd	
Li+	Li	Ce	
Mg+2	Mg	Cf	
Mn+2	Mn, Mn(II)	d	
MoO4-2 Na+	Mo	Cm CN	
Na+ Ni+2	Na Ni	CN	
NI+2 Pb+2	Ni Pb	CNC	
PD+2 PO4-3	P0 P04	CNV	
Sb[OH]6-	sb	Co	
SeO4-2	Se	CO32-	-
Sn+2	Sn		F.
lapped Constitue	nts and mapping order		

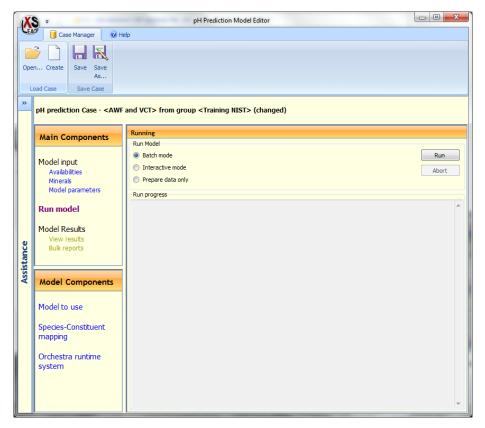
To map TIC on carbonate: click on H2CO3 and double click on TIC.

🔊 😣 🕲		Species to Constituer	nt Mapping Editor		
F ACP	se Manager 🛛 👶 Edit 🗄	View 🕜 Help			
Open Create	Save Save As Save Case				
Species mappin	ng - <unnamed object=""></unnamed>				Available
Species	Constituent mapping			^	Inorganic Organic
Mapped				_	🌲 Name 🔶
Ag+	Ag				Sg
Al+3	Al				Si
Ba+2	Ba				Sm
Br-	Br				Sn
Ca+2	Ca				SO3
Cd+2	Cd			E	SO4 SO4S
Cl-	d				SC45
Co+2	Co				sum heavy
CrO4-2	Cr, Cr(III), Cr(VI)				Ta
Cu+2 DOC	Cu DOC				Tb
F-	F				Tc
re+3	F Fe, Fe(II)				Te
H2CO3	CO32-, TIC				Th
H2C03	As				Thiocyapat
H3BO3	B				П
H4SiO4	si				
K+	ĸ				
Li+	Li				Tm ≡ TOC
Mg+2	Mg				U
Mn+2	Mn, Mn(II)				v -
MoO4-2	Mo				< Ⅲ ►
Na⊥	Na			-	
Mapped Constitue	ents and mapping order				
constituent ma	pping of Species <h2co3></h2co3>				
CO32-	πс				

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).

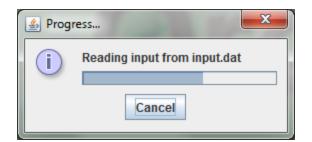
Now all is set to run the model. Click Run model.



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:

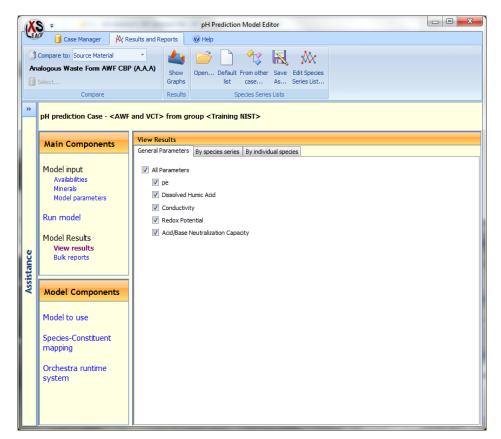
S Orchestra Message Logger	
Reading variables 0.0 s	
Parsing expressions of chemistry1.inp	
Optimizing expressions of chemistry1.inp	
2.044 sec.	
46200 variables, 193790 expressions, 85 equations.	
Switching on: ettr_ss.un: -10.0	
Switching on: Clay_don.logact: 0.0	
Switching on: HA_don.logact: 0.0	
Switching on: HA1.unknown: 0.1	
Switching on: HA2.unknown: 0.1	
Switching on: Hfo_e.logact: 0.0	
Parsing expressions of dissplusdoc.inp	
Optimizing expressions of dissplusdoc.inp	
0.0 sec.	
77 variables, 37 expressions, 0 equations.	
Total Calculation Time: 15.116 sec.	

To close Orchestra and return to LeachXS, hit the cross on the top right hand corner of the main window. Conformation 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.

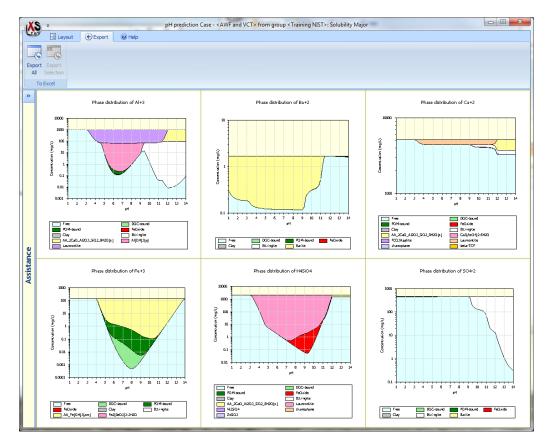


Tick Show graphs to view the results of General parameters, By species series or By Individual species respectively.

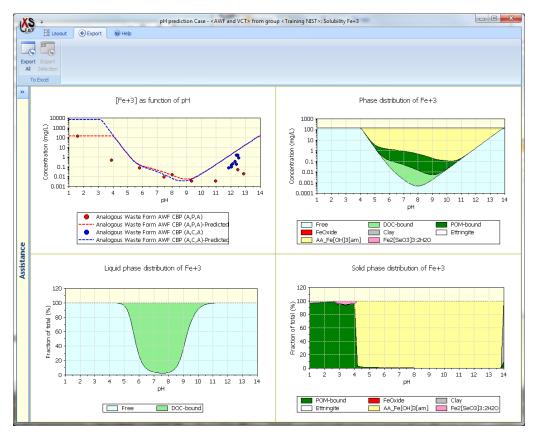
Here are examples of the various views.



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).

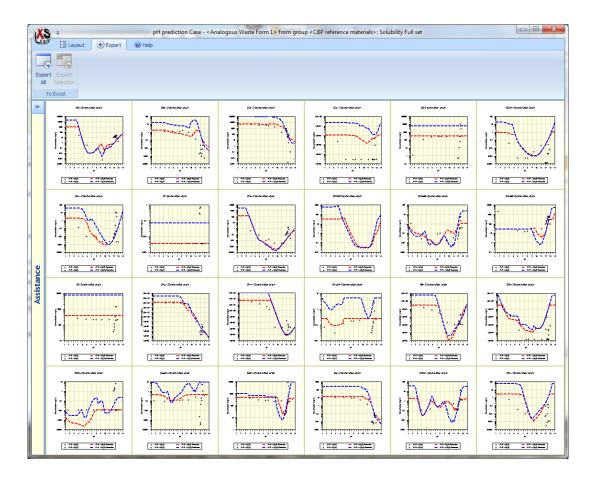


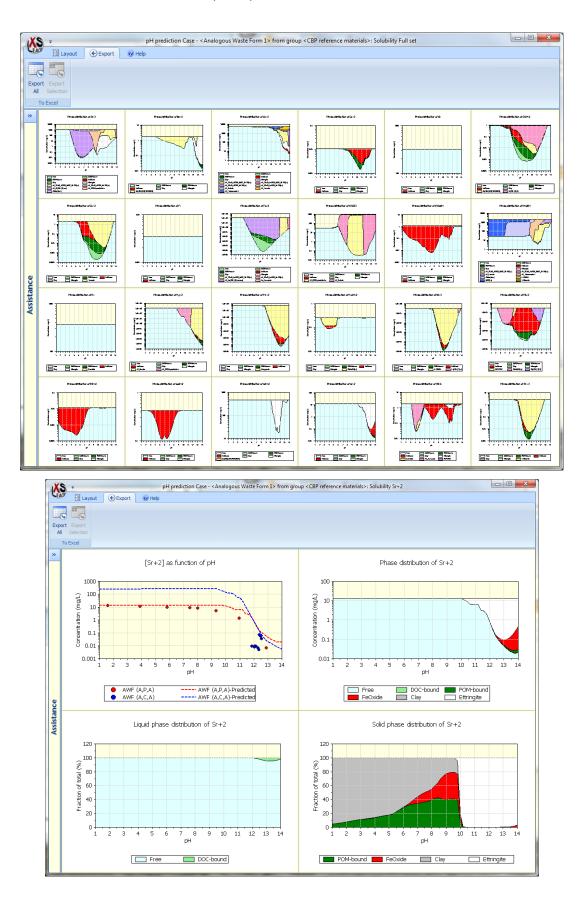
This is a very crucial observation for long term prediction potential.



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.

