LeachXS

User Manual

Energy research centre of The Netherlands
Vanderbilt University, Nashville
DHI Water & Environment, Denmark

This manual was produced using *ComponentOne Doc-To-Help.*™

Contents

Leaching eXpert System

Welcome screen

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.

Main window

The main window gives access to all LeachXS functions. This window has:

- A menu bar, containing a number of general actions. The main menu is explained in section: The main menu bar on page 55.
- A panel displaying the currently selected LeachXS database file specification. Initially, the selected database is the one that is shipped with your version of LeachXS. If you have another LeachXS database, you can select it by using the file menu, explained at Select database… on page 55.
- A panel with a tree-like layout. This panel behaves like a tree-like menu and contains all LeachXS features, grouped by usage. Click on the appropriate entry to continue. A new window will appear, allowing you to choose the parameters to use for that action. Note that your chosen action will be grayed in the main menu, indicating that the parameter window for that action is open. Other actions will still be selectable, allowing you to work on more actions simultaneously.

The panel has the following categorized actions (italicized entries are not implemented in your version of LeachXS):

Leaching data - analysis, presentation and regulatory comparisons.

§ Comparison of different materials and samples for selected constituents.
  - o Granular materials (see Comparison of Granular materials on page 6).
  - o Monolithic materials (see Comparison of Monolithic materials on page 4).

§ Comparison of different constituents from a selected material.
  - o Granular material (see Comparison of constituents (Granular material) on page 12).
  - o Monolithic material (see Comparison of constituents (Monolithic material) on page 10).

- Field monitoring data (time series, full-scale and pilot-scale).
  - Landfills (see Landfill monitoring on page 14).
  - *Road construction projects.*
  - *Ponds and impoundments.*

Acid/base neutralization capacity (ANC/BNC).

  - Acid/base neutralization capacity comparisons (see Acid/base neutralization capacity comparisons on page 17).
  - ANC/BNC calculator (see ANC/BNC calculator on page 17).

L/S to time-scale conversion (see **L/S to timescale wizard on page 19).**

Chemical speciation, equilibrium and transport.

- Chemical speciation finder (see Chemical speciation finder on page 21).
- Leaching prediction wizards (behavior in lab tests).
  - Single materials.
    - pH-dependent (equilibrium) cases (see Leaching prediction, single pH dependent materials on page 24).
    - Percolation cases (see Leaching prediction, single Percolation materials on page 29).
    - *Monolithic cases.*
  - Mixtures of materials.
    - pH-dependent behavior (see Leaching prediction, mixtures of materials on page 35).
    - *Percolation (column flow cases).*
    - *Diffusion (monolith and compacted granular tank leaching cases).*
  - *Scenario calculations (estimating behavior under field conditions).*
    - *Source terms.*
      - *Landfills.*
      - *Road construction.*
    - *Assessment of impact on groundwater.*
      - *Granular and Monolithic materials*

Selection and Use of Methods for Leaching Assessment.

- *Definition of Assessment Goals and Objectives.*
- *Test Methods, Chemical Analyses and Quality Control.*
- *Data Presentation and Evaluation.*
- *Source Term Modeling and Simulation.*

Quality control and compliance monitoring.

Comparison of Monolithic materials

The comparison provided here for the leaching behavior of monolithic materials and compacted granular materials allows selection of both pH dependence leaching test or related information and dynamic leach (tank leaching) test data. The pH dependence test data on the crushed material provide insight in the chemical speciation and pH sensitivity of the monolithic material, whereas the dynamic leach test provides the time dependent release under specified conditions. The four main graphs provided are: pH dependence, concentration in the leachate as function of time, release in mg/m^2 as a function of time and pH in the test as a function of time. Other test data consistent with the general principle of leachant renewal cycles can be selected for comparison. The graphs are generated by element.

You can save all choices you make in this dialog and retrieve them at a later time. Saving and loading choices are disclosed in the Regulations menu entry. See section Regulations editor on page 51 for details. The name of the loaded regulation is displayed in the top pane of the window. The color of the regulation name turns to red if you make changes in the dialog, indicating that there are unsaved changes. If you move the mouse over the regulation name, you'll see a description of the regulation, if you defined one.

Selection of pH dependent materials

Edit the list of the pH dependent materials in this pane. All materials you have selected will appear in a single graph, where the concentration in mg/l of the constituent you have selected in the Selected constituent pane is displayed as a function of pH.

The foreground color of the material name indicates if the constituent you have selected in the Selected constituent pane is measured. Black colored materials contain the constituent, whereas gray colored materials do not.

Use the Select button to bring up the *Select material dialog*, assisting you in the selection of materials. The Clear button removes all materials from the selection list. The Delete button removes those materials you have selected in the selection list.

You can view statistics of the selected materials by pressing the Statistics… button. See section *Statistics* on page 54 for details.

Graphing options

If you have selected any monolithic materials in the Selected monolithic materials pane, you can include them in the pH dependence graph by checking the Include monolithic materials in graph box.

If own pH values of the materials you selected are known or can be calculated from ANC/BNC data, you can check the Include Own pH option to make them visible in the graphs. They will appear as an asterisk in every series.

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.

If you want to display extra guidance lines in your graphs indicating pH or concentration thresholds, you can check the Show Indicator Lines option. For an explanation of indicator lines and how you can define them, see section Indicator lines editor on page 51.

Selection of monolithic materials

Edit the list of the monolithic materials in this pane. All materials you have selected will appear in the.

The foreground color of the material name indicates if the constituent you have selected in the Selected constituent pane is measured. Black colored materials contain the constituent, whereas gray colored materials do not.

Use the Select button to bring up the Select material dialog, assisting you in the selection of materials. The Clear button removes all materials from the selection list. The Delete button removes those materials you have selected in the selection list.

You can view statistics of the selected materials by pressing the Statistics… button. See section *Statistics* on page 54 for details.

Graphing options

Select the desired graphical representation(s) of the monolithic leaching test results in this pane.

The Show time versus concentration in mg/l option produces a graph of the test time (days) versus the leached concentration of the selected constituent

The Show time versus release option produces a graph of the test time (days) versus the cumulative emission in mg/m2 or mg/m2/sec of the selected constituent.

The Show time versus pH option produces a graph of the test time (days) versus the measured pH of the eluate.

Selection of constituent

Use this pane to select your constituent of interest. Use the Select button to bring up the Select constituent dialog, assisting you in selecting a constituent. Use the Clear button to remove the constituent you selected.

Adding directive information to your results

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 for pH dependent materials and mg/m^2 for monolithic materials. Besides choosing from a list of predefined directives, you can create your own directives. Check the appropriate checkbox(es) if you want to use and display directive criteria in your graphs.

Note that a button is enabled only if there are any directives on the selected constituent present in the database.

The Select buttons will enable you to choose the appropriate directives. See the Directive selection dialog on page 44 for details.

For pH dependent materials, define the pH range the directive is imposed on by filling in the Lower pH limit and the Upper pH limit text boxes.

Defining Indicator lines

If you want to display extra guidance lines in your graphs indicating pH or concentration thresholds, you can press the Select button to open a dialog where you can select, modify or create the lines. For an explanation of indicator lines and how you can define them, see section Indicator lines editor on page 51.

Show button

Use this button to display the results from the selected materials. A Graph window on page 48 will appear with all graphs you selected.

Bulk export button

If you want to repeatedly export your data for a number of constituents, but keeping all the other selections and options the same, this button serves as a shortcut to do this in one operation. When pressing this button, the Select constituent dialog will appear where you can select a number of constituents you want to export. Instead of displaying graph windows with results for every constituent, you will be directed to the Export dialog, enabling you to export all constituents in one action.

Note that this operation can be time consuming if you'll export a lot of constituents at once.

Comparison of Granular materials

The comparison provided here for the leaching behavior of granular materials allows selection of both pH dependence leaching test or related information and percolation test data. The pH dependence test data on the granular material provide insight in the chemical speciation and pH sensitivity of the material, whereas the percolation test provides a measure of the time dependent release under specified conditions. The four main graphs provided are: pH dependence, concentration in the leachate as function of liquid to solid ratio (L/S liter/kg dry matter), release in mg/kg dry matter as a function of L/S and pH in the test as a function of L/S. Batch test data at a specified L/S and any other type of percolation data including field data from lysimeters and field studies can be selected for comparison, provided a measure of the L/S can be specified. The graphs are generated by element.

You can save all choices you make in this dialog and retrieve them at a later time. Saving and loading choices are disclosed in the Regulations menu entry. See Regulations editor on page 51 for details. The name of the loaded regulation is displayed in the top pane of the window. The color of the regulation name turns to red if you make changes in the dialog, indicating that there are unsaved changes. If you move the mouse over the regulation name, you'll see a description of the regulation, if you defined one.

Selection of pH dependent materials

Edit the list of the pH dependent materials in this pane. All materials you have selected will appear in a single graph, where the emission in mg/kg of the constituent you have selected in the Selected constituent pane is displayed as a function of pH.

The foreground color of the material name indicates if the constituent you have selected in the Selected constituent pane is measured. Black colored materials contain the constituent, whereas gray colored materials do not.

Use the Select button to bring up the *Select material dialog*, assisting you in the selection of materials. The Clear button removes all materials from the selection list. The Delete button removes those materials you have selected in the selection list.

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.

If own pH values of the materials you selected are known, or can be calculated from ANC/BNC data, you can check the Include Own pH option to make them visible in the graphs. They will appear as an asterisk in every series.

If you want to display extra guidance lines in your graphs indicating pH or concentration thresholds, you can check the Show Indicator Lines option. For an explanation of indicator lines and how you can define them, see section Indicator lines editor on page 51.

You can view statistics of the selected materials by pressing the Statistics… button. See section *Statistics* on page 54 for details.

Display units

You can select the unit of measurement or graphed release in the pH dependent graph. The unit can be in mg/kg or in mg/l.

Composition and availability

Select optional results from total composition and availability for the selected samples if they are available. These results will be plotted as lines in the pH dependent leaching test results.

If the Show total composition checkbox is checked, the total composition (mg/kg dry matter) of the selected samples will be plotted (if the total composition is measured) in the pH versus emission (mg/kg dry matter) graph after clicking the Show button.

If the Show availability checkbox is checked, the availability (mg/kg dry matter) of the selected samples will be plotted (if the availability is measured) in the pH versus emission (mg/kg dry matter) graph after clicking the Show button.

The Details… button reveals detailed information about total composition and availability data of the selected materials. For more information, see the *Total Composition and availability window on page* ***44***.

Selection of percolated materials

Edit the list of the percolation materials in this pane. All materials you have selected will appear in the graphs you have checked in the Graphing options pane. The foreground color of the material name indicates if the constituent you have selected

in the Selected constituent pane is measured. Black colored materials contain the constituent, whereas gray colored materials do not.

Use the Select button to bring up the *Select material dialog*, assisting you in the selection of materials. The Clear button removes all materials from the selection list. The Delete button removes those materials you have selected in the selection list.

You can view statistics of the selected materials by pressing the Statistics… button. See section *Statistics* on page 54 for details.

Graphing options

Select the desired graphical representation(s) of the granular leaching test results for percolated materials in this pane.

Option L/S versus emission produces a graph of the Liquid to solid ratio (L/S) versus the cumulative emission (mg/kg dry matter) of the selected constituent in percolated materials.

Option L/S versus concentration produces a graph of the Liquid to solid ratio (L/S) versus the measured concentrations (mg/l) of the selected constituent in percolated materials.

Option L/S versus pH produces a graph of the Liquid to solid ratio (L/S) versus the measured pH of the eluate in percolated materials.

Curve fitting and weight

Fitted E values option.

Using a simple CSTR model the percolation data are fitted using a least squares fitting routine. Here the cumulative release data are given at the sampled L/S data points. The coefficients are passed on to the excel worksheet upon saving the data. The fit function used is:

$$E_{L/S} = \frac{C_0(1-e^{-\kappa(L/S)})}{\kappa}$$

where L/S is in l/kg and $E_{L/S}$ in mg/kg.

Fitted CSTR values option.

Using a simple CSTR model the percolation data are fitted using a least squares fitting routine. Here 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.

$$CSTR_{L/S} = C_0 e^{-\kappa(L/S)}$$

where L/S is in l/kg and $CSTR_{L/S}$ in mg/l.

The emphasis of the fitting procedure can be placed on the low L/S, intermediate range and high L/S conditions depending on the most relevant conditions for further data evaluation. Standard means no special weight to any of the data points. Use the Weights combo box to select the desired weight:

Weight	Meaning
None	All points have equal weight.
Standard	All points are weighted proportional to their concentration.

Favor low range	The lowest L/S value gets a weight of 10, the highest a weight of 1, the middle one a weight of $10^{1/2}$. Other points get their weight by evaluating a spline, constructed from these three points.
Favor midrange	The lowest L/S value gets a weight of 10, the highest a weight of 10, the middle one a weight of 1. Other points get their weight by evaluating a spline, constructed from these three points.
Favor high range	The lowest L/S value gets a weight of 1, the highest a weight of 10, the middle one a weight of $10^{1/2}$. Other points get their weight by evaluating a spline, constructed from these three points.

Selection of constituent

Use this pane to select your constituent of interest. Use the Select button to bring up the Select constituent dialog, assisting you in selecting a constituent. Use the Clear button to remove the constituent you selected.

Adding directive information to your results

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 the Directive checkbox if you want to use and display directive criteria in your graphs.

Note that this button is enabled only if there are any directives on the selected constituent present in the database.

The Select button will enable you to choose an appropriate directive. See the Directive selection dialog *on page **44*** for details.

Define the pH range the directive is imposed on by filling in the Lower pH limit and the Upper pH limit text boxes.

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.

Defining Indicator lines

If you want to display extra guidance lines in your graphs indicating pH or concentration thresholds, you can press the Select button to open a dialog where you can select, modify or create the lines. For an explanation of indicator lines and how you can define them, see section Indicator lines editor on page 51.

Show button

Use this button to display the results from the selected materials. A *Graph window* will appear with all graphs you selected.

Bulk export button

If you want to repeatedly export your data for a number of constituents, but keeping all the other selections and options the same, this button serves as a shortcut to do this in one operation. When pressing this button, the Select constituent dialog will appear where you can select a number of constituents you want to export. Instead of displaying graph windows with results for every constituent, you will be directed to the Export dialog, enabling you to export all constituents in one action.

Note that this operation can be time consuming if you'll export a lot of constituents at once.

Comparison of constituents (Monolithic material)

A comparison is provided here for the leaching behavior of selected constituents from a monolithic material or a compacted granular material. The selection of both pH dependence leaching test or related information and dynamic leach (tank leaching) test data is possible. The pH dependence test data on the crushed material provide insight in the chemical speciation and pH sensitivity of the selected constituents, whereas the dynamic leach test provides the time dependent release of the selected constituents under specified conditions. The four main graphs provided are: pH dependence, concentration in the leachate as function of time, release in mg/m2 as a function of time and pH in the test as a function of time. Other test data consistent with the general principle of leachant renewal cycles can be selected for comparison.

You can save all choices you make in this dialog and retrieve them at a later time. Saving and loading choices are disclosed in the Regulations menu entry. See Regulations editor on page 51 for details. The name of the loaded regulation is displayed in the top pane of the window. The color of the regulation name turns to red if you make changes in the dialog, indicating that there are unsaved changes. If you move the mouse over the regulation name, you'll see a description of the regulation, if you defined one.