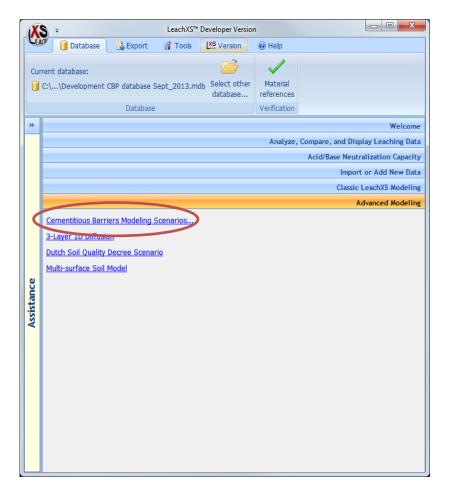
The CSF consists of element availabilities, reactive surface quantification (clay, Iron oxides, and organic matter), minerals and redox status.

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.

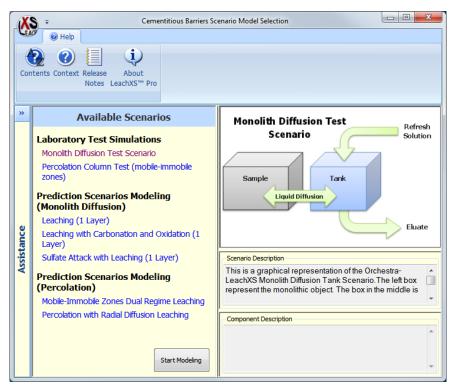


Cementitious Barriers Modeling Scenarios ...

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.

X	S ≠ Cementitious Barriers Sc	enario Model Selection
Cor		
»	Available Scenarios	Leaching with Sulfate Attack
Assistance	Laboratory Test Simulations Monolith Diffusion Test Scenario Percolation Column Test (mobile-immobile zones) Prediction Scenarios Modeling (Monolith Diffusion) Leaching (1 Layer) Leaching with Carbonation and Oxidation (1 Layer)	(1 Layer, unsaturated, no gas interaction) Inflow Suffices Contact Volume (liquid) Contact Volume (liquid) Contact Volume Contact Con
Assis	Sulfate Attack with Leaching (1 Layer) Prediction Scenarios Modeling (Percolation) Mobile-Immobile Zones Dual Regime Leaching Percolation with Radial Diffusion Leaching	Scenario Description This is a graphical representation of the Orchestra- LeachXS Sulfate attack Scenario. The left box represents the cement barrier. The other box represents
	Start Modeling	Click Start Modeling to begin

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.

- 0 X CBP Scenario editor: CBP Sulfate Attack Scenario ÷ 间 Case Manager Nedit 📝 🕜 Help 📕 View Ribbon bar XS <u>[]++/</u> Ęŝ Application Ribbon tab, LeachXS Customize Modify... button Editor... groups and Editor Available Solutions functions Model Input ario Compor Leaching with Sulfate Attack Cement barrier (1 Layer, unsaturated, no gas interaction) Physical **Components** Chemical Navigation Output pane pane No Eko Inflow solution Contact volume (liquid) Cement Refresh barrier Chemical Liquid Diffu Outflow Thickness Output Outflov Global Parameters Strainnarameters Porosity Tortuosity Parameters (textual) Density **Parameter Mapping** Other Classes **Refresh Scheme** Water Composition **Parameters Cell Parameters** pane Solid Composition Model Components Run Model Results <unnamed case>

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:

Save Report	to Excel
Report File 🕜 Help	
Open Create Generate View	
Destination Report File	
C:\Users\Seignette-d\Documents\CBP materials-Con	crete VCO (vaults, CBP)-Case 1 ver 0 (r
This workbook is new.	
Worksheets To Save (double-dick to rename)	Worksheets of Destination Report
Sheet Name	Sheet Name
✓ Report	

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**.

(XS) 🔍 🤇	•	Attac	hed Do	cuments Manager	X
	LEACE U A	ttachment	s 🕜 Help			
		Concerning of the local division of the loca	Show Delete			
	Current Attach	ments				
	Name	Extension	Туре		Original Location	
	DataSelection	.xlsx	Microsoft Excel-w	erkblad	C:\Users\Seignette-d\Documents\DataSelection.xls	x

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**.

- 0 -X CBP Scenario editor: CBP Sulfate Attack Scenario KS. 间 Case Manager Kiew 🕜 Help Nedit 🕺 XS **N++** 1 LeachXS Customize Load model files Modify... Editor... from folder... (notepad++) Editor Model Files Available Solutions Editor Model Input Leaching with Sulfate Attack (1 Layer, unsaturated, no gas interaction) Model Components Infle dutio Model to use Orchestra System Species-Constituent Mapping Contact volume Minerals (liquid) Thickness -> Outflow Minerals Reaction Constant Reaction Name 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+ 1.482E-17 Cem07_Brucite + 2 H+ -> 2 H2O + 1 Mg+2 Cem07 Brucite 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 Model Results Cem07_Syngenite 6.31E-08 Cem07_Syngenite -> 1 Ca+2 + 1 H2O + 2 K+ + 2 SO4-2 <unnamed case>

Navigation pane: Model Components

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

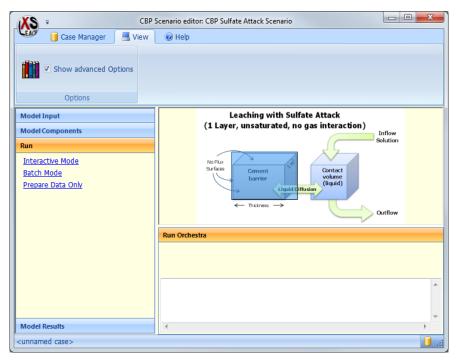
Some model parameters, like concentrations and availabilities, can be obtained from a LeachXS database with leaching data. The name giving of constituents like Na, As or Ba is different from the entities in Orchestra. The Species-to-Constituents Mapping defines which Orchestra species corresponds to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

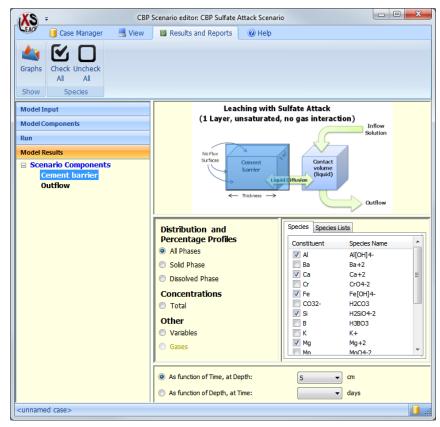
• Batch Mode

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:



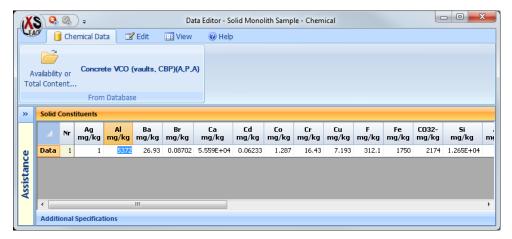
Tab group Model Source Material will only be present if you have opened a scenario for simulating a lab test. By pressing the Select... button you can select an existing lab test. The geometry and other physical parameters of the model will be set to the geometry and physical parameters of your selected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



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:

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	fx Define Range Scheme	Add	Insert Ins Before Aft	ert Delete Delet er Selected All nove steps		All
Order	Duration (da	ays)	Volume (L)	Flowrate (mL/h)	Start At (days)	Stops At (days)
D		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.

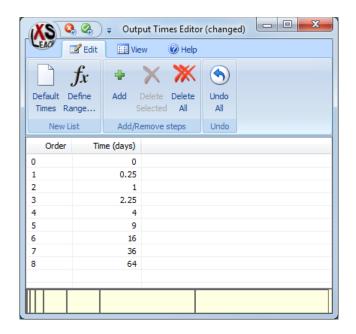
You can undo all your actions and revert to the list as it was when starting the editor by pressing the Undo All button.

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.

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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.

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les subfolder) (notepad++)	CONCOTTINE
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Java executable	java.exe		
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	·		
Description			
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	13 runtime system 2609	92013 with corres	sponding
The Orchestra-LXS 20	13 runtime system 2609	92013 with corres	sponding
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The Orchestra-LXS 20 objects2013. System files Name Root adsmodels.txt cbp_min_2013.txt description.txt	Last Modified 29-06-2007 14:26:00 26-09-2013 21:15:34 28-09-2013 12:24:56	Size 27711 8022 78 38529	sponding
The Orchestra-LXS 20 objects2013. System files Name Root adsmodels.txt cbp_min_2013.txt description.txt ecn_patch_2013.txt	Last Modified 29-06-2007 14:26:00 26-09-2013 21:15:34 28-09-2013 12:24:56 27-09-2013 14:06:08 04-09-2007 14:39:14 18-03-2008 13:54:18	Size 27711 8022 78 38529 31882 149570	sponding
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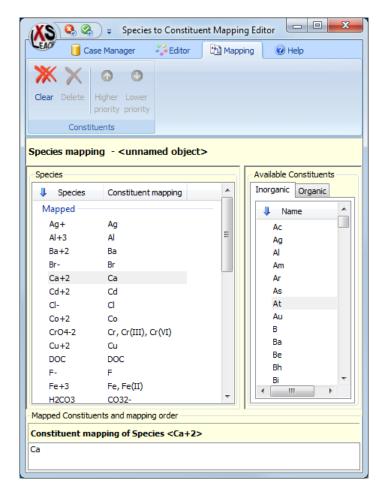
Most functions of this editor are the same as the ones in "The Model Files Editor" on page 91. In addition, you can specify the **Orchestra jar** file this is to be executed for running a model and how the **Java executable** is called in your system.

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.

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	xisting From Chemi ral Pool Speciation Ca Loa	se File(s) File(s					
»	Valid Reactants	-Pool of Available Mir	nerals	Selected Minerals			
	Al+3 Ca+2	Name React	tion Constan	Name	Reaction Constant	Reaction	*
	Cl-			AA_Brucite	1.445E-17	AA_Brucite + 2 H+ -> 2 H2O + 1 M	-
	Fe+3 H4SiO4			AA_Calcite	2.181E-09	AA_Calcite + 2 H+ -> 1 CO2[g] +	
	Mg+2			AA_Fe[OH]3[am]	1E-05	AA_Fe[OH]3[am] + 3 H+ -> 1 Fe+	
	Na+			AA_Gypsum	3.981E+04	AA_Gypsum -> 1 Ca+2 + 2 H2O +	=
	SO4-2			AA_Magnesite	1.647E-09	AA_Magnesite + 2 H+ -> 1 CO2[g]	-
				Cem07_Al[OH]3[am]	5.728E-10	Cem07_Al[OH]3[am] + 3 H+ -> 1	
8				Cem07_Al-ettringite	8.091E-58	Cem07_Al-ettringite + 12 H+ -> 2	
Assistance				Cem07_C2AH8	3.664E-61	Cem07_C2AH8 + 10 H+ -> 2 Al+3	
t I				Cem07_C2FH8	2.535E-54	Cem07_C2FH8 + 10 H+ -> 2 Ca+2	
<u>.</u>				Cem07_C3AH6	7.047E-82	Cem07_C3AH6 + 12 H+ -> 2 Al+3	
< ∎				Cem07_C3AS0.8H4.4	1.356E-69	Cem07_C3AS0.8H4.4 + 12 H+ ->	
				Cem07_C3FH6	9.29E-75	Cem07_C3FH6 + 12 H+ -> 3 Ca+2	
				Cem07_C4AH13	2.582E-105	Cem07_C4AH13 + 14 H+ -> 2 Al+	
				Cem07_C4FH13	1.629E-98	Cem07_C4FH13 + 14 H+ -> 4 Ca+	
				Cem07_CAH10	3.162E-39	Cem07_CAH10 + 8 H+ -> 2 Al+3	
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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:

All	All minerals are shown; minerals having at least one reactant
Having Any Available Reactant	that is not in the list of valid reactants are colored red. A mineral is shown only if it has at least one of its reactants is 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.
Having Available Reactants Only	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 is 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.

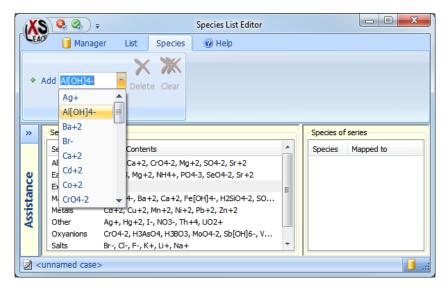
The Species List Editor

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.

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ខ	Earth	H2CO3, Mg+2, NH4+, P		Ba+2	Ba
š I	Major		Fe[OH]4-, H2SiO4-2, SO4-2	Ca+2	
÷ I	Metals	Cd+2, Cu+2, Mn+2, Ni-	· · · · ·	Fe[OH]4-	
Assistance	Other	Ag+, Hg+2, I-, NO3-, T		H2SiO4-2	
4	Oxyanions Salts	CrO4-2, H3ASO4, H3BO Br-, Cl-, F-, K+, Li+, Na	3, MoO4-2, Sb[OH]6-, VO2+ +	SO4-2	SO4, S
<unna< td=""><td>amed case></td><td></td><td></td><td></td><td>I.</td></unna<>	amed case>				I.

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:

X	₽ Manage Text Editors	×
LEAD	🖉 🔞 Help	
Assistance «	Defined Text Editors	
~	Details	
	C:\Windows\notepad.exe	

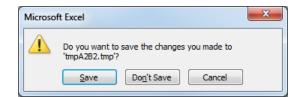
Press the Add... button and browse to the editor you want to use as text editor. In the above example, we've selected two editors as text editor: Notepad and Microsoft Excel[®]. Click on Notepad and press Set As Default to make Notepad your default text editor.

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[®] is used to edit a file, closing Microsoft Excel[®] causes the following message to appear:



When the *Save* button is pressed, Microsoft Excel[®] 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[®], the appropriate action to take for saving edited data is:

Press *File->Save*, and answer *Yes* to the appearing question. Next, close Microsoft Excel[®] 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.

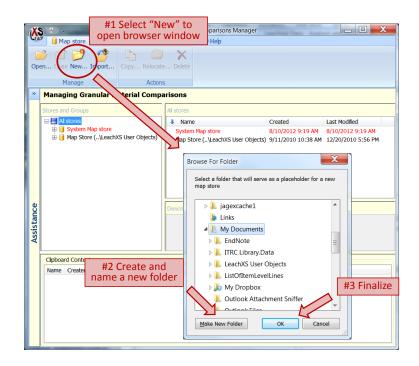
Leaching D.	ata - Analysis and Presentation: Granular Material Compariso	ons 📃 🗖 🛋 🗙	
🥙 📑 Case Manager 🔛 Statistics 🛛 🗵 Graphs Lay	out 🕜 Help		
Dpen Create Save Save			
Load Case Save Case			
Skip this step to exclude pH dependent data	Skip this step to exclude percolation and L/S data	Pick the constituent that is the subject of your comparison	
AFA (P,1,1) Select AFA (P,1,2) Delete GFA (P,1,3) CFA (P,1,1) CFA (P,1,2) CFA (P,1,2) CFA (P,1,3) CFA (P,1,2)	Select Dekte Clear	Clear Use pH Dependent regulatory thresholds Regulatory Thresholds	
Add overall polynomial fit curve	Graphing Options		
Include percolated materials in graph	Show L/S <-> Release (mg/kg) ✓ Show L/S <-> Concentration (mg/L)	Lower pH limit 7.00	
Display Units Show pH <-> Leaching in mg/kg Show pH <-> Leaching in mg/L	Image: Show L/S <-> Concentration (mg/L) Upper pH limit 10.00 Show L/S <-> pH High threshold 0 mg/kg		
Composition and Availability Show total composition, if available Show availabity, if available	Curve Fitting and Weights Show fited E values Show fited exponential model values	Select	
<u>U</u> sage	Weights: None 🔻	Include own pH	
Material Line Scheme	Material Line Scheme	Show indicator lines	
<default></default>	<pre><pre></pre> <pre></pre> <</pre>	Indicator Lines Definition	
Default Edit Select	Default Edit Select	Select	
Step 4: Graph and Export Data			
Click View Graph to generate graphs and export data one contituent at a time.	based on your selections above. Click Bulk Export to generat	e an Excel workbook with graphs and data for more than	
View Gr	ph > Bulk export >		

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.

Ň		lar Material Comparisons Manager	and the local data	
	Map store 🚽 Zip store 🖾 Group	📓 Case 🛛 🞯 Help		
	j 🗋 💋 🔗 🕒 🛑	×		
Ор	en Close New Import Copy Relocate			
	Manage Actions	5		
»	Managing Granular Material Compa	arisons		
	Stores and Groups	All stores		
	□-I Al stores	Name	Created	Last Modified
	System Map store Map Store (\LeachXS User Objects)	System Map store Map Store (\LeachXS User Objects)	8/10/2012 9:19 AM 9/11/2010 10:38 AM	
nce		Description of selected store		
Assistance				
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	Clipboard Contents	J		
	Name Created Last Mod			
	Hame created East Hou			

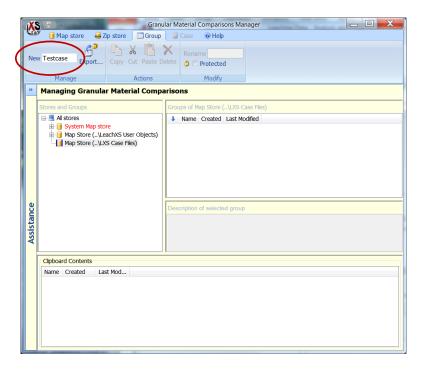
Creating a New Map Store Folder

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.

- Contraction of the second se	
Assistance	Stores and Groups Cases of group Testcase A stores System Map Store System Map Store (LvS Case Files) Highlight group Description of selected case
	Clipboard Contents Name Created Last Mod

These actions results in the following window.