Selection of constituents

This pane will help you in selecting the inorganic and organic to be viewed in your results.

The foreground color of any constituent name indicates if any materials you have selected in the other two panes contain measurements of that constituent. Black colored constituents are measured in at least one of your chosen materials, whereas gray colored constituents are not.

Use the Select button to bring up the *Select constituent dialog*, assisting you in the selection of constituents. The Clear button removes all constituents from the selection list. The Delete button removes those constituents you have selected in the selection list.

Selection of pH dependent material

You select a pH dependent material in this pane. All measured constituents of the material you have selected in the Selected constituents pane will appear in a single graph, where the concentration is displayed in mg/l as a function of pH.

Use the Select button to bring up the Select material dialog, assisting you in the selection of the material. The Clear button clears your selection. No graph will be made in this case.

If own pH values of the materials you selected are known, or can be calculated from ANC/BNC data, you can check the Include Own pH option to make them visible in the graphs. They will appear as an asterisk in every series.

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.

Selection of monolithic material

You select a monolithic material in this pane. All measured constituents of the material you have selected in the Selected Constituents pane will appear in the graphs you selected in the Graphing options pane.

Use the Select button to bring up the *Select material dialog*, assisting you in the selection of the material. The Clear button clears your selection. No graph will be made in this case.

Graphing options

Select the desired graphical representation(s) of the monolithic leaching test results in this pane.

The Show time versus concentration in mg/l option produces a graph of the test time (days) versus the leached concentration of the selected constituents.

The Show time versus release option produces a graph of the test time (days) versus the cumulative release of the selected constituents. The release can be dimensioned as mg/m2 or as mg/m2/sec.

The Show time versus pH option produces a graph of the test time (days) versus the measured pH of the eluate.

Show button

Use this button to display the results from the selected constituents. A *Graph window* will appear with all graphs you selected.

Comparison of constituents (Granular material)

A comparison is provided here for the leaching behavior of selected constituents from a granular material. The selection of both pH dependence leaching test or related information and percolation test data is possible. The pH dependence test data on the granular material provide insight in the chemical speciation and pH sensitivity of the selected constituents, whereas the percolation test provides a measure of the time dependent release of selected constituents under specified conditions. The four main graphs provided are: pH dependence, concentration in the leachate as function of liquid to solid ratio (L/S liter/kg dry matter), release in mg/kg as a function of L/S and pH in the test as a function of L/S. Batch test data at a specified L/S and any other type of percolation data including field data from lysimeters and field studies can be selected for comparison, provided a measure of the L/S can be specified.

You can save all choices you make in this dialog and retrieve them at a later time. Saving and loading choices are disclosed in the Regulations menu entry. See Regulations editor on page 51 for details. The name of the loaded regulation is displayed in the top pane of the window. The color of the regulation name turns to red if you make changes in the dialog, indicating that there are unsaved changes. If you move the mouse over the regulation name, you'll see a description of the regulation, if you defined one.

Selection of constituents

This pane will help you in selecting the inorganic parameters and organic parameters to be viewed in your results.

The foreground color of any constituent name indicates if any materials you have selected in the other two panes contain measurements of that constituent. Black colored constituents are measured in at least one of your chosen materials, whereas gray colored constituents are not.

Use the Select button to bring up the *Select constituent dialog*, assisting you in the selection of constituents. The Clear button removes all constituents from the selection list. The Delete button removes those constituents you have selected in the selection list.

Selection of pH dependent material

You select a pH dependent material in this pane. All measured constituents of the material you have selected in the Selected constituents pane will appear in a single graph, where the emission is displayed in mg/kg as a function of pH.

Use the Select button to bring up the *Select material dialog*, assisting you in the selection of the material. The Clear button clears your selection. No graph will be made in this case.

If own pH values of the materials you selected are known, or can be calculated from ANC/BNC data, you can check the Include Own pH option to make them visible in the graphs. They will appear as an asterisk in every series.

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.

Display units

You can select the unit of measurement or graphed release in the pH dependent graph. The unit can be in mg/kg or in mg/l.

Composition and availability

Select optional results from total composition and availability for the selected material and constituents if they are available. These results will be plotted as lines in the pH dependent leaching test results.

If the Show total composition checkbox is checked, the total composition (mg/kg dry matter) of the selected samples will be plotted (if the total composition is measured) in the pH versus emission (mg/kg dry matter) graph after clicking the Show button.

If the Show availability checkbox is checked, the availability (mg/kg dry matter) of the selected samples will be plotted (if the availability is measured) in the pH versus emission (mg/kg dry matter) graph after clicking the Show button.

The Details… button reveals detailed information about total composition and availability data of the selected materials. For more information, see the *Total Composition and availability window on page **44***.

Selection of percolated material

You select a percolated (column test type) material in this pane. All measured constituents of the material you have selected in the Selected constituents pane will appear in the graphs you selected in the Graphing options pane.

Use the Select button to bring up the Select material dialog, assisting you in the selection of the material. The Clear button clears your selection. No graphs will be made in this case.

Graphing options

Select the desired graphical representation(s) of the granular leaching test results for the selected measured constituents of the selected percolated material in this pane.

Option L/S versus emission produces a graph of the Liquid to solid ratio (L/S) versus the cumulative emission (mg/kg dry matter) of the selected constituents in the percolated material.

Option L/S versus concentration produces a graph of the Liquid to solid ratio (L/S) versus the measured concentrations (mg/l) of the selected constituents in the percolated material.

Option L/S versus pH produces a graph of the Liquid to solid ratio (L/S) versus the measured pH of the eluate in the percolated material.

Curve fitting and weights

Fitted E values option.

Using a simple CSTR model the percolation data are fitted using a least squares fitting routine. Here the cumulative release data are given at the sampled L/S data points. The coefficients are passed on to the excel worksheet upon saving the data. The fit function used is:

$$E_{L/S} = \frac{C_0(1-e^{-\kappa(L/S)})}{\kappa}$$

where L/S is in l/kg and $E_{L/S}$ in mg/kg.

Fitted CSTR values option.

Using a simple CSTR model the percolation data are fitted using a least squares fitting routine. Here 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.

$$CSTR_{L/S} = C_0 e^{-\kappa(L/S)}$$

where L/S is in l/kg and $CSTR_{L/S}$ in mg/l.

The emphasis of the fitting procedure can be placed on the low L/S, intermediate range and high L/S conditions depending on the most relevant conditions for further data evaluation. Standard means no special weight to any of the data points. Use the Weights combo box to select the desired weight:

Weight	Meaning
None	All points have equal weight.
Standard	All points are weighted proportional to their concentration.
Favor low range	The lowest L/S value gets a weight of 10, the highest a weight of 1, the middle one a weight of $10^{1/2}$. Other points get their weight by evaluating a spline, constructed from these three points.
Favor midrange	The lowest L/S value gets a weight of 10, the highest a weight of 10, the middle one a weight of 1. Other points get their weight by evaluating a spline, constructed from these three points.
Favor high range	The lowest L/S value gets a weight of 1, the highest a weight of 10, the middle one a weight of $10^{1/2}$. Other points get their weight by evaluating a spline, constructed from these three points.

Show button

Use this button to display the results from the selected constituents. A *Graph window* will appear with all graphs you selected.

Landfill monitoring

For evaluation of landfill leachate monitoring data, data are displayed as a function of pH to the extent pH dependence data are available for the landfilled material and

as a function of absolute or relative time. This allows visualization of trends in leachate quality with time. This is particularly useful for parameters that change significantly with time such as COD, DOC and NH4 in organic rich waste.

You can save all choices you make in this dialog and retrieve them at a later time. Saving and loading choices are disclosed in the Regulations menu entry. See Regulations editor on page 51 for details. The name of the loaded regulation is displayed in the top pane of the window. The color of the regulation name turns to red if you make changes in the dialog, indicating that there are unsaved changes. If you move the mouse over the regulation name, you'll see a description of the regulation, if you defined one.

Selection of pH dependent materials

Edit the list of the pH dependent materials in this pane. All materials you have selected will appear in a single graph, where the concentration in mg/l of the constituent you have selected in the Selected constituent pane is displayed as a function of pH.

The foreground color of the material name indicates if the constituent you have selected in the Selected constituent pane is measured. Black colored materials contain the constituent, whereas gray colored materials do not.

Use the Select button to bring up the *Select material dialog*, assisting you in the selection of materials. The Clear button removes all materials from the selection list. The Delete button removes those materials you have selected in the selection list.

You can view statistics of the selected materials by pressing the Statistics… button. See section *Statistics* on page 54 for details.

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.

If own pH values of the materials you selected are known, or can be calculated from ANC/BNC data, you can check the Include Own pH option to make them visible in the graphs. They will appear as an asterisk in every series.

If you want to display extra guidance lines in your graphs indicating pH or concentration thresholds, you can check the Show Indicator Lines option. For an explanation of indicator lines and how you can define them, see section Indicator lines editor.

Selection of landfill materials

Edit the list of the landfill materials in this pane. All materials you have selected will appear in a single graph, where the concentration in mg/l of the constituent you have selected in the Selected constituent pane is displayed as a function of time.

The foreground color of the material name indicates if the constituent you have selected in the Selected constituent pane is measured. Black colored materials contain the constituent, whereas gray colored materials do not.

Use the Select button to bring up the *Select material dialog*, assisting you in the selection of materials. The Clear button removes all materials from the selection list. The Delete button removes those materials you have selected in the selection list.

You can view statistics of the selected materials by pressing the Statistics… button. See section *Statistics* on page 54 for details.

Graphing options

In this pane, some aspects of the landfill graph can be changed. Use the Date graphing option to choose between the display of times in absolute dates or in years after start, the first fraction being year 0.

Use the Concentration graphing option to specify a linear or logarithmic concentration axis.

Selection of constituent

Use this pane to select your constituent of interest. Use the Select button to bring up the *Select constituent dialog*, assisting you in selecting a constituent. Use the Clear button to remove the constituent you selected.

Defining Indicator lines

If you want to display extra guidance lines in your graphs indicating pH or concentration thresholds, you can press the Select button to open a dialog where you can select, modify or create the lines. For an explanation of indicator lines and how you can define them, see section Indicator lines editor on page 51.

Show button

Pressing this button will show the results from the selected materials and measured constituents in a *Graph window*. The results are presented in accordance with the graphing options you have chosen.

Bulk export button

If you want to repeatedly export your data for a number of constituents, but keeping all the other selections and options the same, this button serves as a shortcut to do this in one operation. When pressing this button, the Select constituent dialog on page 42 will appear where you can select a number of constituents you want to export. Instead of displaying graph windows with results for every constituent, you will be directed to the Export dialog, enabling you to export all constituents in one action.

Note that this operation can be time consuming if you'll export a lot of constituents at once.

Acid/Base neutralization capacity

The acid/base neutralization capacity as obtained from a pH dependence test according to TS 14429 or TS 14997) or ANC test (ANC or TS 15364) provides the

resistance of a material to pH change either by direct acid or base addition or by exposure to external circumstances (e.g. carbonation of alkaline materials, sulphide oxidation of sulphide bearing materials). The results are expressed in mol/kg dry matter. The ANC/BNC as function of pH allows calculation of the acid or base of certain strength needed to change the pH of a material from one pH to another or to calculate the amount of acid or base it takes to reach a certain user defined-end point. External influences can be quantified in an amount of acid and base neutralizing capacity, which can then be matched with the ANC/BNC information to assess long-term changes in material pH.

There are two wizard involving the calculation and comparison of acid/base neutralization capacities:

- Acid/base neutralization capacity comparisons.
- ANC/BNC calculator.

Acid/base neutralization capacity comparisons

With this option the ANC curves of several samples are compared in a graph. The graph and the individual ANC data can be exported to an Excel spreadsheet. This option can be used when several batches of a material are to be examined or to compare the ANC capacity of several materials.

Select materials

In this first step of the wizard, you select the material(s) you want to do ANC/BNC calculations for. Press the Select button to select the materials in the *Select material dialog*. You may find the Material info window useful here to check if your chosen materials have measured ANC/BNC data. Pressing the Clear button will remove all materials from the selection list.

View materials

If you press the Next button in the wizard, the ANC/BNC data of the selected materials are displayed in a graph. See section Translating, scaling and zooming a chart on page 48 for graph display options.

Export results

If you press the Next button, you can export the graphed data to an Excel workbook for further inspection. See section Export dialog on page 44 for details regarding the export to an Excel workbook.

ANC/BNC calculator

ANC calculations can be used to calculate the amount of acid or base needed to shift the pH from a starting value to a specified endpoint or to calculate a pH shift of a material given a known added amount of acid or base to the material.

Select materials

In this first step of the wizard, you select the material(s) you want to do ANC/BNC calculations for. Press the Select button to select the materials in the *Select material dialog*. You may find the Material info window useful here to check if your chosen materials have measured ANC/BNC data. Pressing the Clear button will remove all materials from the selection list.

Calculation mode

If you have chosen for the Perform calculations option, this is the next step of the wizard. You can choose to:

- **Acid or Base additions**

  ANC calculations can be used to calculate the amount of acid or base needed to shift the pH from a starting value to a specified endpoint. These calculations can be used in preparation of pH dependent leaching tests of materials that have been studied earlier or to study the differences in acid/base amounts between materials needed to reach a specified pH value.

- **Final pH**

  Another option is to calculate a pH shift of a material given a known added amount of acid or base to the material. This option is used to estimate the pH shift in application scenarios of the chosen materials. For example, alkaline materials will tend to neutralize due to carbonation (CO_2 uptake from the air) when the material is in contact with air. The amount of CO_2 can be converted to equivalents acid in order to calculate the effect of carbonation at specific times.

Calculator for Acid or Base additions

This step of the wizard let you calculate the amount of acid or base to add if you want to change the pH from a given start value to an end value.

First, select a material from the list on top of the window, if you had selected more materials in the first step. The calculations will relate to your selected material. The graph will display the pH versus the ANC/BNC (mol/kg). The data of the selected material is plotted as red points connected by a line.

Note that there is another way to provide both the start pH and the end pH:

Move the mouse pointer in the graph to the desired start pH value. Now click and drag the mouse to an end pH value. When you release the mouse button, both text boxes will be filled and the result is calculated.

Now, define a Start pH (e.g. the native pH of the material) and an End pH (e.g. the pH value after the sample will be fully carbonated) by filling in the corresponding text boxes. If you press the Requires button, the result will appear and the graph display will contain a fitted polynomial is represented by a green line. The calculated data points are indicated on the curve by black squares.

If you press the Add to results button, the data is stored for later export to an Excel spreadsheet. You can perform multiple calculations before exporting the whole set to an Excel spreadsheet by pressing this button every time a value has been calculated.

The Reset chart button will clear the graph and will again display the pH versus the ANC/BNC.

See section *Graph window on page **48*** for graph display options.

Final pH calculations

This step of the wizard can be used to evaluate scenarios for application. For example, alkaline materials will tend to neutralize due to carbonation (CO_2 uptake from the air) when the material is in contact with air. The amount of CO_2 can be converted to equivalents acid in order to calculate the effect of carbonation at specific times.

First, select a material from the list on top of the window, if you had selected more materials in the first step. The calculations will relate to your selected material. The graph will display the pH versus the ANC/BNC (mol/kg). The data of the selected material is plotted as red points connected by a line.

Note that there is another way to provide both the start pH and the amount of acid or base to add:

Move the mouse pointer in the graph to the desired start pH value. Now click and drag the mouse upward or downward to define the amount to add. Watch the yellow box in the bottom right corner in the graph. When you release the mouse button, both text boxes will be filled and the result is calculated.