X	Granu	lar Material Comparisons Manager					
LEA	🌋 间 Map store 🛛 😽 Zip store 📰 Group	Case Help					
Net		Kename Cut Paste Delete					
	Manage Actions Modify						
»	Managing Granular Material Compa	risons					
	Stores and Groups	Cases of group Testcase					
Assistance	 ■ Al stores System Map store Map Store (LeachXS User Objects) Map Store (LXS Case Files) □ Testcase 	Name Created Last Modified CCR Comp 8/10/2012 9:19 AM 8/15/2012 10:05 AM Description of selected case					
	Clipboard Contents						
A	Name Created Last Mod						

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.

Skip this step to exclude pH dependent data Select Delete Clear	Skip this step to exclude percolation and L/S data Select Delete Clear	Pick the constituent that is the subject of comparison See C Use pH Dependent regulatory thresholds Regulatory Thresholds
Add overal polynomial ft curve Include percolated materials in graph Display Units Show pH <>> Leaching in mg/kg Show pH <>> Leaching in mg/L	Graphing Options Show L/S <-> Release (mg/kg) Show L/S <-> Concentration (mg/L) Show L/S <-> pH	Lower pH limit 7,00 Upper pH limit 10.00 High threshold 0 mg/kg
Composition and Availability Show total composition, if available Show availability, if available Usage	Curve Fitting and Weights Show fited E values Show fited exponential model values Weights: None	Sel
Material Line Scheme <pre></pre>	Material Line Scheme <pre></pre>	Show indicator lines Indicator Lines Definition See

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.

	Granular Material So	#3 Open "Case" menu ribbon
#4 Click on the		Ap Rename Protected Modify
	Granular Material Comparisons: select case to oper	
	Stores and Groups Cases of group Tests A stores A stores Name Crea CCR Comp (4) C Map Store ()LaschXS User Objects) Map Store ()LXS Case Fies Map Store (tted Last Modfied //2012 9:19 AM 8/15/2012 10:05 AM #2 Highlight cast
	Clpboard Contents Name Created Last Mod	

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.

X	🙄 🗧 Granular M	laterial Comparisons Manager				
LEA	🧖 📔 Map store 🛛 😽 Zip store 📰 Group	📑 Case 🛛 🔞 He	łþ			
Nev	Open Report Export Copy	Cut Paste Delete	Rename			
	Manage	Actions	Modify			
»	Granular Material Comparisons: select ca	ise to open				
	Stores and Groups	Cases of group CBP r	naterials			
Assistance	System Map store CPP materials Template GP materials GP materials GP materials Example cases Template		l material comparison materials vs WW statistical data	Created 06-11-2013 1:15 PM 06-11-2013 1:15 PM	Last 06-1 06-1	
Assist		•	III		Þ	
		Description of selecte	d case			

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.

Organize ▼ New folder 🔠 ▼ 🔞						
쑦 Favorites 📃 Desktop	Documents library My Documents Arrange by: Folde	r *				
Downloads Downloads Downloads Documents Music Pictures Videos	Name My Projects My PSP Files My References My Shapes My Snapfire Shows My Videos Nested Lists					
File name: RegMatGr Save as type: Exported c	Notes Petra-MonsterAdmin <	+				

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**.

X	÷ LeachXS™ Pro					
CEA	🖉 🔋 Database 🔹 Export 🦷 Tools 🛛 🔀 Version 🖉 Help					
	erial Line Chart X-Grid Interpolation Indicator Species Case Importer Layouts Manager Lines Lists Editors					
»		Welcome				
	Analyze, Compare, and Dis	play Leaching Data				
	Compare Materials for Selected Constituents					
	Granular Materials (pH and L/S Dependence)					
	Monolithic Materials (pH and Time Dependence)					
	Compare Constituents from a Selected Material					
	Granular Materials (pH and L/S Dependence)					
	Monolithic Materials (pH and Time Dependence)					
Assistance	Field Monitoring Data					
ista	View Time Series, Full- and Pilot-Scale					
Ass	Statistics and Quality Control					
	Compare Materials to Statistics of a Reference Data Set					
	Quality Control for Leaching Evaluation of Materials and Products					
	And d/Derry March	- l'anti- Caracitu				
		ralization Capacity t or Add New Data				
		LeachXS Modeling				
		Advanced Modeling				

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.

XS =	Case Importer	
(i) Help		
File containing cases to import		
C: \Users\Seignette-d\Desktop	\RegMatGra-exported case.zip	Select
File contents information		
Cases type	Granular Material Comparisons	
Type Description	Definitions for comparing granular materials.	
		Import

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.

X.		pH prediction Case Manager		_ X
CEA	🚺 Map store 🛛 🝓 Zip store 🕅 Group	🛛 Case 🛛 🞯 Help		
	n Close New Import	e Delete Rename		
	Manage	Actions		
»	pH prediction Case: select case to	open		
	Stores and Groups	All stores		
	All stores	👃 Name	Created	Last Modified
	System Map store Map Store (\LeachXS User Objects)	System Map store Map Store (\LeachXS User Object	8/10/2012 9:19 AM cts) 11/18/2010 5:07 PM	8/10/2012 9:19 AM 11/18/2010 5:07 PM
Assistance		Description of selected store		
1	Clipboard Contents			
	Name Created Last Mod			

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.

Browse For Folder	X
Select a folder that will serve as a store	placeholder for a new zip
🧮 Desktop	<u> </u>
Dibraries	
🛛 🗟 Homegroup	=
4 🥦 Hans	=
🖻 퉲 AppData	
🔓 Contacts	
🛛 📔 Desktop	
🛛 📜 Downloads	
🛛 🍌 Dropbox	
Favorites	
👔 Links	_
	•
Make New Folder	OK Cancel

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.

Image Store Image Copy Image Copy Image Copy Image Copy Image Copy
Open Close New Import Copy Relocate Delete Rename Manage Actions * PH prediction Case: select case to open Stores and Groups Groups of New PhPredictCase Zp store * System Map store * System Map store * Name Created Last Modified * New PhPredictCase Zp store * Name Created Last Modified * New PhPredictCase Zp store
PH prediction Case: select case to open Stores and Groups Stores and Groups Image: Store
Stores and Groups Groups of New PhPredictCase Zp store Image: System Rap store Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified Image: Name Created Last Modified
A stores System Map store System Map store Way Store (Lueachts) User Objects) Map store (Lueachts) User Objects) Description of selected group
Opposed Contents
Clipboard Contents

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.

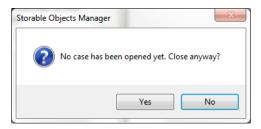
X				pH prediction	Case Manager				• X
LEA	🧖 🧻 Map store	😹 Zip store	💷 Group	🔄 Case 🛛 🕜 Help					
New	ı	Copy Cut Pas		Rename					
	Manage	Actions		Modify					
»	pH prediction	Case: select c	ase to ope	n					
	Stores and Groups			Groups of Map Store (\LeachXS	User Objects)				
	- All stores			Name	Created	Last Modified			
Assistance	Ca CB CB CB CB CB CB CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CB CC CC	ore (LeachXS User Silicate P April P reference materials F Loncnar A CCR A VAL EaFA port trar W Landgraaf testing cycled concret		CaSilicate CBP April CBP reference materials EAF Loncnar EPA VAL EAFA Const Mining waste Motar MSW Landgraaf RA testing Recycled concrete aggregate Sol EPA CBP	26-1-2012 16:02 26-1-2012 16:02 26-1-2012 16:02 26-1-2012 16:02 26-1-2012 16:02 26-1-2012 16:02 26-1-2012 16:02 26-1-2012 16:02 26-1-2012 16:02 26-1-2012 16:02	8-4-2012 14:09 26-1-2012 16:02 27-3-2012 20:43 24-3-2012 19:51 8-4-2012 16:02 26-1-2012 16:02 26-1-2012 16:02 15-3-2012 0:36 26-1-2012 16:02			
Assi				Test LT Description of selected group	25-1-2012 21:26	rag case	e name to n ' case Zip St	nove tore	

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

X	; (@ (pH prediction Case Manager	
CEA	Map store	🤬 Zip store 🛛 🛄 Group	🚡 Case 🛛 🔞 Help	
New		Copy Cut Paste Delete	Rename and a second sec	
	Manage	Actions	Modify	
»	pH prediction	Case: select case to op	en	
	Stores and Groups		Cases of group Export	
1	All stores	Map store	Name Created Last Modified	
Assistance	⊕ - U Mas New P	ore (. UsedNXS User Objects) PredictCase Zip store	Analogous Waste Form 1 8-4-2012 14:30 8-4-2012 14:30	
			Description of selected case	
	Clipboard Conten	3		
	Name Create	d Last Modified		

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.

X	÷ Leaching Dat	a - Analysis, Presentation and Data Comparisons	
LEA	Case Manager 🔀 Graph	s Layout 🛛 🕡 Help	
Con	ase (mg/kg) centration (mg/L) Concentration (mg/L) H Dependent Percolation and L/S		
»	Granular Materials Comparison - <unna< th=""><th></th><th></th></unna<>		
Assistance	Selected pH Dependent Data (7) Analogous Waste Form AVIF CBP Caerent. concrete Vault 1 and 4\ Cement. concrete Vault 2 VCT CE Cement. concrete Vault 2 VCT CE Cement. concrete Vault 2 VCT CE Add overall polynomial fit curve Include percolated materials in graph Display Units Show pH <> Leaching Img/kg mg/L Composition and Availability Show votal composition, if available Show availability, if available Show availability, if available Composition and Availability Default Edt From selection	Selected Percolation and L/S Data Clear Delete Select Graphing Options Show L/S <> Release (mg/kg) Show L/S <>> Concentration Show L/S <>> pH Curve Fitting and Weights Show fitted Evalues Show fitted exponential model values Weights: None Weights: None Default Edit From selection	Selected Constituent Clear Ca Select Ca Select Ca Select Chocked pH dependent regulatory thresholds Chocked pH dependent regulatory thresholds Chocked pH dependent regulatory threshold Upper pH limit 7.00 Upper pH limit 7.00 Upper pH limit 9.00 Right threshold 0 mg/kg Select Inducator Lines Definition Select Enduced own pH Show indicator lines Bulk export Show

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).

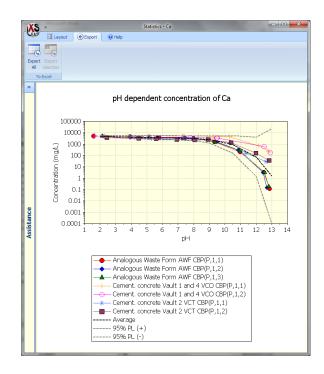
Statistical results are shown in the tabbed display at the lower right corner of the window with options for showing distributions, graphs, confidence intervals, etc.

Spline Calculate Statistics On Nearest point Normal Values Nearest point Ligarithmic Values Titted polynomial Ligarithmic Values X-values Gridpoints Confidence Limits 2, 4, 5.5, 7, 8, 9, 10.5, 12, 13 No Limits Edit Prediction Limits No Limits Confidence Interval general science Single Value Statistics Analogous Waste Form AWF CBP(P, 1, 1) Analogous Waste Form AWF CBP(P, 1, 2) Analogous Waste Form AWF CBP(P, 1, 3) Entity Cement. concrete Vault 1 and 4VCO CBP() Entity Cement. concrete Vault 1 and 4VCO CBP() Stil Deviation Cement. concrete Vault 1 and 4VCO CBP() Stil Deviation Cement. concrete Vault 1 and 4VCO CBP() Stil Deviation Comment. concrete Vault 1 and 4VCO CBP() Notes Comment. concrete Vault 1 and 4VCO CBP() Stil Deviation	onstituent	
June June	K Values Interpolation	Y Values Statistics
Clear Diversion Confidence Interval Prediction Limits Avalues Gridpoints Z, 4, 5, 5, 7, 8, 9, 10, 5, 12, 13 Edit Defined Series Defined Series Defined Series Defined Series Defin	Spline	Calculate Statistics On
Pitted polynomial X-values Gridpoints 2, 4, 5, 5, 7, 8, 9, 10, 5, 12, 13 Edit Defined Series Materials Analogous Waste Form AWF CBP(P, 1, 1) Analogous Waste Form AWF CBP(P, 1, 2) Analogous Waste Form AWF CBP(P, 1, 2) Cement. concrete Vault 1 and 4VCO CBP(Cement. concrete Vault 1 and 4VCO CBP(P, 1, 2) Cement. concrete Vault 2 VCT CBP(P, 1, 2) Variance 0.009316 Mediam 3.71 Count 7 Mediam 3.54 95% confidence 0.187	Linear	Normal Values
X-values Gridpoints Confidence Limits 2, 4, 5, 5, 7, 8, 9, 10.5, 12, 13 Prediction Limits Befined Series Single Value Statistics Materials Prediction Limits Analogous Waste Form AWF CBP(P, 1, 2) Single Value Statistics Analogous Waste Form AWF CBP(P, 1, 2) Frequency Bins Cement. concrete Vault 1 and 4VCO CBP(Cement. concrete Vault 1 and 4VCO CBP(Cement. concrete Vault 2 VCT CBP(P, 1, 2) Value Cement. concrete Vault 2 VCT CBP(P, 1, 2) Value Cement. concrete Vault 2 VCT CBP(P, 1, 2) Value Cement. concrete Vault 2 VCT CBP(P, 1, 2) Value Verage 3.55 Std Devalion 0.0957 CV 0.0277 Std Error 0.0362 Variance 0.030916 Minimum 3.71 Count 7 Medan 3.54	Nearest point	 Logarithmic Values
2, 4, 5, 5, 7, 8, 9, 10, 5, 12, 13 Image: Construction of the second	Fitted polynomial	Limits Showing
Edt On Limits Edt Confidence Interval 95.00 % Defined Series Single Value Statistics Materials pH to inspect 7.00 in range (2, 13) # Analogous Waste Form AVF CBP(P, 1, 1) Analogous Waste Form AVF CBP(P, 1, 2) For frequency Bins # Analogous Waste Form AVF CBP(P, 1, 2) For frequency Bins 5 # Cement. concrete Vault 1 and 4VCO CBP(Feer figures Distribution Graph Confidence Series # Cement. concrete Vault 2 VCT CBP(P, 1, 2) Key figures Distribution © Cement. concrete Vault 2 VCT CBP(P, 1, 2) Std Deviation © Cement. concrete Vault 2 VCT CBP(P, 1, 2) Uariance Ø Cement. concrete Vault 2 VCT CBP(P, 1, 2) Uariance Ø Construction 0.09516 Waimum 3.71 Count 7 Medan 3.54 95% confidence 0.187	X-values Gridpoints	Confidence Limits
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Defined Series Single Value Statistics Materials PH6 inspect 7.00 Analogous Waste Form AVF CBP(P, 1, 1) Analogous Waste Form AVF CBP(P, 1, 2) If Frequency Bins Ø Analogous Waste Form AVF CBP(P, 1, 2) If Grequency Bins S Ø Cement. concrete Vault 1 and 4VCO CBP(Entity Value Ø Cement. concrete Vault 2 VCT CBP(P, 1, 2) Entity Value Ø Cement. concrete Vault 2 VCT CBP(P, 1, 2) Common S Stat Devaltion Ø Cement. concrete Vault 2 VCT CBP(P, 1, 2) Common S Stat Devaltion Ø Cement. concrete Vault 2 VCT CBP(P, 1, 2) Common S Stat Devaltion Ø Cement. concrete Vault 2 VCT CBP(P, 1, 2) Common S Stat Devaltion Ø Common S Stat Devaltion 0.09516 Minimum 3.71 Count 7 Median 3.54 95% confidence 0.187		- No Limits
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Image: Construction CV 0.027 Std Error 0.0362 Variance 0.00916 Minimum 3.41 Maximum 3.71 Court 7 Median 3.54 95% confidence 0.187	Cement. concrete Vault 2 VCT CBP(P, 1, 1)	
Std Error 0.0362 Variance 0.00916 Minimum 3.41 Maximum 3.71 Count 7 Median 3.54 95% confidence 0.187	Cement. concrete Vault 2 VCT CBP(P, 1, 2)	
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Median 3.54 95% confidence 0.187		Maximum 3.71
95% confidence 0.187		Count 7
		Median 3.54
95% prediction 0.2		95% confidence 0.187
		95% prediction 0.2
		Bulk export
Bulk expo		

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.

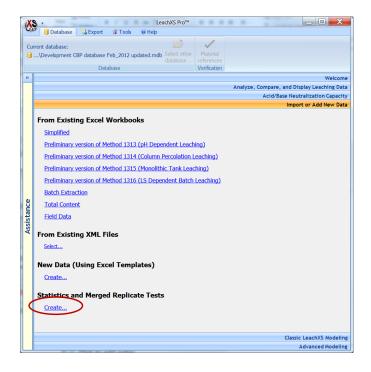
	he constituent ayed statistics
X Values Interpolation Spline Linear Nearest point Fitted polynomial X-values Gridpoints 2, 4, 5.5, 7, 8, 9, 10.5, 12, 13	Y Values Statistics Calculate Statistics On Normal Values Light Showing Confidence Limits Prediction Limits Confidence Interval Confidence Interval Statistics Confidence Interval Statistics Confidence Interval Statistics Confidence Interval Statistics Stat
Defined Series Material Analogous Waste Form AWF CBP(P, 1, 1) Analogous Waste Form AWF CBP(P, 1, 2) Analogous Waste Form AWF CBP(P, 1, 2) Cament. concrete Vault 1 and 4 VCO CBP(Cement. concrete Vault 1 and 4 VCO CBP(Cement. concrete Vault 2 VCT CBP(P, 1, 2) Cement. concrete Vault 2 VCT CBP(P, 1, 2)	Single Value Statistics pH to inspect # of Frequency Bris 5 Key figures Distribution Graph Confidence Std Deviation 0.0957 CV 0.0277 Std Error 0.0352 Variance 0.00916
Change the data series in the statistical calculations and displays	Minimum 3.41 Maximum 3.71 Count 7 Median 3.54 95% prediction 0.187 95% prediction 0.2 Export statistics to Excel workbook
	Bulk export

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.