Specify the amount of acid or base that is added to the material in the adding textbox. Specify the start pH value of the material, e.g. the native pH of the material, in the to pH textbox. If you press the Yields button, the result will appear and the graph display will contain a fitted polynomial is represented by a green line. The calculated data points are indicated on the curve by black squares.

If you press the Add to results button, the data is stored for later export to an Excel spreadsheet. You can perform multiple calculations before exporting the whole set to an Excel spreadsheet by pressing this button every time a value has been calculated.

The Reset chart button will clear the graph and will again display the pH versus the ANC/BNC.

See section Translating, scaling and zooming a chart on page 48 for graph display options.

Export results

If you press the Next button, you can export the graphed data to an Excel workbook for further inspection. See section Export dialog on page 44 for details regarding the export to an Excel workbook.

L/S to timescale wizard

The L/S data obtained in a percolation test can be related to a time scale through the general relationship:

$$t = \frac{(L/S) \cdot h \cdot d}{N}$$

with t as time in years, L/S is the cumulative amount of water leached (l/kg), h as height of application (m), d as density (kg/m^3) and N as net infiltration in mm/year.

This is an approximation as in reality the annual rain will occur intermittently and with varying intensity. However, for many purposes this approximation is a useful simplification.

The L/S to timescale wizard will let you define and change scenarios. The scenarios are persistent, so you can re-use them in another session.

Selecting or adding a scenario

In the first step of the L/S to timescale wizard you can manipulate the set of scenarios.

The Add button is used to create a new scenario. A dialog window is presented to you where you can give a name and description to the scenario. The Rename button will allow you to change the name and description for the scenario you selected in the list of persistent scenarios. Finally, the Delete button removes the selected scenario from disk.

Edit values

The second step of the L/S to timescale wizard is used to define the scenario. All adjustable parameters are grouped into three panes:

- **General parameters**

  The input for the conversion of L/S to time and visa versa can be given here.

- **Fixed infiltration parameters**

  Using fixed infiltration, a constant infiltration over the years is assumed

- **Varying infiltration parameters**

Using a varying infiltration input some flexibility in variations in infiltration related to e.g. linear performance or other factors that may affect infiltration can be specified here.

General parameters

In the Density text box, provide bulk density in kg/m^3.

In the Height text box, provide the height of the application in m.

In the Minimum L/S text box, provide the minimum L/S ratio that is of interest for the case.

Fixed infiltration parameters

In the Infiltration rate text box, provide average annual infiltration rate in mm/year as a constant input over the years.

In the Maximum L/S text box, provide maximum value of L/S for the case.

Varying infiltration parameters

The More button allows input of up to 5 time periods with associated infiltration rate.

The Less button reduces the number of time periods by one.

The None button removes all entries.

Graphing options

This step of the wizard will let you choose options for the graphical presentation of the fixed and varying infiltration series.

In the Series pane, you can select the series you want to see.

In the Scales pane, you can choose the scale type used for the time and L/S axes. Checking an option will use a logarithmic scale for that axis, while unchecking it makes the scale linear.

In the X-axis pane, you can select whether you want to have the L/S values or the time value along the X-axis.

The calculator

This step of the L/S to timescale wizard displays a graph with the series you selected. Below the graph, there are two input boxes: one for typing an L/S value and one for a time value.

If you type an L/S value and press the Enter or TAB key, the associated times for fixed and varying infiltration rates are calculated and presented in the boxes below.

If you type a time value and press the Enter or TAB key, the associated L/S values for fixed and varying infiltration rates are calculated and presented in the boxes below.

There is an alternate way of supplying L/S and time values: move the mouse pointer to a coordinate having the L/S or time value you want to calculate and press the right mouse button. The coordinate values are copied in the input boxes and the corresponding values are calculated.

For translating, scaling or zooming in on the graph, see *Translating, scaling and zooming a chart on page **48***.

Chemical speciation finder

Provided sufficient major, minor and trace elements have been measured in a sample, the saturation indices (SI) for all minerals in the mineral database can be determined with ORCHESTRA taking into account DOC interaction through the

NICA Donnan model. These SI units (0 represents full equilibrium, negative values represent undersaturation and positive values represent oversaturation) can be used to select relevant minerals for a subsequent chemical speciation prediction run.

With the wizard, you can define and calculate many different scenarios. Scenarios are persistent and can be used for later reference.

In the next sections, all steps in the wizard are described. By pressing the Next button of the wizard, you will leave the current step, the data for the step is saved and the next step is displayed. Pressing the Back button will bring you to the previous step.

Session definition

In this first step of the Chemical speciation wizard you can:

- modify existing scenarios;
- create new scenarios;
- delete scenarios;
- select a scenario to work with.

When an SI run is attempted on a scenario that has already been made before and subsequently processed using the prediction tool, then a message will appear, warning you that changes will not be kept. This is to ensure that stored cases built upon the scenario can be retrieved. A suitable course of action is to copy the scenario and select it.

The window contains three lists and a number of buttons. The Previously defined scenarios list contains all persistent scenarios. The buttons beside it act upon this list. The Minerals list displays all selected minerals of the scenario that is selected in the top list, whereas the Materials list shows all materials in the scenario.

The Delete button removes the selected scenario from the list of persistent scenarios.

The Copy button makes a copy of the selected scenario to be modeled in a different fashion or after obtaining new results.

The name of a selected scenario can be changed to provide a clearer distinction for future reference. This is done with the Rename button.

Note that a scenario will be stored as a file in the file system of your computer with a name identical to the name of the session. Therefore, only use characters in the name that are valid filename characters.

The New session button makes a new scenario. A dialog will pop up asking you to give a name to the new session. The name must be unique within the list of already present scenarios.

The Last used button selects the scenario you used the last time you entered the wizard.

Material selection

The calculation of saturation indices can be carried out for any type of test data, leachate, groundwater or field data provided the relevant parameters to carry out such calculation are available. This generally implies information on pH, major, minor and trace elements. It is generally not very useful to run widely different materials in one run. A suitable combination is to evaluate the same material as a function of pH and as a function of L/S or time. This highlights possible relevance of minerals at for instance low L/S, which are not observed in the relatively high L/S used in the pH dependence test.

You select pH dependent materials by marking the corresponding checkbox and clicking the Select… button. The *Select material dialog* will appear, assisting you in making the selection.

If you want to include materials of another type, mark the corresponding checkbox and select one of the options below the checkbox: Column test materials, Monolithic materials or Landfill materials. Then, click the Select… button. The *Select material dialog* will appear, assisting you in making the selection.

The success of a chemical speciation calculation depends on the presence of concentrations of the main speciation materials in the constituents you select. The main speciation constituents are: Al, Ca, Si and S or SO_4. If you check the box before Allow selection of main constituents only, the material selection dialog boxes will display only the materials having all main constituents.

Inspect or edit material concentrations

The concentrations as obtained from the database can be inspected here and modified, if necessary. See the Concentration editor on page 46 for a description of the editing of concentrations. This modification is not maintained in a subsequent run: if you change anything that will cause the model to rerun, such as adding a material or a mineral, the concentrations are reset to those that are present in the database. If a number in the database is obviously wrong, in spite of data checks at input, then the administrator must change this data in the database after adequate justification of the change. Sometimes additional data are available and not yet entered in the database, and then this input sheet allows inserting these data.

DOC adsorption

Ticking this option is only relevant when DOC data are available. In case data are not available, the program will run normally, but it just takes longer to complete the run as all equations for DOC interaction are loaded for nothing.

Running interactively

Running interactively allows the experienced user to make some changes in Orchestra prior to actually running the program. Ticking this box implies that calculation only starts after the RUN button of Orchestra has been activated.

Defining the mineral set

Based on the saturation indices and expert knowledge a selection of possibly relevant minerals can be made. The currently selected minerals are displayed in the list. Press

the Select button to bring up the Mineral selection dialog, assisting you in selecting the minerals.

Viewing and exporting speciation results

The results of the selected minerals and DOC interaction, when DOC interaction was selected, can be viewed in comparison with the measured concentrations. This allows a judgment of the suitability of the model fit. It should be noted that a curve shaped very much like the measured data, but lying above or below the measured data can still be a good fit.

You select subject reactant in the result in the top left list that contains all reactants known to LeachXS. If you select one, the selected minerals that contain that reactant are checked in the minerals pane to the right of the reactant list. Check or uncheck the minerals you want to include in or exclude from the result set.

Below the list of reactants, there is the list of materials. Check at least one material to be included.

The results can be shown with and without DOC interaction, as the model is run twice to calculate the SI units with and without DOC interaction in cases where DOC is present. Check the box before the label Include DOC concentration to include it in the results. This option is only available when DOC has been included from the beginning.

You will see a graph with results by pressing the View button. A *Graph window* will appear.

Leaching prediction, single pH dependent materials

This wizard uses the saturation indices (SI) generated in the chemical speciation wizard as a starting point to allow prediction of measured pH dependence leaching tests results. At the same time the partitioning between dissolved (free and DOC bound) and solid phases (minerals, Fe-oxide sorption, clay sorption and particulate organic matter interaction) is obtained. The fractionation of dissolved constituents in solution and the fractionation of constituents over particulate phases can be obtained in percentage distribution allowing identification of most relevant controlling phases in specific pH domains. The combination of the availabilities of elements, the mineral selection, the specific DOC, DOM, Fe and Al and clay properties form a chemical speciation fingerprint for the material at hand. When a proper match between measurement and model can be achieved, this information can be used as input for chemical reaction/transport modeling describing release in specific scenarios.

In the next sections, all steps in the wizard are described. By pressing the Next button of the wizard, you will leave the current step, the data for the step is saved and the next step is displayed. Pressing the Back button will bring you to the previous step.

Case definition

In the first step of the wizard you can:

- Create a new case based on an existing chemical speciation setting;
- Modify an existing case;
- Remove, copy or rename existing cases.

In the top left pane, the Available speciation session pane, all currently defined chemical speciation sessions are listed. Below this, the Existing pHStat Cases pane displays a list of cases already created from the session selected in the top pane.

The panes to the right display available minerals and materials. If a case is selected, the panes display data from the case. If only a session is selected, the panes display data from the session.

All buttons act upon a selected case. Use the Delete button to delete a case.

The Copy button can be used to copy a case, which can be useful if you want to run a new case that resembles an already defined case closely.

The Rename button will show a dialog requesting you to give a new name to the case.

The New case button will create a new case based on the selected chemical speciation session. You will be prompted to give a name to the new case.

By pressing the Last used button the case you used the previous time you used the wizard will be selected.

Material selection

Select a single material for which pH dependence test data is available.

Specifying model input

In this step of the wizard you define all quantities that are relevant to the solubility prediction model. The quantities are grouped into tab pages:

- In the **Material** tab page, you can inspect or edit reactant concentrations;
- In the **Humic acid** tab page, you can inspect or edit Humic Acid concentrations;
- In the **Parameters** tab page, you can inspect or edit parameters used by the model.

Reactant concentrations

The reactant concentrations used are the maximum values as obtained in the pH dependence test. Normally the lower pH is set at pH 4. For soils with a substantial fraction of organic matter, the availability obtained this way is not adequate for several metals. In that case a lower pH should be used in the pH dependence test (pH 1.5 - 2).

Changing the concentration of a component may be relevant, if a parameter has not been measured and a phase controlling several elements is missing. This parameter

should subsequently be measured, but to see its effects a figure from other experiments can be used. Double-click the entry to change or press the F2-button.

In case of concrete and comparable matrices the ratio between Al, Si, Ca, and SO4 may be crucial. Adaptation of Al may lead to more consistent results when ettringite type phases are formed.

You can change the presentation to showing reactants or constituents by selecting the appropriate radio button.

The Reset concentrations button resets values to the original database concentrations.

Humic acid concentrations

This tab page is used to define the Solid Humic acid concentration and the dissolved concentrations.

The total amount of Humic Acid (HA) in the solid sample (kg HA/kg sample) is typed in the text box on the top of the tab page.

Dissolved humic acid concentrations are obtained from DOC concentrations, as obtained from the database. Two additional points (pH and concentration) are provided to be able to correct the polynomial when needed. DOC cannot be below 0, as the program will halt. This is avoided by not allowing values below 0.

If DOC values are present, the pane contains a graph, displaying the DOC concentration, the DHA concentration and a polynomial fit through the DHA concentrations.

The bottom of the pane reveals the polynomial coefficients that are used to fit the DHA concentrations. You can input the polynomial order or the coefficients. You can use the Edit… button to use the DHA concentration editor. See the *Dissolved Humic acid editor on page **50*** for details.

Note that a polynomial fit is created by fitting the logarithm of the DHA concentrations. Therefore, the coefficients can only be used to obtain the logarithm of a fitted DHA concentration.

The bottom of the pane reveals the polynomial coefficients that are used to fit the DHA concentrations. You can input the polynomial order or the coefficients. You can use the Edit… button to use the DHA concentration editor. See the *Dissolved Humic acid editor on page **50*** for details.

Model parameters

In this input field generic parameters can be provided to initiate clay sorption and Fe-oxide sorption parameters to be loaded. In addition the redox status of the material can be provided.

- **Sum of pH and pe**
  Definition of the redox status of the system:

Redox status	pH + pe
Oxidized	> 15
Mildly reducing	Between 10 and 15
Reducing	< 10

- **L/S**

  The Liquid to Solid (L/S) ratio (l/kg) that was used in the leaching test. To the right of this parameter you'll find the average L/S value of the material you have selected. By pressing the **Copy** button you can set the L/S parameter to this value.

- **Clay**

  The amount of clay in the sample (kg clay/kg sample) measured as the fraction < 2 µm (lutum).

- **HFO**

- The amount of Hydrous Ferric Oxide (HFO) in the sample (kg HFO/kg sample).

- **Modeling Low L/S**

  Often the high L/S as applied in the pH dependence test does not reflect the proper condition for modeling field scenarios or the initial stages of a column experiment. To get an impression how well the set of minerals and other parameters describes the release behavior at low L/S, it is possible to carry out a simulation at the L/S corresponding with the first fraction of a column test on the same material. Check the box and a selection appears (it is necessary to select the column test together with the pH dependence test in the Speciation wizard for this choice to appear). Double click on the L/S value and this value will be selected for the calculation.

- **Running interactively**

  Check this box to run ORCHESTRA interactively to be able to adjust model parameters before the calculations start.

Editing the set of minerals

The set of mineral to be taken along in the prediction is based on the suitability of the data fit. Many factors play a role as different elements are affected by the same parameter and a selected mineral to improve the prediction of one constituent may deteriorate the prediction for another. This multi-component fitting is an iterative process requiring some experience. The solution converges generally, as the closer the fit for all elements simultaneously the shorter the run time to reach a solution.

The Reactants pane allows selection of reactants actually measured or in case another relevant set of phases may need to be factored in selection of minerals from the entire thermodynamic database. Sometimes carbonate is not measured. This may lead to the situation that none of the carbonate minerals are taken along. By inserting a carbonate level, it is possible to identify, if carbonate is crucial for one or more elements.

The Current set of minerals pane shows the currently selected minerals. Press the Select button to select minerals by revisiting the SI output from the foregoing speciation run in the *Mineral selection dialog*.

You can also remove minerals by selecting the minerals to remove and subsequently pressing the Delete button.