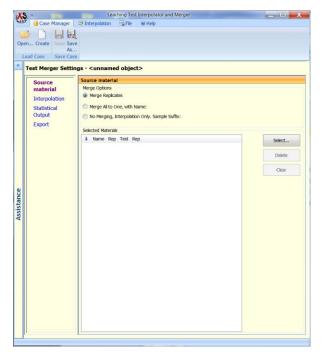


Statistical Calculations from the Import or Add New Data Roll-up Menu

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.

X	÷	Leaching Test Interpolator and Merger	
CEA	🥙 间 Case Manager 🛛 🛃	Interpolation 🗧 File 🕡 Help	
»	Test Merger Settings -	<unnamed object=""></unnamed>	
	Source material	Source material	
	Interpolation Statistical Output Export	Merge Options Merge Replicates Merge All to One, with Name: No Merging, Interpolation Only. Sample Suffix: Selected Materials	
		Vame Rep Test Rep	Select Delete
ce			Clear

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

X	S	Leaching Test Interpolator and Merger
CEA	🥙 📋 Case Manager 🛛 🐺	Interpolation 🗧 File 🎯 Help
»	Test Merger Settings -	<unnamed object=""></unnamed>
Assistance	Source material Interpolation Statistical Output Export	Interpolation data X Values Interpolation Type Spline Nearest point Interpolation grid points 2, 4, 5.5, 7, 8, 9, 10.5, 12, 13 Interpolation Threshold Edit Interpolation Threshold Interpolate, if: Relative distance from grid is less than: Absolute distance from grid is less than: Absolute distance from grid is less than: Always interpolate Minimum Concentration Value Half of the Detection Limit As Calculated Maximum Concentration Value Maximum in Data Interpolate using logarithmic values Y Values Use log values for interpolation and statistics

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:

XS =	Interpolation an	d Ext	rapol	ation	Previ	ew				
CEACH 2	Edit 🕜 Help									
Copy Entire Grid Copy										
		2	4	5.5	7	8	9	10.5	12	13
Concrete V	CO (vaults, CBP) (P,1,1)	Ext	Int	Int	Int	Int	Int	Int	Int	Ext
Concrete V	CO (vaults, CBP) (P,1,2)	Int	Int	Int	Int	Int	Int	Int	Int	Ext
Concrete V	T (vaults, CBP) (P,1,1)	Ext	Int	Int	Int	Int	Int	Int	Int	Ext
Concrete V	T (vaults, CBP) (P,1,2)	Ext	Int	Int	Int	Int	Int	Int	Int	Ext
Legend										
Int	The value is reached by i	nterpo	latior							
Ext										
A Not reachable by interpolation or extrapolation										

You can choose to perform the interpolation on the x-values on a logarithmic bases. This is especially apropriate 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.

	Test Merger Settings -	-				
	Source material	Statistics and Interpolation O Statistical Value(s) to Merge	utput			
	Interpolation					
	Statistical Output	Single Statistics Values Nested	Statistics Values			
	Export	Target	Material suffix	Confidence %	Percentile %	-
		Parametric Statistics				- 11
		Mean	X			
		Std Deviation (-)	[SD-]	95.00		
		Std Deviation (+)	[SD+]	95.00		
		Mean - Std Deviation	[X-SD]	95.00		
		Mean + Std Deviation	[X+SD]	95.00		
		Confidence Limit (-)	[CL-]	95.00		
		Confidence Limit (+)	[CL+]	95.00		=
		Prediction Limit (-)	[PL-]	95.00		
2		Prediction Limit (+)	[PL+]	95.00		
		Non-Parameteric Statistics				- 11
		Minimum	[Min]			
2		Lower Percentile	[LPx]		5	
		Median	[Med]			
		Upper Percentile	[UPx]		90	
		Maximum	[Max]			
						-
		Interpolation results				
		Output interpolated tests				
		Suffix for interpolated	tosts Into			
		Surfix for interpolated	iesis inp			

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:

<u> XS 8 8</u>	🖵 🗧 Edit Statistics Merge Value Settings 📃 🔲 🗮 🏹
CEAO @ He	lp
Name	Std Deviation (+)
Туре	Parametric Statistics
Suffi	x SD+ Default ([SD+])
Confidence	e 95.00 %
# of Sigma	s 1.96

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.

	Case Manager	Leaching Ter	st Inter		r and M) Help	lerger	_ 0 _ X
» T	Fest Merger Settings -	<unnamed ol<="" th=""><th>ject:</th><th>> (ch</th><th>anged</th><th>d)</th><th></th></unnamed>	ject:	> (ch	anged	d)	
	Source material Interpolation Statistical Output Export	Source materi Merge Options Merge Replic Merge All to No Merging, Selected Materi	ates One, w Interpo			ample Suffix:	
		Selected Materia Name		Test	Rep		 Select
		AFA (P,1,0) - AFA AFA AFA	1 1 1	P P	3 2 1		Delete
Assistance		BPB (P,1,0) - BPB BPB BPB	1 1 1	P P P	3 2 1		
As		BPT (P,1,0) - BPT BPT BPT	1 1 1		3 2 1		
					*		

The Sample Selector

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

Application menu Ca	ncel or Save too	olbar	Ribbon toolba	ir		
Samples	Y= Filtering @ Help	Sample Se	lect			
Open Save As	Save Selection Select all as Favorites		V			
Load Sample Selection Save Sample Selection	Favorites					Selected Samples (0)
All Available Often Used Favorites					_ [Name
Name Analogous Waste Form AWF CBP (P, 1, 1) Analogous Waste Form AWF CBP (P, 1, 2) Analogous Waste Form AWF CBP (P, 1, 2) Backfill Grout Mortar BGM CBP (P, 1, 1) Backfill Grout Mortar BGM CBP (P, 1, 1) Backfill Grout Mortar BGM CBP (P, 1, 2) CEM II/A-V + CrO4 reduction + 17%FA (M, 1, 1) CEM II/A-V + CrO4 reduction + 17%FA (M, 2, 1) CEM II/A-V + CrO4 reduction + 17%FA (P, 2, 1) CEM II/A-V + CrO4 reduction + 17%FA (P, 2, 1) CEM II/A-V + CrO4 reduction + 17%FA (P, 2, 1) CEM VI/A 32.5 N 32% GBF5 + 20% FA 2 (M, 1, 1) CEM V/A 32.5 N 32% GBF5 + 20% FA 2 (M, 2, 1) CEM V/A 32.5 N 32% GBF5 + 20% FA 2 (M, 1, 1) CEM V/A 32.5 N 32% GBF5 + 20% FA 2 (M, 1, 1) CEM V/A 32.5 N 32% GBF5 + 20% FA 2 (M, 1, 1) CEM V/A 32.5 N 32% GBF5 + 20% FA 2 (M, 1, 1) CEM V/A 32.5 N 32% GBF5 + 20% FA 2 (M, 1, 1) Cement mortar CEM V/L D slag-1 (P, 1, 1) Cement mortar CEM V/L D slag-1 (P, 1, 1)) Monolithic leach) pH Dependence) pH Dependence U pH Dependence) Monolithic leach) Monolithic leach	Test Subtype US-EPA Method 1313 US-EPA Method 1313 US-EPA Method 1313 US-EPA Method 1313 US-EPA Method 1313 NEN 7345 ANC 14429 ANC 14429 NEN 7345 NEN 7345	Category Cementitious Materials Cementitious Materials	Subcategory Stabilized waste Stabilized waste Stabilized waste Stabilized waste Grout Grout Mortar Mortar Mortar Mortar Mortar Mortar Mortar Mortar		<no samples="" selected=""></no>
Available Samples panel]		Selected Sa	mples pane	el	Database icon

- 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 en 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.