The Reset button will restore the mineral selection to the list of the underlying speciation session.

Running the model

If you have changed any of the data or selections in one of the previous steps, Orchestra will run, performing the task you requested with the data you supplied. When this task is carried out successfully, you will automatically be directed to the next step.

Note that if you didn't change any data, this step will be skipped.

Selecting reactants of interest

The graphical display of data generated by modeling does not allow display of many graphs simultaneously as detail is lost to make choices on relevance of phases. This implies that 6 constituents can be shown simultaneously. For this a selection of constituent groups can be defined, which are useful to view together as they often are interrelated.

The top pane displays the currently defined reactant series. The bottom pane reveals the contents of a selected reactant series in the top pane.

The Delete series button removes a selected series from the list of defined reactant series.

Note that the maximum number of reactants in a series is 6.

The Add series button adds an unnamed series to the list and selects it. You can give a name to the series in the selected reactant series pane and add or remove reactants. Double-click an entry in the Available reactants list to add a reactant. Double-click an entry in the Selected reactants list to remove it.

If you have built a set of series, you can save them for use in other cases by pressing the Save as default sets button. You can load them later in other cases by pressing the Load default sets button.

View general model data

If you press the General View… button, a *Graph window* will appear with 5 graphs, comparing input data and model data:

- pe as function of pH;
- Dissolved Humic Acid in kg/l as function of pH;
- Conductivity in mS/cm as function of pH;
- Acid/Base neutralization capacity in mol/kg as function of pH;
- Redox capacity in mol O_2/l as function of pH.

Viewing and exporting prediction results

In this stage of the wizard you can choose which results you like to visualize. You can view:

- **Solubility prediction results**

  Comparison of measured test data and modeled solution composition (free + DOC associated)

- **Solid and liquid phase partitioning**

  Visualization of partitioning of the constituent between free, DOC associated, clay-bound, Fe-oxide bound, solid organic mater bound (POM), mineral precipitate or incorporated in a solid solution.

- A combination of solubility prediction and partitioning for a specific reactant in the selected reactant series. Two extra graphs will show:
  - Solid phase partitioning;
  - Liquid phase partitioning.

Concentrations can be shown on a log scale and on a linear scale. The first presentation mode allows viewing the partitioning at low concentrations, whereas the linear scale gives an impression of the absolute relevance of a specific phase. Select the appropriate scale in the Graphing options pane. This option is not available for the combination graphs.

Hitting the View button will reveal the *Graph window* with the desired results.

Bulk export button

If you want to repeatedly export your data for a number of reactants, but keeping all the other selections and options the same, this button serves as a shortcut to do this in one operation. When pressing this button, the Select reactants dialog will appear where you can select a number of reactants you want to export. Instead of displaying graph windows with results for every constituent, you will be directed to the Export dialog, enabling you to export all constituents in one action.

This option is available only for solubility prediction results and reactant overviews.

Note that this operation can be time consuming if you'll export a lot of reactants at once.

Leaching prediction, single Percolation materials

This wizard uses the chemical speciation fingerprint as generated in the Leaching prediction wizard for the Leaching prediction, single pH dependent materials on page 24 as a starting point for the prediction of measured percolation test or lysimeter test results. In addition to the concentration as a function of time or L/S at the outlet of the column, the partitioning between dissolved (free and DOC bound) and solid phases (minerals, Fe-oxide sorption, clay sorption and particulate organic matter interaction) is obtained within the column as a function of time at a specified depth in the column or as a function of depth at a specified time. When a proper match between measurement and model can be achieved, this information can be used as basis for chemical reaction transport modeling of field scenarios adding another level of complexity.

Next, all steps in the wizard are described. By pressing the Next button of the wizard, you will leave the current step, the data for the step is saved and the next step is displayed. Pressing the Back button will bring you to the previous step.

Case definition

In the first step of the wizard you can:

- Create a new case based on an existing prediction case for pH dependent materials;
- Modify an existing case;
- Remove, copy or rename existing cases.

In the top left pane, the Available speciation session pane, all currently defined chemical speciation sessions are listed. Below this, the Dependent pHStat Cases pane displays a list of cases already created from the session selected in the top pane.

The bottom left pane, the Dependent Percolation cases pane, displays all prediction cases that depend on the case you have selected in the pane above it.

The panes to the right display available minerals and materials. If a case is selected, the panes display data from the case. If only a session is selected, the panes display data from the session.

All buttons act upon a selected case. Use the Delete button to delete a case.

The Copy button can be used to copy a case, which can be useful if you want to run a new case that resembles an already defined case closely.

The Rename button will show a dialog requesting you to give a new name to the case.

The New case button will create a new case based on the selected pH dependent case. You will be prompted to give a name to the new case.

By pressing the Last used button the case you used the previous time you used the wizard will be selected.

Material selection

Select a single material for which percolation test data is available.

Specifying model input

In this step of the wizard you define all quantities that are relevant to the solubility prediction model. The quantities are grouped into tab pages:

- In the **Material** tab page, you can inspect or edit reactant concentrations;
- In the **Humic acid** tab page, you can inspect or edit Humic Acid concentrations;
- In the **Parameters** tab page, you can inspect or edit parameters used by the model.
- In the **Solution** tab page, you can inspect or edit initial reactant concentrations in the percolation solution.
- In the **Refresh data** tab page, you can change the flow speed for every step in the percolation process.

Reactant concentrations

The reactant concentrations used are the maximum values as obtained in the pH dependence test. Normally the lower pH is set at pH 4. For soils with a substantial fraction of organic matter, the availability obtained this way is not adequate for several metals. In that case a lower pH should be used in the pH dependence test (pH 1.5 - 2).

Changing the concentration of a component may be relevant, if a parameter has not been measured and a phase controlling several elements is missing. This parameter should subsequently be measured, but to see its effects a figure from other experiments can be used. Double-click the entry to change or press the F2-button.

In case of concrete and comparable matrices the ratio between Al, Si, Ca, and SO4 may be crucial. Adaptation of Al may lead to more consistent results when ettringite type phases are formed.

You can change the presentation to showing reactants or constituents by selecting the appropriate radio button.

The Reset concentrations button resets values to the original database concentrations.

Humic acid concentrations

This tab page is used to define the Solid Humic acid concentration and the dissolved concentrations.

The total amount of Humic Acid (HA) in the solid sample (kg HA/kg sample) is typed in the text box on the top of the tab page.

Dissolved humic acid concentrations are obtained from DOC concentrations, as obtained from the database. Two additional points (pH and concentration) are provided to be able to correct the polynomial when needed. DOC cannot be below 0, as the program will halt. This is avoided by not allowing values below 0.

The pane contains a graph, displaying the DOC concentration, the DHA concentration and the polynomial fit through the DHA concentrations.

The bottom of the pane reveals the coefficients that are used to fit the DHA concentrations. The following function is used in the fitting process:

$$DHA_{L/S} = Q_2 + Q_0 e^{-Q_1(L/S)}$$

You can modify the weighting scheme used in the fitting process by selecting the appropriate option in the Weights list. The scale to display in the graph can be linear or logarithmic. Furthermore, you can use the Edit… button to modify the DHA concentrations. See the *Dissolved Humic acid editor on page **50*** for details.

Model parameters

In this input field generic parameters can be provided to initiate clay sorption and Fe-oxide sorption parameters to be loaded. In addition the redox status of the material can be provided.

- **Sum of pH and pe**
  Definition of the redox status of the system:

Redox status	pH + pe
Oxidized	> 15

Mildly reducing	Between 10 and 15
Reducing	< 10

- **Clay**

  The amount of clay in the sample (kg clay/kg sample) measured as the fraction < 2 µm (lutum).

- **HFO**

  The amount of Hydrous Ferric Oxide (HFO) in the sample (kg HFO/kg sample).

- The **Defaults** button.

  This button will set the Sum of pH and pe, the Clay, the HFO and the SHA parameters to the values as found in the underlying pH dependent solubility prediction case.

- **Initial pH**

  The initial pH must be given here. Generally a value close to the pH in the first fraction of the column is inserted here.

- **Porosity fraction**

  This property describes the water filled pore volume in the packed column (saturation assumed) expressed as a fraction of the total volume (dimensionless).

- **Density**

  Insert the density of the solid matrix in kg/dm^3. The Calculate button will try to calculate the density from the material data that are present in the LeachXS database.

- **Column length**

  Insert the length of the column in cm.

- **Relative volume stagnant phase**

  Insert here an estimate of the fraction of the column content where pore water is stagnant and only contribution through diffusion from the stagnant zone to the flow channel is occurring.

- **Effective distance between phases**

  This property is a measure of the transfer between stagnant zone and the flow channel. A common default value is 3 cm.

- **Running interactively**

  Check this box to run ORCHESTRA interactively to be able to adjust model parameters before the calculations start.

Solution

The composition of the leachant can be modified. Default is demineralised water with very low concentrations of all parameter and an initial pH of 7. In the Initial pH field you can specify the initial pH value of the solution.

Refresh data

In this table the leachant collection stages expressed as time after the start of the percolation test are given as extracted from the database. The flow rate is calculated

based on the volume of eluate collected in a given time period. Modifications of the values in the table will be stored with the case file. The Reset button will reset the values to those that were defined before you entered this stage of the wizard. The Reload from DB button will reset the values to those present in the LeachXS database.

Editing the set of minerals

The set of mineral to be taken along in the prediction is based on the suitability of the data fit. Many factors play a role as different elements are affected by the same parameter and a selected mineral to improve the prediction of one constituent may deteriorate the prediction for another. This multi-component fitting is an iterative process requiring some experience. The solution converges generally, as the closer the fit for all elements simultaneously the shorter the run time to reach a solution.

The Reactants pane allows selection of reactants actually measured or in case another relevant set of phases may need to be factored in selection of minerals from the entire thermodynamic database. Sometimes carbonate is not measured. This may lead to the situation that none of the carbonate minerals are taken along. By inserting a carbonate level, it is possible to identify, if carbonate is crucial for one or more elements.

The Current set of minerals pane shows the currently selected minerals. Press the Select button to select minerals by revisiting the SI output from the foregoing speciation run in the *Mineral selection dialog*.

You can also remove minerals by selecting the minerals to remove and subsequently pressing the Delete button.

The Reset button will restore the mineral selection to the list of the underlying speciation session.

Running the model

If you have changed any of the data or selections in one of the previous steps, Orchestra will run, performing the task you requested with the data you supplied. When this task is carried out successfully, you will automatically be directed to the next step.

Note that if you didn't change any data, this step will be skipped.

Selecting reactants of interest

The graphical display of data generated by modeling does not allow display of many graphs simultaneously as detail is lost to make choices on relevance of phases. This implies that 6 constituents can be shown simultaneously. For this a selection of constituent groups can be defined, which are useful to view together as they often are interrelated.

The top pane displays the currently defined reactant series. The bottom pane reveals the contents of a selected reactant series in the top pane.

The Delete series button removes a selected series from the list of defined reactant series.

Note that the maximum number of reactants in a

The Add series button adds an unnamed series to the list and selects it. You can give a name to the series in the selected reactant series pane and add or remove

series is 6.

reactants. Double-click an entry in the Available reactants list to add a reactant. Double-click an entry in the Selected reactants list to remove it.

If you have built a set of series, you can save them for use in other cases by pressing the Save as default sets button. You can load them later in other cases by pressing the Load default sets button.

View general model data

If you press the General View… button, a *Graph window* will appear with 5 graphs, comparing input data and model data:

- pH as function of L/S;
- pe as function of L/S;
- Dissolved Humic Acid in kg/l as function of L/S;
- Conductivity in mS/cm as function of L/S;
- Acid/Base neutralization capacity in mol/kg as function of L/S;
- Redox capacity in mol O_2/l as function of L/S.

Viewing and exporting prediction results

In this stage of the wizard you can choose which results you like to visualize. You can view:

- **Leachate concentrations**
- In this graph the concentrations as obtained in the percolation or lysimeter test are given as extracted from the database together with the predicted concentration as a function of L/S and the concentration as predicted for the collected fractions (diamonds).
- **Cumulative release**

  In this graph the cumulative leached amount as a function of L/S as derived from the percolation or lysimeter test data in the database are compared with the predicted cumulative release.
- **Concentration profiles at a specified time**

  In this graph the partitioning between dissolved (free and DOC bound) and solid phases (minerals, Fe-oxide sorption, clay sorption and particulate organic matter interaction) is given as a function of the depth in the column at a specified time (to be selected).
- **Concentration profiles at a specified depth**

  In this graph the partitioning between dissolved (free and DOC bound) and solid phases (minerals, Fe-oxide sorption, clay sorption and particulate organic matter interaction) is given at a given depth in the column as a function of time (to be selected).
- **Animated time profiles for a single reactant**

  This option allows an animation to be generated of the partitioning of a constituent between dissolved (free and DOC bound) and solid phases (minerals,

Fe-oxide sorption, clay sorption and particulate organic matter interaction) as a function of depth in the column over the time span of the percolation test.

Concentration profiles can be shown on a log scale and on a linear scale. Select the appropriate scale in the Graphing options pane. This option is not available for the display of Leachate concentration graphs and Cumulative release graphs.

Hitting the View button will reveal the *Graph window* with the desired results.

Bulk export button

If you want to repeatedly export your data for a number of reactants, but keeping all the other selections and options the same, this button serves as a shortcut to do this in one operation. When pressing this button, the Select reactants dialog will appear where you can select a number of reactants you want to export. Instead of displaying graph windows with results for every constituent, you will be directed to the Export dialog, enabling you to export all constituents in one action.

This option is not available for Animated time profiles.

Note that this operation can be time consuming if a lot of reactants are exported at once.

Leaching prediction, mixtures of materials

Once chemical speciation fingerprints as defined by the combination of the availabilities of elements, the mineral selection, the specific DOC, DOM, Fe and Al and clay properties for specific material are available from the Leaching prediction, single pH dependent materials on page 24 it is possible to evaluate the leaching behavior of a mixture of materials under the assumption that the availabilities and sorptive surfaces are additive. The minerals assumed to be relevant are the combination of all minerals occurring in any of the constituting materials. Assumptions are needed for the DOC response as a function of pH. This aspect requires further study as precipitation of DOC and mobilization may occur.

In the next sections, all steps in the wizard are described. By pressing the Next button of the wizard, you will leave the current step, the data for the step is saved and the next step is displayed. Pressing the Back button will bring you to the previous step.

Case definition

In the first step of the wizard you can:

- Create a new case;
- Modify an existing case;
- Remove, copy or rename existing cases.

The left pane shows all existing pH dependent mixture cases available.

The panes to the right display the selected minerals and the material mixture. If a case is selected, the panes display data from the case. All buttons act upon a selected case. Use the Delete button to delete a case.

The Copy button can be used to copy a case, which can be useful if you want to run a new case that resembles an already defined case closely.

The Rename button will show a dialog requesting you to give a new name to the case.

The New case button will create a new mixture case. You will be prompted to give a name to the new case.

By pressing the Last used button the case you used the previous time you used the wizard will be selected.

Mixture definition

This step helps you to define or modify the composition of the material mixture.

In the top left pane, the Available speciation session pane, all currently defined chemical speciation sessions are listed.

Next to this pane, the Existing pHStat Cases pane displays a list of cases already created from the session selected in the left pane. Below this pane, you can see the pH dependent material that was selected in the selected pH dependent case.

In the bottom half of the window, the Mixture composition pane displays the currently defined material mixture: the name of the material, the pH dependent case it originates from and the percentage the material contributes to the mixture.