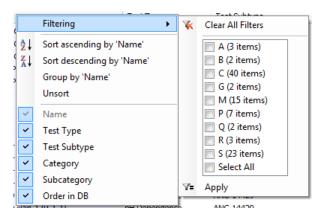
Manipulating the Sample List

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:

Il Available Often Used Favorites		
Name	Test Type	Test Subtyp
A [3 items]		
Analogous Waste Form AWF CBP (P, 1, 1)	pH Dependence	US-EPA Meth
Analogous Waste Form AWF CBP (P, 1, 2)	pH Dependence	US-EPA Met
Analogous Waste Form AWF CBP (P, 1, 3)	pH Dependence	US-EPA Meth
B [2 items]		
Backfill Grout Mortar BGM CBP (P, 1, 1)	pH Dependence	US-EPA Meth
Backfill Grout Mortar BGM CBP (P, 1, 2)	pH Dependence	US-EPA Meth
C [40 items]		
CEM II/A-V + CrO4 reduction + 17%FA (M, 1, 1)	Monolithic leach	NEN 7345
CEM II/A-V + CrO4 reduction + 17%FA (M,2,1)	Monolithic leach	NEN 7345
CEM II/A-V + CrO4 reduction + 17%FA (P,3,1)	pH Dependence	ANC 14429
CEM II/A-V + CrO4 reduction + 17%FA (P,4,1)	pH Dependence	ANC 14429
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:

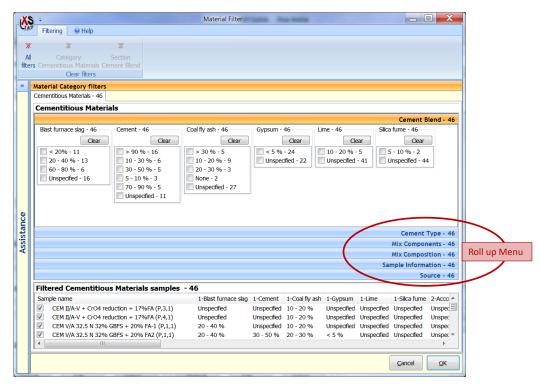
KS & & =		Sample Selector
🛯 📔 Sample Manager 🛛 📥 Samp	oles 🛛 🍞 = Filtering 🛛 🔞 He	lp
A Part of Name:	7	y y
🛣 Clear Filter	Filter Displayed Samples	Filter Displayed Filter Selected Samples Samples
Filter by Typing	Sample Category Properties	Other Attributes

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:

XS 🔒 🍓 🗧				Sample Select	tor			
🐠 🧻 Sample Manager 🛛 🕹 Samp	les 🛛 🍞 🖓 Filteri	ng 🛛 🕜 He	lp					
∛ Part of Name: slag X Clear Filter	Filter Disp Sample		Filter Displayee Samples	J Filter Selecte Samples	d			
Filter by Typing Available Samples All Available Often Used Favorites	Sample Catego	ry Properties	Other /	Attributes			ſ	Selected Samples (0)
Name C C [2 items] Cement mortar CEM I with LD glag (P, 1, 1) Cement mortar CEM I with LD glag 1 (P, 1, 1) Cement mortar CEM I with LD glag 1 (P, 1, 1)		Test Type	Test Su	btype	Category	Subcategory		
		pH Dependence pH Dependence			Cementitious Materials Cementitious Materials			
G [2 items] Granulated Blast furnace Slag BFS CBP (P, 1, 1) Granulated Blast furnace Slag BFS CBP (P, 1, 2)		pH Dependence pH Dependence		Method 1313 Method 1313	Construction Construction	CEM CEM		<no samples="" selected=""></no>
٠		m				4		
								[]

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:

🖳 Material Characteristics							
Cement. concrete V	ault 1 and 4 VCO CBP (P,1,2)						
Characteristic	Information						
Full name	<unspecified></unspecified>						
Description	Strucutral concrete cylinders representative of Vault						
Test type	pH Dependence, US-EPA Method 1313						
Category	Cementitious Materials, Concrete						
Origin	Savannah River National Laboratory						
Supplier	Savannah River National Laboratory						
Lab	Unspecified						
Standard	Unspecified						
Remarks	<unspecified></unspecified>						
LIMSBo×Nr	<unspecified></unspecified>						
Measured fractions	9						
Has ANC data	True						
Total composition measured	True						
Availability measured	False						
Testtypes of material	C: Percolation, US-EPA Method 1314						
	M: Monolithic leach, US-EPA Method 1315						
	P: pH Dependence, US-EPA Method 1313						
	T: Total composition, HF acid mix						
Measured constituents	39						
· ·	• II						
Measured constituents:							
Al Be Co DIC K Mo	P Sb SO4 U						
As Ca Cr DOCLi Na B Cd Cs F Mo Ni	Pb Se Sr V Re Si Ti Zn						
Ba Cl Cu Fe Mn NO3							

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

Application menu	Cancel or Save toolbar	
Ribbon toolbar	Constituent Selector	
	Open From Species Save List Save Selection Select all as Favorites Load Selection Save Selection Available Constituents Favorites All Often Used Name Inorganic [6 items]	
Available Constituents panel	Inorganic [49 items]	Selected Constituents panel
		Database icon

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.

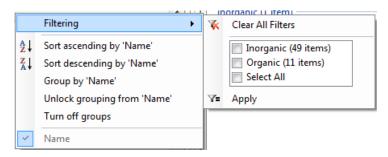
If you are done with selecting constituents, click on the small green button with the checkmark on the **Cancel or Save** toolbar. The **Constituent Selector** will close and pass the selected constituents to its caller. If you want to leave the **Constituent Selector** without using the selection, click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

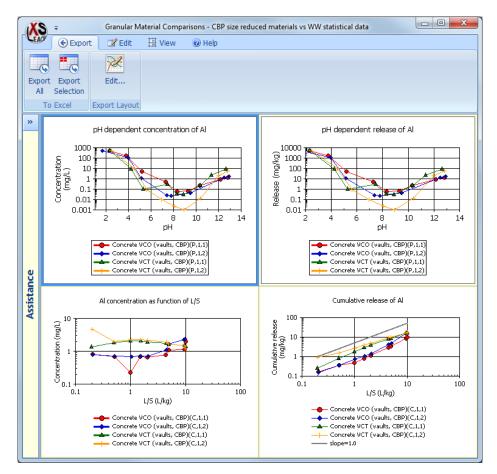
You can make a list of selected constituents your favorite list by saving the list with button **Save Selection as Favorites** on the **Favorites** tab group of ribbon tab **Constituent Manager**. If you have designated a list of constituents to be your favorite, you will always have these constituents 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 you 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:

(C	n Create	Manager	Const Const Save Sa	Į.	Lines 🖗 He	łp			Edit	licator line se	t						
L T	Constituent	or Lines	Save Ca														
1	Name	# Hor.	# Vert.	Constituent	Label	Appearance	Direction	Line Type	Line Weight	Line Color	рН	L/S (L/kg)	Time (days)	Concentration (mg/L)	Release (mg/kg)	Cum, Rel. (mg/m²)	Flux (mg/m²/sec)
l	Al	2	2	Al	MDL		Horizontal	DashDot	Thin	Black	-		-	0.001	-		
l	As	3	2	A	ML		Horizontal	Dot	Thin	Black				0.003			
l	в	3	2	Al	95%		Vertical	Continuous		Red	12.4				-	-	
l	Ba	3	2	Al	5%		Vertical	Continuous		Red	5.4		-			-	
l	Cd	3	2	As	MDL		Horizontal	DashDot	Thin	Black				0.00064			
l	Co	2	2	As	ML		Horizontal	Dot	Thin	Black			-	0.002	-	-	
l	Cr.	3	2	As	MCL or DWEL		Horizontal	Dot	Medium	Blue	-		-	0.01	-		
l	Default	5	2	As	95%		Vertical	Continuous		Red	12.4						
l	Hg	3	2	As	5%		Vertical	Continuous		Red	5.4		-	-	-	-	
l	Mo	3	2	B	MDL		Horizontal	DashDot	Thin	Black	-		-	0.001			
l	Pb	3	2	в	ML		Horizontal		Thin	Black				0.003			
l	Sb	3	2	в	DWEL		Horizontal	Dot	Medium	Blue			-	7	-	-	
l	Se	3	2	в	95%		Vertical	Continuous	Thin	Red	12.4						
l	п	3	2	в	5%		Vertical	Continuous		Red	5.4						
l			-	Ba	MDL		Horizontal	DashDot	Thin	Black		-	-	0.00057	-	-	
l				Ba	ML		Horizontal	Dot	Thin	Black		-		0.0018			
				Ba	MOL		Horizontal	Dot	Medium	Blue				2			
l				Ba	95%		Vertical	Continuous	Thin	Red	12.4	-		-	-	-	
1				Ba	5%		Vertical	Continuou	Thin	Red	5.4	-		-	-	-	
l	•			ba	MDL		Horizontal	DashDot	thin	Black				0.00017			
	Dpene			Const	ituents	nanel	1 1		es pan							Data	Dase ico

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.

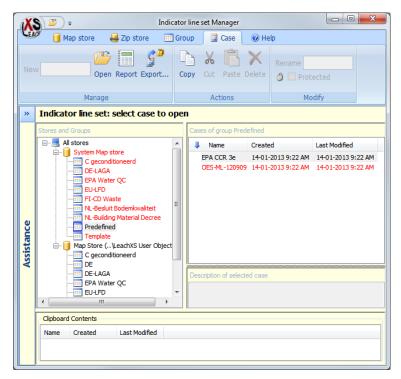
Loading and saving indicator lines

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:

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

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

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

Cumulative Release (mg/m²)A cumulative release.Flux (mg/m²/sec)A flux.

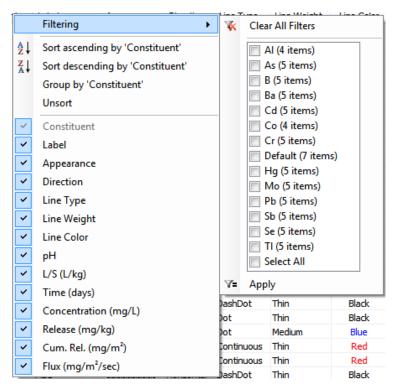
One of first three fields is usually used for vertical lines, since these quantities usually are plotted along the x-axis. The other fields are common for horizontal lines.