You can add a material to the mixture by pressing the Add button next to field that contains the name of the material of the selected pH dependent material. You'll be prompted to enter the contribution percentage of the material in the mixture. This percentage can be changed by double-clicking the material entry in the Mixture composition pane or by pressing the Percentage… button.

The Delete button removes the selected material in the composition pane, whereas the Clear button removes all entries.

Finally, the Normalize button will scale all percentages in order to add up to 100 percent.

Specifying model input

In this step of the wizard you define all quantities that are relevant to the solubility prediction model. The quantities are grouped into tab pages:

- In the **Material** tab page, you can inspect or edit reactant concentrations;
- In the **Humic acid** tab page, you can inspect or edit Humic Acid concentrations;
- In the **Parameters** tab page, you can inspect or edit parameters used by the model.

Reactant concentrations

The reactant concentrations used are the maximum values as obtained in the pH dependence test. Normally the lower pH is set at pH 4. For soils with a substantial

fraction of organic matter, the availability obtained this way is not adequate for several metals. In that case a lower pH should be used in the pH dependence test (pH 1.5 - 2).

Changing the concentration of a component may be relevant, if a parameter has not been measured and a phase controlling several elements is missing. This parameter should subsequently be measured, but to see its effects a figure from other experiments can be used. Double-click the entry to change or press the F2-button.

In case of concrete and comparable matrices the ratio between Al, Si, Ca, and SO4 may be crucial. Adaptation of Al may lead to more consistent results when ettringite type phases are formed.

You can change the presentation to showing reactants or constituents by selecting the appropriate radio button.

The Reset concentrations button resets values to the original database concentrations.

Humic acid concentrations

This tab page is used to define the Solid Humic acid concentration and the dissolved concentrations.

The total amount of Humic Acid (HA) in the solid sample (kg HA/kg sample) is typed in the text box on the top of the tab page.

Dissolved humic acid concentrations are obtained from DOC concentrations, as obtained from the database. Two additional points (pH and concentration) are provided to be able to correct the polynomial when needed. DOC cannot be below 0, as the program will halt. This is avoided by not allowing values below 0.

If DOC values are present, the pane contains a graph, displaying the DOC concentration, the DHA concentration and a polynomial fit through the DHA concentrations.

Note that a polynomial fit is created by fitting the logarithm of the DHA concentrations. Therefore, the coefficients can only be used to obtain the logarithm of a fitted DHA concentration.

The bottom of the pane reveals the polynomial coefficients that are used to fit the DHA concentrations. You can input the polynomial order or the coefficients. You can use the Edit… button to edit the DHA concentrations. See the *Dissolved Humic acid editor* for details.

Model parameters

In this input field generic parameters can be provided to initiate clay sorption and Fe-oxide sorption parameters to be loaded. In addition the redox status of the material can be provided.

- **Sum of pH and pe**
  Definition of the redox status of the system:

Redox status	pH + pe
Oxidized	> 15
Mildly reducing	Between 10 and 15
Reducing	< 10

- **L/S**

The Liquid to Solid (L/S) ratio (l/kg) that was used in the leaching test. To the right of this parameter you'll find the average L/S value of the material you have selected. By pressing the **Copy** button you can set the L/S parameter to this value.

- **Clay**

  The amount of clay in the sample (kg clay/kg sample) measured as the fraction < 2 µm (lutum).

- **HFO**

  The amount of Hydrous Ferric Oxide (HFO) in the sample (kg HFO/kg sample).

- **Running interactively**

  Check this box to run ORCHESTRA interactively to be able to adjust model parameters before the calculations start.

Editing the set of minerals

The set of mineral to be taken along in the prediction is based on the suitability of the data fit. Many factors play a role as different elements are affected by the same parameter and a selected mineral to improve the prediction of one constituent may deteriorate the prediction for another. This multi-component fitting is an iterative process requiring some experience. The solution converges generally, as the closer the fit for all elements simultaneously the shorter the run time to reach a solution.

The Mixture composition pane displays the mixture definition. You can view the minerals that are defined in a specific mixture component by selecting a component. The defined minerals in that component are colored blue.

The Reactants to show pane allows selection of reactants actually measured or in case another relevant set of phases may need to be factored in selection of minerals from the entire thermodynamic database. Sometimes carbonate is not measured. This may lead to the situation that none of the carbonate minerals are taken along. By inserting a carbonate level, it is possible to identify, if carbonate is crucial for one or more elements.

The Current set of minerals pane shows the currently selected minerals. Press the Select button to select minerals by revisiting the SI output from the foregoing speciation run in the *Mineral selection dialog*.

You can also remove minerals by selecting the minerals to remove and subsequently pressing the Delete button.

The Reset button will restore the mineral selection to the list of the underlying speciation session.

Running the model

If you have changed any of the data or selections in one of the previous steps, Orchestra will run, performing the task you requested with the data you supplied. When this task is carried out successfully, you will automatically be directed to the next step.

Note that if you didn't change any data, this step will be skipped.

Selecting reactants of interest

The graphical display of data generated by modeling does not allow display of many graphs simultaneously as detail is lost to make choices on relevance of phases. This implies that 6 constituents can be shown simultaneously. For this a selection of constituent groups can be defined, which are useful to view together as they often are interrelated.

The top pane displays the currently defined reactant series. The bottom pane reveals the contents of a selected reactant series in the top pane.

The Delete series button removes a selected series from the list of defined reactant series.

Note that the maximum number of reactants in a series is 6.

The Add series button adds an unnamed series to the list and selects it. You can give a name to the series in the selected reactant series pane and add or remove reactants. Double-click an entry in the Available reactants list to add a reactant. Double-click an entry in the Selected reactants list to remove it.

If you have built a set of series, you can save them for use in other cases by pressing the Save as default sets button. You can load them later in other cases by pressing the Load default sets button.

Viewing and exporting prediction results

In this stage of the wizard you can choose which results you like to visualize. You can view:

- **Solubility prediction results**

  Comparison of measured test data and modeled solution composition (free + DOC associated)

- **Solid and liquid phase partitioning**

  Visualization of partitioning of the constituent between free, DOC associated, clay-bound, Fe-oxide bound, solid organic mater bound (POM), mineral precipitate or incorporated in a solid solution.

- A combination of solubility prediction and partitioning for a specific reactant in the selected reactant series. Two extra graphs will show:
  - Solid phase partitioning;
  - Liquid phase partitioning.

- **General data**

  5 graphs will show, comparing input data and model data:
  - pe as function of pH;
  - Dissolved Humic Acid in kg/l as function of pH;
  - Conductivity in mS/cm as function of pH;
  - Acid/Base neutralization capacity in mol/kg as function of pH;
  - Redox capacity in mol O_2/l as function of pH.

Except from the Solid and liquid phase partitioning, you must select a material to compare model data with measured data that is present in the LeachXS database.

You can select a Component from the mixture or an Other material from the database. Press the Select button to select a material from the appearing Select material dialog.

Concentrations can be shown on a log scale and on a linear scale. The first presentation mode allows viewing the partitioning at low concentrations, whereas the linear scale gives an impression of the absolute relevance of a specific phase. Select the appropriate scale in the Graphing options pane. This option is not available for the combination graphs.

Hitting the View button will reveal the *Graph window* with the desired results.

Bulk export button

If you want to repeatedly export your data for a number of reactants, but keeping all the other selections and options the same, this button serves as a shortcut to do this in one operation. When pressing this button, the Select reactants dialog will appear where you can select a number of reactants you want to export. Instead of displaying graph windows with results for every constituent, you will be directed to the Export dialog, enabling you to export all constituents in one action.

This option is available only for solubility prediction results and reactant overviews.

Note that this operation can be time consuming if you'll export a lot of reactants at once.

Assessment of impact on groundwater, granular and monolithic materials

Sorry, no help available yet.

Other dialogs and windows

Select material dialog

The Select material dialog assists you in selecting one or more materials. The left pane of this dialog shows all materials that are selectable for the situation from which the dialog is called. The right pane shows the currently selected material(s).

The left pane has three tabs. Every tab reveals a way of looking at the list of available materials:

- **Materials by category** tab

In this tab materials are organized by the main category and subcategory they belong to.

- **Materials by test type** tab

  In this tab materials are organized by the main test type and subtype they belong to.

- **Alphabetic list of materials** tab

  In this tab the materials are listed alphabetically.

The way you select materials depends on how many materials you are allowed to select. If you are allowed to choose only one material, you select a material by clicking on it. Any previously selected material will be replaced by the one you clicked on.

When you are allowed to select multiple materials, you can select them by checking the box in front of it. The checked material will be added to the list of selected materials. Unchecking a material will remove the material from the list.

If a multiple selection is allowed, you can select all materials belonging to a (sub)category or test (sub)type by checking the box before the category or test type.

The OK button will close the dialog and update your material selection. The Cancel button will close the dialog without updating your selection.

Apart from the panes and buttons, the dialog has a menu bar with filtering and material information options.

Materials menu

This menu contains an entry named Show Information. Selecting this entry will reveal details about the selected material in the left or right pane. The *Material info window* containing information of the material will pop up. The window remains on the screen until you press the close button in the window or selecting the menu entry again. If you select another material, the contents of the material information window will be changed to information about the newly selected material.

Depending on the context, the menu may contain another entry, named Propose… This entry may be present if you are selecting materials in one of the regulatory comparison windows. If it is present, LeachXS has found one or more materials you might be looking for. Selecting this entry will bring up another instance of the Select material dialog with proposed materials. If you select one or more proposed materials and press the OK button, the second instance of the dialog closes an the selected materials are added to the current selection.

Filter menu

If there are a lot of materials in the database, the lists of available materials can be extremely large. You can make the selection of materials easier by applying filters on test types or categories. In this way, you can limit the materials to be displayed to the materials that are of interest to you. You can define a filter on a number of test types, categories or you can limit the materials that are displayed by materials containing a certain constituent. You define filters by using the Define menu entry and then select the appropriate filter type. A Material selection filter dialog or Select constituent dialog will pop up, enabling you to define the filter.

After you have created a filter, you can activate or deactivate it by checking one of the appropriate menu entries.

You can see if a filter is imposed on test types, categories or constituent occurrence by inspecting the icons to the left of the buttons pane.

Delete button

This button deletes the material(s) you have selected in the right pane.

Go to button

The go to button will highlight the material that is selected in the right pane in the left pane. First select a material in the right pane, and then click on a tab in the left pane. Now, if you press the Go to button, the material is highlighted in the left pane.

Select constituent dialog

The Select constituent dialog assists you in selecting one or more constituents. The left pane of this dialog shows all constituents, categorized by organic or inorganic nature of the constituent. The right pane shows the currently selected constituents(s).

The way you select constituents depends on how many constituents you are allowed to select. If you are allowed to choose only one constituent, you select a constituent by clicking on it. Any previously selected constituent will be replaced by the one you clicked on.

When you are allowed to select multiple constituents, you can select them by checking the box in front of it. The checked constituent will be added to the list of selected constituents. Unchecking a constituent will remove it from the list.

The OK button will close the dialog and update your constituent selection. The Cancel button will close the dialog without updating your selection.

Delete button

This button deletes the constituent (s) you have selected in the right pane.

Go to button

The go to button will highlight the constituent that is selected in the right pane in the left pane. First select a constituent in the right pane, and then click on a tab in the left pane. Now, if you press the Go to button, the constituent is highlighted in the left pane.

Select reactants dialog

The Select Reactants dialog assists you in selecting one or more reactants. The left pane shows all reactants, grouped by reactant series in which they are defined. The right pane shows all currently selected reactants.

The OK button will close the dialog and update your reactant selection. The Cancel button will close the dialog without updating your selection.

This dialog will pop up if you want to do a bulk export from one of the Leaching prediction wizards. If you want to bulk export a general view of the prediction results along with the results you selected, check the Include Material overview checkbox.

Material info window

The Material info window reveals details about a material.

Below the name of the material you will find a table with some characteristics of the material, stored in the database:

Material characteristic	Meaning
Full name	The full name of the material.
Description	A description of the material.
Test type	The test type and subtype of the material.
Category	The category and subcategory of the material.
Origin	An indication where the material was originated.
Supplier	The company or institute that supplied the material.
Lab	The laboratory that performed the tests on the material.
Standard	The standard procedure that has been followed.
Remarks	Any additional remarks to the material, if any.
Measured fractions	The total number of measured fractions. Note that this not necessarily means that all constituents have been measured in all fractions.
Has ANC data	Indicates if any Acid/Base neutralization capacity data is present on the material.
Total composition measured	Indicates if total composition data has been measured.
Availability measured	Indicates if availability data has been measured.
Test types of material	All tests performed on the material.
Measured constituents	The total number of constituents that have been measured. Note that this not necessarily means that all constituents have been measured in all fractions.

At the bottom of the window there is a list of all measured constituents of the material.

You can adjust:

- the location of the window. Drag the window to a screen position of your preference.
- the size of the window. Move the mouse pointer to an edge or corner of the window and drag the mouse to resize it.
- the width of the columns of the table with material characteristics. Move the mouse pointer to the border between the column headers and drag the mouse to resize the column to the left of it.
- the ratio of the size of the characteristics table and the list of constituents. Move the mouse pointer to the ruler above the caption of the list of constituents and drag the mouse to divide the space between the two panes.

All your adjustments are saved if you close the window. If you open the window at another time, your saved adjustments will be applied.

Total Composition and availability window

This window will reveal a table with details about availability and total composition data of selected materials.

For every selected material, the table contains the measured test types of the data. If availability or total composition is measured by different test types, there will be multiple, blue colored entries for that material. Before showing results, you will have to select the desired test types to be used for every material having multiple test types measured.

Directive selection dialog

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

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

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

Note that only user defined directives can be edited.

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. A Select constituent dialog 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.

Export dialog

The Export dialog facilitates the reporting of results and graphs. The results will be presented in a Microsoft Excel workbook. You can choose an existing or a new workbook as a storage holder for your results. A workbook typically contains a number of worksheets, each containing (a part of your) results.

Every workbook with results will have two additional sheets. One sheet contains administrative data about your results and is called Index. On the other sheet, all graphs belonging to the results are kept. This sheet is called Charts. The results resulting from a single export action will be stored on a single sheet. All graphs belonging to the results will occupy a single row in the Charts sheet. The rows will be in the same order as the tab order with results. You can consult the Index sheet as well to view the row on which the graphs to your results are.

You can choose to show the results immediately after the exporting process has been finished.

Specifying a workbook

You can specify a workbook by using File entry on the menu bar. You can make a new workbook, select an existing workbook, or pick a recently used workbook. If you select an existing workbook, be sure to select one that already has LeachXS results. If you select another one, LeachXS will complain about not finding the administration sheet later on.

Specifying a worksheet name

Be aware that Microsoft Excel imposes some restrictions on naming a sheet. The characters in the set { \/?,'" } are prohibited and the name should be less than 30 characters.*

Your results will be kept on a separate sheet in the workbook. LeachXS proposes a sheet name (or several names if you accessed this dialog from a bulk export operation) that is displayed in the top pane. If you are not happy with a proposed name, select it and press the Rename button right to the pane.

All worksheet names are prepended with an icon, indicating the status of the sheet. A red bullet with a cross indicates that the name for the sheet is not valid. You will need to rename the sheet. A yellow triangle with an exclamation mark will indicate that a sheet with that name is already present in the selected workbook. You can check this by inspecting the Existing worksheets pane. If you don't rename the sheet, the existing sheet will be overwritten. A green check mark will indicate that the sheet name is valid and that the sheet doesn't exist in the workbook.

Manipulating existing worksheets

The Existing worksheets pane shows all the sheets in the workbook. You can rename, delete or reorder the sheets by selecting a sheet name and press the appropriate button.

Excel graphs layout

Before exporting the results you can change some aspects of the graphs to be exported. If you are happy with the default appearance, select the Default option button. If you want to use a previously defined layout or edit the layout, select the User defined option button. Hitting the Define… button will show the Edit Excel chart layout dialog, enabling you to change the layout.

Defining alternative names for materials

The names of materials are constructed in such a way that they are unique within the list of all present materials in the database. This will assist you in identifying the different materials. However, you may want to change material names for presentation purposes. If you check the Use alternative material names checkbox the alternative names you chose for the materials present in your results will be reported. You can create or edit the alternative names with the *Alternative names for materials dialog* that will pop up if you press the Define button.

Open workbook after export

If you check this option, the workbook you chose will be opened after you leave this dialog.

Export button

By pressing Export button you will start the actual reporting process. This process will take a while, especially when large amounts of data are to be reported or you are bulk exporting data. If the workbook the results are exported to is currently opened in Microsoft Excel, close it first. LeachXS is not able to export to an opened workbook.

Concentration editor

The Concentration editor is used to edit concentrations and related data of materials that are selected in the *Chemical speciation finder*.

For every material and fraction the concentrations of all reactants that have representatives in the database are listed. Beside these concentrations pH and pe values are shown for every fraction.

For Landfill and Monolithic materials, an extra column Time (days) is present, whereas Column test materials have an L/S column.

Unmeasured quantities that should have a value are displayed in red: you have to specify them in order to produce results. Concentrations may be "not measured": you can edit them, but this will not be mandatory.

Press the OK button to save your changes and leave the editor. By pressing the Cancel button you quit the editor as well, discarding the changes.

Editing a value

You edit a value by double-clicking a value or pressing the F2 key after selecting a cell in the presented table.

Mineral selection dialog

Based on the saturation indices and expert knowledge a selection of possibly relevant minerals can be made. The figure of merit (FOM) is a parameter, that weighs the observed indices based on the number of observations between the indicated upper and lower limit for the accepted SI values (major reduction of possible mineral phases) and the closeness of the SI to 0. Weighing factors are available to modify the selection criteria.

By clicking a possible mineral the model description and the measured data can be compared. The selection of a mineral requires some specialist knowledge and experience as phases may seem relevant, that cannot be formed under the conditions in the experiment (e.g. high temperature minerals). In addition, in some cases minerals with very similar composition can be identified. In such cases, one with the closest fit should be selected.

The dialog contains a list of all minerals that are known to LeachXS. For every mineral, the SI values for every fraction of every selected mineral are displayed. You

can select a mineral or remove it from the selection by checking or unchecking the box before the mineral.

You can control the minerals that are displayed in the list by selecting a reactant in the top left Reactants pane. Only those minerals that contain the selected reactant are displayed. Selecting a reactant doesn't change the currently selected set of minerals: it just limits the number of minerals to be displayed. A complete list of the minerals that comprise the mineral selection is displayed in the Selected minerals pane.

You can control the visibility of SI values by setting an upper and lower bound and choosing colors for SI values inside and outside the range defined by these bounds. This will assist you in inspecting the SI values.

Define the SI range in the Saturation Index coloring pane: type the upper and lower bounds in the text boxes and press the Change… buttons in the Used Colors pane to change the colors of the values inside or outside the range. The colors of the labels before the buttons display the currently selected colors.

If you press the OK button, the dialog closes, saving your mineral selection. The Cancel button will cause to close the dialog as well, keeping the originally selected set of minerals intact.

Figure of merit (FOM)

To assist you in selecting minerals with a good set of SI values, a figure of merit is calculated for every combination of material and mineral. This figure will give you an indication of how well SI values are near zero (the *Fit* part of the figure) and how many SI values are inside the SI range you have defined (the *Hit* part of the figure). Both parts of the FOM are scaled to a range from 0 to 100, weighted according to the weights you have defined in the Figure of Merit pane and combined to a final number between 0 and 100.

You can sort the list of minerals on the FOM by clicking on a FOM column header. The FOM consists of three numbers, the first being the combined FOM, the second is the *FIT* FOM and the third is the *HIT* FOM.

The Hit *figure of merit*

The Hit figure of merit is the number of the SI values inside the defined SI range divided by the total number of SI values, multiplied by 100.

If there is only one SI value within the range and it is the value of the first or last fraction of the material, it is counted twice to give it a higher figure than a single hit in the middle of the range.

The Fit *figure of merit*

The first step is to find the first and last SI values that are within the defined range. Note that there may be SI values outside the defined range between those two points. Furthermore, if only one SI value is in the range (so the first and last point denotes the same SI value, an extra SI point is added: the one adjacent to the found point with the best SI value).

Then, the fit is defined by taking the root of the sum of squared SI values between the first and last found point, divided by the number of values in the range. This number is scaled between 0 and 100.

The combined figure of merit

The combined figure of merit is:

$$FOM_{COMBINED} = \frac{W_{FIT} \cdot FOM_{FIT} + W_{HIT} \cdot FOM_{HIT}}{W_{FIT} + W_{HIT}}$$

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.

Note that any changes you make in a graph will not be present in results you export. They will only be present in graphs you save to disk or to the Windows Clipboard.

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.

Although the layout of the graphs cannot be changed, you can resize the entire window by moving the mouse pointer to an edge or corner of the window and dragging it.

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.

Saving a chart

If you click the right mouse button on a graph, a menu will pop up, allowing you to:

- Save the graph on the Windows clipboard in JPEG or Enhanced Metafile format.
- Save the graph on disk, formatted as in JPEG or Enhanced Metafile. The file will be saved in your **My Pictures** folder and named after the title of the graph you selected.

Note that an existing file with the same name on that location will be overwritten without notification.

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.

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

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 scaling 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.

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.

Changing the appearance of a chart

*Note that any changes in appearance will not be undone by pressing the **r** key.*

You can change a few basic properties of a graph by pressing the p key, after you have clicked on the graph you want to change the properties of. A dialog will appear, in which you can change:

- The appearance of every series;
- The location and visibility of the legend;
- The axis titles, graph title and graph footer.

Legend font size

If you have a lot of series in a graph, the legend may be bigger than the graph itself. You can type a smaller font size to reduce the legend area. The default font is 8.25 points.

Export button

You export calculated results and accompanying graphs by pressing the Export button. The *Export dialog* will pop up, enabling you to provide details about the export process.

Alternative names for materials dialog

The names of materials are constructed in such a way that they are unique within the list of all present materials in the database. This will assist you in identifying the different materials. However, you may want to change material names for presentation purposes. The Alternative names for materials dialog will let you define alternative names for them. LeachXS keeps a list of all materials you have given an alternative name.

In the dialog, a table is presented that contains that list, together with entries for the materials that were selected at the time the dialog was brought up. You can change existing alternative names or create new names for those materials that have not been given one.

You can recognize the currently selected materials by their color: the foreground color of the rows containing them is black, whereas the foreground color of the other materials in the table is gray.

The OK button will close the dialog, effectuating all changes made. The Cancel button closes the dialog, discarding all changes.

Clear Used button

The Clear Used button will remove all alternative names of the currently selected materials.

Clear Unused button

The Clear Unused button will remove all alternative names of the not currently selected materials.

Reset button

The Reset button will restore the table to the state when it was opened.

Material selection filter dialog

To limit the number of test types or categories when selecting materials, you can define filters. The Material selection filter dialog will enable you to define these filters.

Note that your material selection may change if you change filters: selected materials that are not visible by the imposed filters will be removed from the selection list.

The dialog displays a hierarchical view of the test types or categories, depending on the pane that was selected in the *Select material dialog*. Any entry that is checked in the view will be included in the filter. Unchecked entries are excluded and materials belonging to that entry will not show up.

The No Filter button will check all entries, so all materials will show up.

Dissolved Humic acid editor

The Dissolved Humic acid concentration editor enables you to edit the reactive fraction of DOC towards sorption of elements. This information is used to calculate the polynomial describing reactive DOC at intermediate pH values.

You can specify a fraction for every measured pH. For polynomial fit purposes, additional points of pH values 1 and 14 are added to control the fit procedure. However you can remove any of these values by selecting the concentration cell to the right of the pH and pressing the Delete button.

Change a concentration or fraction by selecting a cell and pressing the F2 key or by double-clicking a cell.

You can use the text boxes below the table to:

- Change all DOC concentrations to a certain value;
- Change all DHA fractions to a certain value;

Type the value in the appropriate text box and press the corresponding Set button.

Press the Reset button to reset the values to the ones at the time the editor was called.

Note that every time you change a value, the graph on the window from which the editor is called is updated dynamically.

The OK button will close the editor, saving the changes you made. The Cancel button will close it without saving the changes.

Regulations editor

All regulatory comparisons that can be done in the analysis, presentation and regulatory comparisons entry in the main LeachXS pane can be saved and re-used at a later time. The Regulations editor will assist you in inspecting and selecting previously saved comparisons. The editor is accessible from the menu bar in any of the regulatory comparison dialogs. It is context sensitive in the sense that it will display only those comparisons that were previously saved in the same dialog.

The editor contains three panes and a menu bar. With the entries in the menu bar, you can create new comparisons or rename, delete or copy existing ones.

You leave the editor by pressing the Cancel or OK button. By using this last button, the currently selected regulation will be loaded into the regulations dialog from which you started the editor.

The Saved Regulation definitions pane displays all regulations you have saved, along with the date you created them and the last time they were modified.

The Description pane shows a description of the selected regulation. You can edit the description in this pane. This description will show up as a tooltip in the regulatory comparison dialog as you move the mouse over the name of the comparison in the heading pane.

The Details pane reveals the selected constituent(s) and material(s), the latter ones grouped by type.

Indicator lines editor

Indicator lines are horizontal or vertical lines in a graph, from the start to the end of the graph scale.

Indicator lines can be defined in pH-dependent graphs only and have a color, a thickness, a pattern, a value and optionally a label. Vertical indicator lines have a pH value and horizontal indicator lines can have a concentration in mg/l, and a release value in mg/kg.

To ease the application of indicator lines in a series of graph, indicator lines are grouped into definitions. You can create one or more named definitions with the Indicator lines editor.

In a definition, you can add sets of lines for every LeachXS constituent you like.

All sets can be edited, thus allowing using a different set of lines for every constituent.

When a new definition is created, it will contain a default set of lines. This set serves as a template for all constituent line sets that are added after the creation of the definition.

This default set may come in handy if you want to build a consistent definition with sets of lines.

Editor Layout

If you activate the editor from one of the regulation dialogs, a dialog will pop up with a number of panes.

The Available Definitions pane contains all currently defined line definition sets. If there was a previously selected set in the regulation dialog at the time you started the

Indicator lines editor, this pane will have two tab pages: one called All, displaying all sets known to LeachXS and one called Selected with the currently selected set. Note that this last set can by a physical copy of a set in the All tab page. It can be edited independently from the one it is copied from, without changing its originator.

Below this pane is the Definition description field. If a definition is selected, you can modify this description.

The Line indicators pane shows the lines that are defined for a selected constituent or the default line set of a definition in the Available Definitions pane. Note that this pane is not visible if a definition is selected.

The pane contains a number of buttons to manipulate the displayed lines:

- The Clear button removes all lines.
- The Default button will change the line set to the default set. If a constituent is selected in the Available Definitions pane, the set will be made equal to the set of default lines that are defined for the definition in effect. If the default line set is selected, the set will be made equal to the general default line set, having two horizontal and two vertical lines.
- The Edit button will show a dialog for editing an individual line. Not that you can edit the concentration and pH values of the line in the Quick edit values pane as well.
- The Add button will help you in adding a new line by showing the same dialog as when pressing the Edit button.
- Finally, the Delete button deletes the line that is currently selected.

Example

As an example, let's say you want to create a new definition, named "*My Definition*", for a number of constituents having the following lines:

- All graphed constituents will have three lines, two vertical lines and one horizontal.
- The vertical lines should be red, thick, dashed and have a label. They should be drawn at pH values 5 and 9.
- The horizontal line should be green, thick and dotted, without label. The concentration or release values (whichever value is displayed) vary at different constituents.

From a regulatory comparisons editor, press the Select… button in the **Indicator lines definition** group box, and select the **All** tab.

Now, select **Root**, press the right mouse button and select **Add definition…**

Type **My Definition** in the appearing dialog box.

A new definition with the above name is created. Expand the node by pressing the plus sign before the definition and select the **Default lines** node. You'll see that a set of four lines is created for you: two horizontal and two vertical lines. Since we need only one horizontal line, delete one of the horizontal ones by selecting one and pressing the **Delete** button.

The dialog window should look like this:

Now, we will format the lines properly. Select the horizontal line and press **Edit**.

Because the system color

In the appearing dialog window, change the **Type** to *Dot*, the **Weight** to *Thick*

set is different from and much larger than the Microsoft Excel color set, the color you selected may appear slightly different in Excel.

and the color to your favorite green color by pressing the … button.

The Label field should be left blank, while the concentration and release values remain unfilled, because these values will vary for every constituent we will define later on.

Now, edit the vertical lines analogous to the horizontal line.

The **Type** should be *Dash*, the **Weight** *Thick.* Fill the **Label** field with *pH=5* and the **pH value** box with *5*.

Edit the other line like the previous one, but now for *pH=9*.

We will now add some constituents.

Select *My Definition* in the **Available Definitions** group box, press the right mouse button and select **Add/remove constituents**.

Select the constituents *Al*, *Ba* and *Ca* in the constituent selection dialog window. When you press **OK**, you will notice that the constituents are added to the definition.

Now, you can define release or concentration values for the individual horizontal lines for each individual constituent. You can type the values right into the **Conc** and/or **Release** field in the **Quick edit** values group box, after you have selected a constituent and the horizontal line.

When done, press the **Save and Close** button. The definition is ready to be used.

Don't forget to check the **Show Indicator Lines** checkbox in the regulatory comparisons editor dialog window.

Further remarks

- Lines will show up only for constituents that are present in the definition.
- Lines that haven't been given a pH, concentration or release value won't show.
- Changing the *Default lines* line set will have effect only on constituents that are added after the changing.
- Notice the two tab pages in the **Available Definitions** group box: all definitions in the **All** tab page are stored apart from the current regulatory comparison dialog window and are available in other dialog windows too. Modifying the definition in the **Selected** tab page will only change the definition copy in the current regulatory comparison dialog window.
- If you select a definition in the **All** tab page, a copy of that definition will be saved within the current regulatory comparison object.

Edit Excel chart layout dialog

With the aid of this dialog, you can change a number of aspects of graphs that are to be exported to Microsoft Excel.

You can change backgrounds, borders or fonts and hide or show gridlines, legend or axis titles and labels.

A chart on this dialog will give you an impression of the result of all the aspects you change. The Default button will restore all settings to their default values.

Statistics

When comparing a lot of samples, the statistical module can assist you in judging the distribution of your data. You can calculate statistical quantities for a single x-value and display average and confidence levels for the entire x-value range.

- The statistical module is implemented in the following LeachXS windows:
- Comparison of granular and monolithic materials.
- Comparison of landfill data.