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	pН	L/S (L/kg)	Time (
AI [4 items	;]								
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	-	-	
As [5 item:	s]								
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 [5 items]									
в	95%		Vertical	Continuous	Thin	Red	12.4	-	
в	5%		Vertical	Continuous	Thin	Red	5.4	-	
в	DWEL		Horizontal	Dot	Medium	Blue	-	-	
в	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 (m
Horizo	ntal [5 items]									-
Al	ML		Horizontal	Dot	Thin	Black	-	-	-	0
Al	MDL		Horizontal	DashDot	Thin	Black	-	-	-	0
Cr	MCL		Horizontal	Dot	Medium	Blue	-	-	-	
Cr	ML		Horizontal	Dot	Thin	Black	-	-	-	0.0
Cr	MDL		Horizontal	DashDot	Thin	Black	-	-	-	0.
Vertica	l [4 items]									
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	-	-	
<			III							

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:

(S) 🥝 🗞)	Ŧ		
🚧 📝 Edit	🕜 Help		
Line Label			
Label	I		(multiple values)
Line Appearence			
Line Direction	Horizontal	•	
Line Type		•	(multiple values)
Line Weight		•	(multiple values)
Line Color		Change	(multiple values)
Appearance			(multiple values)
Horizontal Line Va	lues		
Concentration	- mg	J/L	(multiple values)
Release	- mg	j/kg	
Cum. Release	- kg	/m²	
Flux	- kg	/m²/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:

EAC	📔 Case Manager 🛛 💊 Constitu	ients	🗛 Line	es 🔞 He	lp						
Add											
»	Constituents	Lin	es								_
	Name # Hor. # Vert.	Co	nstituent	Label	Appearance	Direction	Line Type	Line Weight	Line Color	pН	L/S
	Default Lines 3 0	De	fault Lines	unnamed2		Horizontal	Continuous	Thin	Red	-	
		De	fault Lines	unnamed1		Horizontal	Continuous	Thin	Red	-	
		De	fault Lines	unnamed		Horizontal	Continuous	Thin	Red	-	

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

LEA	🖉 🧻 Case Mai	nager 🤇	👌 Constitu	ents	🗛 Lines	🕜 Hel	р						
9			•	<i>/</i> /\/									
Ad	d Remove Rena		et Lines Ad Default Lir										
	Cons	stituents											
»	Constituents			-Li	nes								
	Name	# Hor.	# Vert.	0	Constituent	Label	Appearance	Direction	Line Type	Line Weight	Line Color	pН	L/S (L/k
	Default Lines	1	2	C	efault Lines	Low		Vertical	Continuous	Medium	Red	4	
				0	efault Lines	High		Vertical	Continuous	Medium	Red	11	
				0	efault Lines	Safe		Horizontal	Dot	Medium	Green	-	

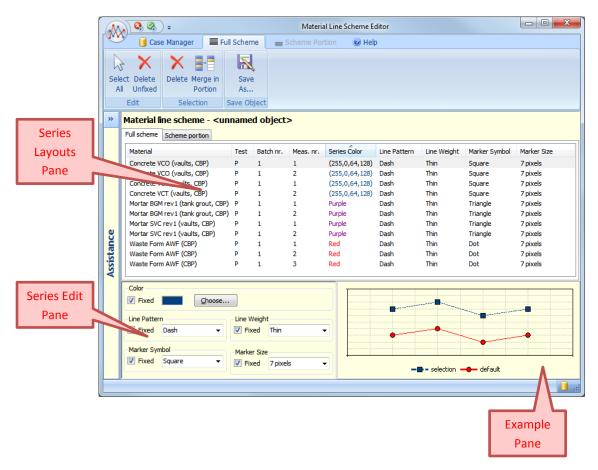
If you add constituents, every constituent will get this set of lines. Add extra constituents with the **Constituent Selector** by pressing the **Add** button on tab group **Constituents** of ribbon tab **Constituents**. All you have to do is filling in concentrations for every horizontal line.

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.

<u>Pi</u> rectives <u>E</u> dit			
Directives	Constituents		
System User defined	Name	Upper	
All directives	As	2	
C geconditioneerd	Ba	100	
DE-LAGA ■ EU-LFD	Br	34	
H FI-CD Waste	Cd	0.06	=
II-CD waste II-CD waste II-NL-BBK	Cl	8800	
Closed Application	Co	2.4	
Granular	Cr	7	
Open Application	Cu	10	
	F	1500	
	Hg	0.08	
	Mo	15	
	Ni	2.1	
Directive description	Pb	8.3	
Building materials decree 2007, unclosed storageBuilding materials decree 2007, closed storage			
Copy Rename Remove Add		Remove	A <u>d</u> d

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.

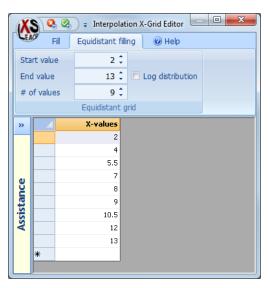
If you want to create statistical data sets from existing samples, the sample series all need to be brought to a common set of x-values in order to be properly evaluated. The **Interpolation Grid Editor** helps you to define such a set.

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.

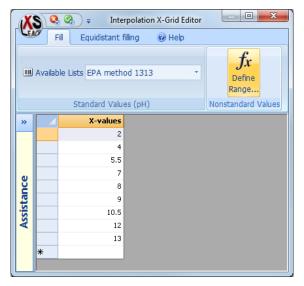


You can add a value by typing it in the row starting with an asterisk. Delete a value by selecting the row to be deleted and press the **Delete** button of your keyboard. To edit a value, double-click it and type the new value.

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 uniformely 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.

	🗧 🗸 Grid Interpolat	ion Lists Manager
LEA	Lists 🕜 Help	
Nev List.		
»	I Name	X-Axis Values
	pH Draft EPA method 1313 L/S	2, 4, 5.5, 7, 8, 9, 10.5, 12, 13
	CEN EN 12457 Part 3	2, 8
	Draft EPA method 1314 Draft EPA method 1316	0.2, 0.5, 1, 1.5, 2, 4.5, 5, 9.5, 10
Assistance	ISO/TS 21268-3	0.5, 1, 2, 5, 10 0.1, 0.2, 0.5, 1, 2, 5, 10
a l	NEN 7343	0.1, 0.2, 0.5, 1, 2, 5, 10
sis	NEN 7373	0.1, 0.2, 0.5, 1, 2, 5, 10
I X	NVN 7344	0.1, 0.2, 0.5, 1, 2, 5, 10
	PrEN 14405	0.1, 0.2, 0.5, 1, 2, 5, 10
	Time	
	CEN TC 292 Monolith	0.08, 1, 2.25, 8, 14, 15, 28, 36
	Draft EPA method 1315	0.08, 1, 2, 7, 14, 28, 42, 49, 63
	NEN 7345	0.25, 1, 2.25, 4, 9, 16, 36, 64

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.

List Generator					
Create a list of	X-values values				
🔘 Linear,	9 steps,	ending at	20		
 Factorial, 	8 steps,	ending at	20		
	with	a factor of	1.50		
Manually	this semicolon- o	r space-sepa	arated list:		
	0.406; 1.02; 1.9	3; 3.3; 5.35	; 8.44; 13.1; 20		
Resulting va					Refresh
0.406; 1.02;	1.93; 3.3; 5.35; 8	.44; 13.1; 2	0	*	
				Ŧ	
	·			 ОК	Cancel

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
[Install location]	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.
[Application data]	C:\Users\ <username>\AppData\Roaming\LeachXS Lite</username>
[Local Application data]	C:\Users\ <username>\AppData\Local\ECN_TSC</username>
[User data]	C:\Users\ <username>\Documents\LeachXS User Objects</username>
[Template location]	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 your 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:

Number of points.
Index of point (between 1 and N).
<i>ith</i> L/S value.
ln(<i>C_i</i>).
Concentration of <i>i</i> th point.
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: $Sig_i = 1$ for i between 1 and N. Standard weighting: $Siq_i = 0.05 * Y_i$ Favor low/midrange/high L/S values: First, create 3 XW values: $XW_1 = In(X_1)$ $XW_3 = In(X_N)$ $XW_2 = 0.5 * (XW_1 + XW_3)$ Now, create 3 YW values, depending on the range to favor: Favor low L/S values: $YW_1 = 1$, $YW_2 = SQRT(10)$, $YW_3 = 10$. Favor midrange L/S values: $YW_1 = 10, YW_2 = 1, YW_3 = 10.$ Favor high L/S values: $YW_1 = 10, YW_2 = SQRT(10), YW_3 = 1.$

Then, a polynomial of degree 2 is fitted through the three points (XW_i, YW_i) . The uncertainties are constructed by:

Sig_i = Polynomial(In(X_i))