Module layout

The module has four panes. The top pane of the module holds a number of parameters that determine how the statistical data is gathered. The bottom pane shows all the materials that were initially selected for statistical analysis. The middle pane on the left side displays a graph with a schematic distribution of the x-values of the selected materials and a line indicating the number of datapoints available at a certain x-value. The middle pane on the right is used to reveal a statistical analysis of a given x-value. You can view some key figures, frequency distribution data or a graphed frequency distribution.

The top pane

This pane has a number of parameters to control the analysis.

Confidence percentage	Determines the percentage of confidence that is used to calculate confidence levels around the average of the data.
Number of frequency bins	Determines the number of bins to use in order to make a frequency distribution graph when calculating statistical data for a single x-value. Note that the actual number of bins used might be a bit larger or smaller in order to create nice bin intervals.
Interpolation mode	If you compare a lot of materials at a certain x-value, it is unlikely that all data have measured values at that specific point. An estimation of the y-value at that point can be obtained by interpolating the dataset linearly, by evaluating linear bicubic splines through the y-values, or by taking the nearest measured value.
Y-values statistics calculation	You can choose to calculate statistical data on the y-values or on the 10-based logarithm of the y-values.
Number of x-values to use for interpolation	This number affects the smoothness of the average and confidence level curves drawn. The larger the number, the smoother the curves will be.

The bottom pane

This pane shows all materials that can be included in a statistical analysis. Every material has a checkbox. If a material is checked, it is included in the analysis data and graphs. Uncheck it if you want to exclude the subject material from the analysis.

The middle left pane

This pane will assist you in getting an idea of the number of y-values are present for analysis at a certain x-value. Every red line represents a schematic view of the range of x-values of a certain material, the top line being the first selected material. The blue line indicates the number of y-values available at a certain x-value. If you click on an endpoint of a red line, the corresponding material in the bottom pane will be colored red, helping you to identify the data series.

The middle right pane

In this pane you can calculate and visualize statistical data for a certain x-value. At the top, you can specify the x-value. To the right of this field, the allowable range of x-values is displayed.

The results are grouped in three tab pages. The first tab contains a number of statistical entities. The second tab shows the frequency distribution. The last tab contains a graphical representation of the distribution. You can inspect the materials in a distribution bin by clicking on any bar; the materials in the clicked bin are colored red in the bottom pane.

Some notes on calculations

Interpolation

How spline interpolation is carried out depends on the distribution of your y-values. If the values are usually displayed on a logarithimic scale, splines are calculated by using the 10-based logarithm of the existing y-values. This is done in order to prevent undesirable oscillation of the splines, especially at low y-values.

If your x-values are usually shown on a linear scale (e.g. pH-values) the x-values where interpolation is done are distributed evenly: the interval between successive values is kept constant. However, if the values are usually shown on a logarithmic scale (e.g. L/S or time), the interval between the logarithm of successive values is kept constant.

The main menu bar

The main menu bar gives you access to actions that are not specifically related to any of the actions in the tree-like panel.

File

Select database…

This entry enables you to change the database where LeachXS retrieves all materials and their related data. A file dialog will appear. Locate your database in the appearing dialog and select it.

Warning: If you change the database, all previously saved chemical speciation sessions and solubility prediction cases may become unusable, because your selected materials may not be present in the selected database.

From now on, all actions you take in LeachXS will use the newly selected database.

Verify materials…

Many LeachXS objects hold references to materials that are defined in a LeachXS database. A material reference consists of a unique ID and a name, as it appeared in the database at the time the material was selected in the object. In some situations, these references may not be pointing to the correct database entries. For instance, if you rename a material in your database or if you remove or update one. Although LeachXS is not capable of detecting these changes, you can check all material references with this function.

This option starts the material verifier and enables you to correct the references in the following cases:

- if the name in the reference appears in the database, but the unique ID does not match;
- if the unique ID of the reference appears in the database, but the name does not match.

A dialog will assist you in correcting the references that are not fully matched in the database that is currently active in LeachXS.

View

LeachXS clipboard

LeachXS contains a private clipboard that can be used to copy and paste mineral selections. The Chemical speciation finder and every leaching prediction wizard contain a step where you can select minerals. All the list boxes that hold the currently selected minerals have a context menu that enables you to copy some or all minerals to this clipboard or paste minerals from it, if it is not empty. The context menu is accessed by pressing the right mouse button.

You can display the current contents of the mineral clipboard by selecting the LeachXS clipboard from the View menu.

This small dialog contains a button to Clear the clipboard, to Delete the minerals you selected in the list or to Hide the clipboard again.

Report

The primary export function of LeachXS reports graphs and results to Microsoft Excel. Sometimes, however, you may want to incorporate exported graphs into a word processor. If you ever tried this, you'll probably agree that scaling and positioning graphs on a page neatly is very tedious. For this purpose, LeachXS has a

built-in utility to copy graphs from any Excel workbook to a Microsoft Word document. This utility is especially designed for copying a large number of graphs to one or more pages in Word format.

Overview

With the LeachXS Image report builder, you can open any Excel workbook that contains graphs (including workbooks not created by LeachXS) and copy graphs from the workbook to one or more Word document pages. The size and layout of the pages can be changed, as well as the number of graphs per page. The page format can be defined manually or you can select an existing Word document from which the layout is to be copied.

In addition, you can optionally add a figures title to each page in any font you like.

It is not possible to add the graphs to an existing document directly. LeachXS creates a new, separate Word document. However, this document is easily insertable in an existing document.

The Image report builder

The report builder has four sections and a menu bar.

The LeachXS Export workbook pane displays the name and graphs contained in the Excel workbook that is opened with the Open Export Workbook… entry in the File menu. If a LeachXS workbook was opened, thumbnails of all graphs in the *Charts* worksheet are displayed. For a non-LeachXS workbook, the thumbnails are arranged by worksheet: one row of graphs per sheet.

Next to this pane a larger image is displayed of the selected thumbnail, or, if the Information tab is selected, some information on the graph, if present.

The LeachXS Report document section contains an image of the Word document to be created. A Page browser lets you browse through the pages to be generated.

To the right of this image is the Report Layout pane that is used to define the format of the Word document.

On tab page named Pages you can define the size and layout of the pages: specify Paper size, Nr of pages, page Orientation and all Margins. You can choose to define the margins in inches or in centimeters. If you already have a Word document or document template that will incorporate the generated report, you may find it handy to take over the layout of that document by selecting it by means of the From template… button.

The space on a report page that is left for displaying graphs is the printable area that remains if the margins and the space for a figures title are taken into account. This area is filled with graph slots. The Number of graph slots across and down the area and the Width/Height ratio of a single graph can be defined on the Graphs tab page.

On the third tab page, named Footer you can define a figures title. If you want a figures title to appear, mark the Include Figure title and type a text in the field below. The figure title will appear at the bottom of each report page. You can change the font of the text by pressing the Font… button.

On the last tab page, named Alignment, you can set a horizontal and vertical alignment of the area enclosing the graph slots with respect to the page area within the page margins.

You can add graphs to the report by selecting a number of graphs from the LeachXS Export workbook pane and dragging them with the right mouse button to the

displayed page of the LeachXS Report document. The dragged graphs will be appended to the page, starting with the first free graph slot. Note that the graphs can only be dragged to the current report page. If more graphs are dragged to the page than there are free slots, excessive graphs are not placed.

With the Clear button at the bottom right side of the editor, all graphs are removed from the currently displayed report page. The Delete button deletes any selected graphs on the report page, moving up all graphs in order to fill the vacancies.

You can switch between different Excel workbooks to fill your report: simply open a new workbook from the File menu and keep on dragging.

Don't be mislead by the appearance of the graphs in the Word document. The graphs are optimized for printing.

Finally, if you're happy with your report, save it with the Save Report As… menu entry in the File menu. Note that this may be a rather lengthy operation if you have dragged a lot of graphs to your report.

Help

Contents

This entry will display the help manual you are reading now.

About LeachXS…

This entry will display an about box with the LeachXS version number and release date, along with the name of the licensed user.

Technical topics

LeachXS data organization

Apart from the LeachXS database, the LeachXS software uses other sources of information to perform its tasks and to save and retrieve dialog settings, speciation sessions and solubility prediction cases. This section briefly describes these sources and their locations. LeachXS uses the following locations:

1. **the application installation folder**

   This is the folder that you specified during the installation of LeachXS. The default location is the Leaching folder below the Program Files folder. A typical example is: `c:\Program Files\Leaching`.

2. **the version dependent user application data folder**

   This is a unique folder for every user, application and application version on the system the software is installed on. For version 1.0.4.1 of LeachXS, this folder might look like this: `C:\Documents and Settings\<username>\Application Data\ECN`

TSC\LeachXS\1.0.4.1, where <username> is the name you used when you logged on to your computer.

3. **the version independent user application data folder**

   This is a unique folder for every user, and application on the system the software is installed on. For version 1.0.4.1 of LeachXS, this folder might look like this: C:\Documents and Settings\<username>\Application Data\LeachXS, where <username> is the name you used when you logged on to your computer.

4. **the My Documents folder**

   This is a unique folder for every user on the system. It is used to save documents and pictures. Note that this is a virtual folder the operating system allows you to place this folder anywhere you want.

Main software components

The main software components are located in **the application installation folder**. They have the extension dll. These are used to perform specific tasks, such as:

- showing a data grid;
- showing a wizard;
- building graphs;
- interacting with Microsoft Excel.

Other main components are LeachXS.exe (the executable) and LeachXS.chm (the online help manual).

Orchestra software components

LeachXS utilizes Orchestra to run your chemical speciation sessions and solubility prediction cases. The Orchestra software components are installed along with the installation of LeachXS. The components are installed in a subfolder of **the application installation folder**, named Orchestra.

LeachXS database

When installing LeachXS, a sample database is installed as well. This database is named LeachXS.mdb and is installed in **the version independent user application data folder**. If LeachXS is started for the first time, this database is used. If you want to, you can move the database to another place, e.g. a place that other users can access as well. Use the File menu in the main window of LeachXS to specify the location of the database to use.

Minerals and mineral reactions

Both LeachXS and Orchestra use minerals and mineral reactants. There are three files that provide information about minerals and reactants to exchange information. They are installed in **the application installation folder** and are called MineralReactions.xml, ReactantMapper.xml and LeachXSConstituents.xml.

The first file defines all minerals that can be used and the reactants to form the minerals. The second file defines the mapping of reactants to the constituents that are defined in the LeachXS database. The third file defines all the LeachXS constituents.

Dialog settings

If you use a dialog, its state is saved when you leave it. If you use it again, the saved state of the dialog is loaded. The states of all dialogs are stored in **the version dependent user application data folder**, in binary format. The state of the About box containing your licensed username and key is encrypted as well for obvious security reasons. Every dialog has its own file with its saved state, having the extension `lxs`. Because these states are version dependent, they become useless if you install a new version of LeachXS. Note that when you uninstall LeachXS, the states will not be removed. So if you reinstall the same version of LeachXS, they will be used again.

Chemical speciation sessions

All chemical speciation sessions and all the solubility prediction cases that are dependent on them are stored in a subfolder of **the version dependent user application data folder**. This folder is called `CSPSessions`.

A definition of a chemical speciation session is contained in a file in this folder, with a name equal to the name of the session and the extension xml. Data related to the session is kept in a subfolder of the `CSPSessions` folder, named after the name of the session. The related data comprise:

- Mineral reactions and reactant mapping that is used for the session;
- Calculated data from Orchestra, if the session has been run;
- Dependent solubility prediction cases, if there are any.

Although all this information is stored in **the version dependent user application data folder**, they might be used in a later version of LeachXS. Consult the installation notes for that version of LeachXS for details.

If sessions are compatible in a higher version, follow these steps to make them available in the higher version:

1. The higher version of LeachXS must have been started in order to the version dependent user application data folder to be created.
2. Copy the `CSPSession` folder and all its files and subfolders from **the version dependent user application data folder** of the previous version to **the version dependent user application data folder** of the current version.

Note that you can exchange sessions with other users by giving them the session folder and its files and subfolders along with the session file with the same name.

Tables of LeachXS entities

Material categories and types

Air	
Atmospheric dust	Atmospheric dust samples

Construction	
ASP	Asphalt
CEM	Cement
MBA	Bottom ash
OTH	Other building materials
PCA	Coal fly ash
SLA	Slag
SLU	Sewage sludge
SOI	Soil
Treated wood	Treated wood for preservation purposes

Fuel	
Biomass	Biomass products and residues

Landfill	
APC	APC residues
BIO	Bioreactor
HZW	Hazardous waste
MSW	Municipal solid waste
NHZ	Nonhazardous materials
PIW	Predominantly inorganic waste
STW	Stabilized waste

Ore	
NHZ	Nonhazardous materials

Soil	
Amendment	Soil amendments for increased structure or fertilizer use
Biomass	Biomass products and residues
Compost	Compost

SED	Sediment
SLU	Sewage sludge
SOI	Soil

Construction	
C&D	Construction and demolition waste
HAZ	Hazardous waste
ISL	Industrial sludge
MBA	Bottom ash
MFA	Fly-ash and APC
OTH	Other building materials
SBW	Sand blasting waste
SLA	Slag
SLU	Sewage sludge
SOI	Soil

Test types and subtypes

B	Batch Leaching	
	Acetic acid for Soil	Acetic acid extraction test for soil
	AFNOR X310	AFNOR X310
	ASLP	Australian Standard Leaching Protocol
	AV002.1	AV002.1 (Availability at pH 7.5 with EDTA)
	Bodemsattigungs extract	Bodemsattigungs extract
	CaCl2 extraction for soil	CaCl2 extraction test for soil
	CEN EN 12457 Part 1	1-step leaching test at L/S=2 for materials < 4mm
	CEN EN 12457 Part 2	1-step leaching test at L/S=10 for materials < 4mm
	CEN EN 12457 Part 4	1-step leaching test at L/S=10 for materials < 10mm
	Concise	Concise test (L/S=1 en L/S=10 extraction own pH)
	DIN 384141 S4	DIN 384141 S4
	Draft availability leaching	Draft availability leaching test for hydrophobic organic contaminants (1000 mg/L Aldrich humic acid, pH=12; L/S=100)
	DTPA extraction for Soil	DTPA extraction for soil
	EDTA extraction for Soil	EDTA extraction for Soil
	ISO/AWI 21268	ISO/AWI 21268 – 1 and 21268-2 L/S=2 and L/S=10 ISO/TC 190
	JLT-13	JLT-13
	LS100 extraction	Batch leaching test, L/S=100, 48 hours, native pH.
	NaNO3	NaNO3 extraction test
	NordTest	Danish batch leaching test

	Porewater test	Porewater test (extraction, pressure-filtration, centrifugation, immiscible displacement etc., to be specified by qualifier)
	QC leaching test	Short compliance leaching test, L/S=2 at native pH for one hour.
	SR003	SR003.1 (Solubility and Release as a Function of LS Ratio)
	Swiss TVA	Swiss TVA
	TCLP	TCLP
	Tenax-extraction	Tenax-extraction test for hydrophobic organic contaminants (Cornelissen et al.; Shor et al.)

K	Kinetic experiments	
	Batch	Kinetic experiments in batch leaching tests to test time dependency

L	Landfill measurments	
	Groundwater	Groundwater measurements
	Lysimeter Monolithic	Lysimeter experiments
	Percolation	Percolation water measurements
	Pilot Monolithic	Pilot experiments for monolithic materials

M	Monolithic leach	
	ANS 16.1	ANS 16.1
	CEN TC 292 Dynamic	Dynamic leach test CEN TC 292 (in development)
	CEN TC 292 Monolith	Monolith compliance leaching test Cen TC 292
	Lysimeter Monolithic	Lysimeter experiments
	MT001.1	MT001.1 (Mass Transfer Rates in Monolithic Materials)
	MT002.1	MT002.1 (Mass Transfer Rate in Granular Materials)
	NEN 7345	Tank leach test
	NEN 7345 pH7	Tank test pH driven by CO_2
	NEN 7345 Short	Short tank leach test (24h)
	NVN 7347	Compacted granular leach test
	OECD guideline 1	OECD guideline for the testing of chemicals proposal for a new guideline (I)
	OECD guideline 2	OECD guideline for the testing of chemicals proposal for a new guideline (II)
	Unspecified Monolith	Unspecified test monolithic test

C	Percolation	
	ISO/AWI 21269-3	ISO TC 190 WG6

	Lysimeter Percolation	Lysimeter experiments
	NEN 7343	NEN 7343
	NEN 7394	Column leaching test under anaerobic conditions
	NEN7383	Leaching characteristics - Determination of the cumulative leaching of inorganic components from granular materials with a simplified procedure of the columm test - Solid earthy and stony materials
	NVN 7344	NVN 7344 for (RIVM; hydrophobic organic contaminants)
	Pilot Experiments	Pilot Experiments
	PrEN 14405	CEN TC 292

P	pH Dependence	
	ANC	PrEN 14429 ANC test
	Concise leach	Concise leach test (pH controlled steps)
	pHStat	pH stat test CEN TC 292 WG6
	SR002	SR002.1 (Alkalinity, Solubility and Release as a Function of pH)

E	Sequential chemical extraction	
	SCE BCR	SCE BCR
	SCE Tessier	SCE Tessier

S	Serial Batch	
	Availability	Availability test
	Cascade	Cascade test
	CEN EN 12457 Part 3	EN 12457-3 (incl. modified procedure for hydrophobic organic contaminants)
	Leachant renewal	Serial batch test with leachant renewal
	Solid renewal	Serial batch test with solid renewal

T	Total Composition	
	Acid neutralization	Acid neutralization test CEN TC 292
	Actually-soluble organic carbon	Actually-soluble organic carbon (DOC at neutral pH); draft standard ANVM247
	Aqua regia	37% HCl + 65% HNO3
	Ascorbic acid extraction	Ascorbic acid extraction (HFO specific)
	B1	
	B1/B8	
	B5	

	B8	
	Dithionite extraction	Dithionite extraction (crystalline Fe)
	DOC neutral pH	DOC at neutral pH (biodegradability test)
	GC-MS	GC-MS
	HCLP	HCLP
	HF acid mix	HF acid mix
	HF+aqua regia	Digestion with mixture of HF and aqua regia
	HNO3	HNO3
	IHSS procedure	IHSS procedure (humic and fulvic acids; solid/leachate; incl. FAST/SUPERFAST)
	Inert carbon	Inert carbon (draft standard ANVM247)
	LiBO3 melt	LiBO3 melt
	Monolithic character	Monolithic character test CEN TC 292
	MT	
	N1	
	NAA	NAA
	Non-water soluble organic carbon	Non-water soluble, potentially degradable organic carbon; draft standard ANVM247
	NVN7348	NVN7348 redox capacity test
	Oxalate extraction	Oxalate extraction (amorphic/poorly-crystalline Fe and Al)
	pH001.0	pH001.0 (pH Titration Pretest)
	Potentially-soluble organic carbon	Potentially-soluble organic carbon (DOC at high pH after acid treatment); draft standard ANVM247
	PS001.1	PS001.1 (Particle Size Reduction)
	S1	
	S1/Aquaregia	LiBO4 melt and aquaregia
	Unspecified total	Unspecified total composition test
	XRD	XRD
	XRF	XRF

Constituents

Inorganic constituents

Ac	Cr(III)	La	Po	Th
Ag	Cr(VI)	Li	PO4	Thiocyanates
Al	Cs	Lr	PO4P	Ti
Am	Cu	Lu	Pr	Tl
Ar	Db	Md	Pt	Tm

As	DIC	Mg	Pu	U
At	Dy	Mn	Ra	V
Au	Er	Mn(II)	Rb	W
B	Es	Mo	Re	Xe
Ba	Eu	Mt	Rf	Y
Be	F	N	Rh	Yb
Bh	Fe	Na	Ru	Zn
Bi	Fe(II)	Nb	S	Zr
Bk	Fluoride free	Nd	S2-	
Br	Fm	Ne	S2O3	
C	Fr	NH3	Sb	
Ca	Ga	NH4	Sc	
CaCO3	Gd	NH4N	Se	
Cd	Ge	Ni	Sg	
Ce	H	No	Si	
Cf	He	NO2	Sm	
Cl	Hf	NO3	Sn	
Cm	Hg	Np	SO3	
CN	Ho	O	SO4	
CNC	Hs	Os	Sr	
CNT	I	P	sum heavy metals	
CNV	In	Pa	Ta	
Co	Ir	Pb	Tb	
CO32-	K	Pd	Tc	
Cr	Kr	Pm	Te	

Organic constituents

(p+m)-Xylene	Chlorobenzenes non-volatile	ONB_sum
1,1,1,2-Tetrachloroethane	Chlorobenzenes volatile	OPB_sum
1,1,1-Trichloroethane	Chloroform	o-PO4
1,1,2,2-Tetrachloroethane	Chlorophenol	Organotin (sum)
1,1,2-Trichloroethane	Chloropyrifos-Ethyl	O-Xylene
1,1-Dichloroethane	CHR	PAH WCA
1,1-Dichloroethene	Cis-1,2-dichloroethene	PAH-Bornhef
1,1-Dichloroethylene	CIS-1,2-DICHLOROETHYLENE	PAH-EPA
1,1-Dichloropropene	Cis-1,3-Dichloropropene	PAH-VROM
1,2,3,4-Tetrachlorobenzene	Cis-chlordane	PAK-VROM
1,2,3-Trichlorobenzene	Cis-heptachloroepoxide	Parathion-Ethyl
1,2,3-Trichloropropane	Citric acid	Parathion-Methyl
1,2,4-Trichlorobenzene	COD	PCA sum

1,2,4-Trimethylbenzene	COD unfiltered	PCB_sum
1,2-Dibromide-3-chloropropane	coronene	PCB101
1,2-Dibromideethane	Cresols	PCB118
1,2-Dichlorobenzene	Cyclohexanon	PCB138
1,2-Dichloroethane	DAA	PCB153
1,2-Dichloroethene	DBA	PCB180
1,2-Dichloropropane	DCM	PCB28
1,2-Trichloroethylene	DDD TOT	PCB52
1,3,5-Trimethylbenzene	DDE TOT	PCP
1,3-Dichlorobenzene	DDT TOT	Pentachlorobenzene
1,3-Dichloropropane	delta HCH	Pentanoic acid
1,4-Dichlorobenzene	DFA	Pesticides sum
1235/1245-Tetrachlorobenzene	DHA	PHE
1-methyl-NAP	DHY	Phenol
2,2-Dichloropropane	Diazinon	Phenol index
2,3-Dimethylphenol	Dibromidechloromethane	Phenol sum
2,4 DDD	Dibromidemethane	Phthalates (sum)
2,4 DDE	Dichlorodifluoromethane	PolySulphide
2,4 DDT	Dichloromethylene	Prometon
2,4/2,5-Dimethylphenol	Dichlorophenols	Prometryn
2,6-Dimethylphenol	Dichlorovos	Propazine
2-Chlorotoluene	Dieldrin	Propiconazole
2-Ethylphenol	Dimethoate	Propionic acid
2-methyl-NAP	Disulfoton	p-Xylene
2-Methylphenol	DOC	PYR
3,4-Dimethylphenol	DOC Unfiltered	Pyridine
3,5-Dimethylphenol	DOC_AV	Pyruvic acid
3+4-Ethylphenol	DOC_HA	Resorcinol
3+4-Methylphenol	Drins	sec-Butylbenzene
4,4 DDD	Endrin	SFA
4,4 DDE	EOCL	SHA
4,4 DDT	EOX	SHY
4-Chlorotoluene	Ethylbenzene	Simazine
4-Isopropyltoluene	Fatty acids	Styrene
ACE	Fenthion	Sulphide sum
Acetic acid	FLA	Sum non-volatile Chlorobenzenes
ACY	FLT	Sum volatile Chlorobenzenes
Aldrin	FLU	Sum_ONB/OPB
alfa HCH	Formic acid	Suspended particles
alfa-Endosulfan	gamma HCH	TDS
ALK	Halogenated hydrocarbons sum	Tebuconazole

Alkylphenols sum	HCH (sum)	telodrin
Ametryn	HCO3	Terbutryn
Amoniacal copper quat	Heptachlor	tert-Butylbenzene
ANT	heptachloroepoxide	Tetrachloroethene
Aromatic hydrocarbons sum	Hexachloro 1,3-butadiene	Tetrachloromethane
Atrazine	Hexachlorobenzene	Tetrahydrofuran
BAA	Hexanoic acid	Thiofuran
BAP	Hydrocarbons sum	Toluene
BBF	Hydrochinon	Trans-1,2-dichloroethene
BBF+BKF	Indamprest	TRANS-1,2-DICHLOROETHYLENE
Benzene	IPY	trans-1,3-Dichloropropene
BEP	Isodrin	Trans-chlordane
beta HCH	Isopropylbenzene	Trans-heptachloroepoxide
beta-Endosulfan	Lactic acid	Tribromidemethane
BGP	M/P-Xylene	Trichloroethene
BKF	Malathion	Trichloroethylene
BOD	Maneb	Trichlorofluoromethane
BOD20	Methylene chloride	Trichloromethane
BOD5	mevinphos	Valeric acid
BPE	Min_oil	Vinylchloride
Bromidebenzene	Min_oil C10-C12	Volatile fatty acids
Bromidechloromethane	Min_oil C12-C22	VOX
Bromidedichloromethane	Min_oil C22-C30	VOX minus DCM
Bromophos-Ethyl	Min_oil C30-C40	Xylene
Bromophos-Methyl	Monochlorobenzene	
BTEX	m-Xylene	
Butyric acid	NAP	
C-2 Alkyl phenols	Naphtol	
C-3 Alkyl phenols	n-Butylbenzene	
C-4 Alkyl phenols	N-Kj	
Carbaryl	Non-chlorinated pesticides	
Carbofuran	n-Propylbenzene	
Catechol	NVOC	
Chlooraniline (sum)	O2	
Chloornaftaleen (sum a, b)	OCB_sum	
Chlorobenzene	Oil	

Glossary of Terms

acid neutralization capacity

The amount of acid, expressed in mol/kg, required to neutralize a given weight of material to a stable neutral pH.

availability

The quantity of a constituent that can be leached from a material under conditions that under extreme conditions could be reached in the environment or at the very long term.

base neutralization capacity

The amount of base, expressed in mol/kg, required to neutralize a given weight of material to a stable neutral pH.

batch tests

Leaching tests which are carried out on a single portion of material using a single portion of leachant i.e. there is no renewal of leachant during the test.

buffer

A solution containing both a weak acid and its conjugate weak base whose pH changes only slightly on addition of acid or alkali.

carbonation

Uptake of carbondioxide in an alkaline material

cation

An ion with a positive charge.

complexation

The formation of an ion into a molecular structure consisting of a central atom bonded to other atoms by coordinate covalent bonds

concise test

Combination of selected batch leaching tests to cover 3 pH conditions and 2 L/S conditions in 4 extractions as a concise characterisation of a materials leaching behaviour.

DIC

See dissolved inorganic carbon.

diffusion

The spontaneous mixing of one substance with another when in contact or separated by a permeable membrane or microporous barrier.

dissolution

Molecular dispersion of a solid in a liquid.

dissolved inorganic carbon

This usually represents carbonate species.

dissolved organic carbon

Natural or artificial organic matter remaining in dissolved state in solution (e.g. humic and fulvic acids).

DOC

See dissolved organic carbon.

E_H

A measure of the oxidation reduction potential. See **oxidation/reduction**.

eluate

As **leachate** but usually in the context of a laboratory test.

emission

Release of substances from one environment, medium or phase to another.

equilibrium

Chemical equilibrium is a condition in which a reaction and its opposite or reverse reaction occur at the same rate resulting in a constant concentration of reactants.

Physical equilibrium is exhibited when two or more phases of a system are changing at the same rate so the net change in the system is zero.

extraction

A separation operation that may involve three types of mixture:

3. a mixture composed of two or more solids
4. a mixture composed of a solid and a liquid - as in this context
5. a mixture of two or more liquids.

One or more components of such a mixture are removed (extracted) by exposing the mixture to the action of a solution or solvent in which the component to be removed is soluble.

infiltration

The movement of water (usually rainwater) into and through a solid material.

inorganic

Chemicals that are generally considered to include all substances except hydrocarbons and their derivatives or all substances which are not compounds of carbon with the exception of carbon oxides and carbon disulphide.

ionic strength

A measure of the concentration of ions in solution.

leachant

Liquid in contact with or which will be brought in contact with a solid which extracts soluble components of the solid.

leachate

Liquid containing soluble components extracted from a solid (usually linked to field conditions; e.g landfill leachate).

leaching

The process by which the soluble components of one phase (usually a solid) are transferred to another phase (usually a liquid).

liquid to solid ratio

The liquid to solid ratio relates to the amount of liquid used in a batch leaching test to extract a given amount of solid. Abbreviation: L/S Unit : l/kg

organic

Chemicals that are generally considered to include all compounds of carbon except carbon oxides and sulphides.

oxidation/reduction potential

A measure of the ability of a system to cause oxidation or reduction reactions. Oxidation and reduction are reactions in which electrons are transferred. Oxidation and reduction always occur simultaneously (redox reactions). The substance that gains the electrons is termed the oxidizing agent and the substance that loses the electrons is termed the reducing agent.

partitioning

The distribution of molecules in different states or phases in a system for example as solid, liquid or gas or as separate chemical entities, such as minerals, sorbed phases or solid solutions.

pE

A measure of the redox potential.

percolation

The movement of a liquid through a solid.

pH

pH is a value taken to represent the acidity or alkalinity of an aqueous solution.

pH static leach test

A leaching tests consisting of a number of individual extractions of sub-samples of the same material at pH values fixed by addition of acid or base as required.

POM

Particulate organic matter.

porosity

The relative volume of void space to the total volume occupied by a material.

potential leachability

The quantity of a constituent that can be leached from a material under conditions that under extreme conditions could be reached in the environment or at the very long term.

precipitation

The settlement of small particles out of a liquid or gaseous suspension by gravity or as the result of a chemical reaction.

redox

See oxidation/reduction potential.

solubility

The ability or tendency of one substance to blend uniformly with another e.g. solid in liquid, liquid in liquid, gas in liquid, gas in gas. Solids vary from 0% to 100% in their degree of solubility in liquids depending on the chemical nature of the substances.

sorption

A surface phenomenon that may be either absorption, adsorption or a combination of the two. The term is often used when the specific mechanism is not known.

speciation

Determination of the precise chemical form of a substance present in a solid material, in a liquid or in a gas.

standard

A documented method or specification to which activities should conform.

Index

N

O

P

R

S

T

U

V

W

X

Y