

# The LeachXS Material Exchange System

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## Introduction

The LeachXS Material Exchange System has been designed to exchange information about leaching data, obtained from laboratory tests or field samples.

The heart of this system is an XML-structured file that contains all measured data of one or more lab or field samples. In this document, such a file is called: a Central Data Store, or CDS.

The exchange system has two types of modules:

- *Reader* modules read data from some kind of data container (e.g. an Excel workbook, or a laboratory database) and transform the contents or part of it to a central data store.
- *Writer* modules write the contents of a central data store to some kind of data container (e.g. a LeachXS database, or a Word document).

The exchange system is capable of loading reader and writer modules dynamically. In fact, new modules can be developed and added to the system. Because of the nature of the modules, they are called plug-ins. Throughout this manual, reader and writer modules will be called plug-in readers and plug-in writers.

The current Material Exchange System that is shipped with this document contains one Reader and one Writer. The plug-in reader creates a CDS from a specially formatted Excel workbook containing leaching data. The structure of this workbook is described in detail in one of the next chapters in this workbook. The plug-in writer adds the contents of a CDS to a LeachXS database.

### ***Adding your measured data to a LeachXS database***

As explained in the previous section, if you want to add your own data to a LeachXS database, you'll need to take the following steps:

1. Create an Excel workbook and fill it with your data;
2. Start the Material Exchange software;
3. Load and run the plug-in reader that will create a CDS from your workbook;
4. Load and run the plug-in writer that will put the data from the CDS into your LeachXS database.

This might be a bit cumbersome, but there are advantages:

- The CDS that is created during the process can be used as a platform independent vehicle to exchange leaching information with other people or systems.
- Plug-ins that can read from or write to other data storage systems can easily be developed.

## The software

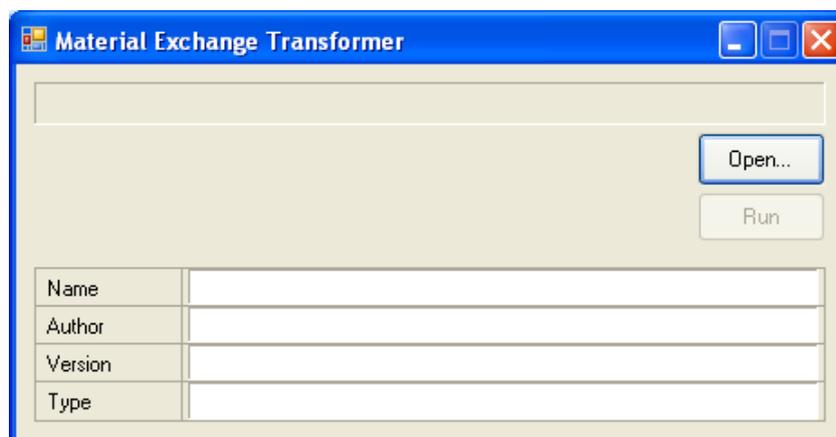
### Installing

The material exchange software will be installed when you execute `setup.exe`, which you will find in the same directory as this document. This will install:

- **The Material Exchanger.**  
This is the part that can load and execute readers and writers. By default, it will be installed in subdirectory `LeachXS` of your `Program Files` map.
- **A plug-in reader named StandardExcel.**  
This plug-in is capable of creating a CDS from a specially formatted Excel workbook containing leaching data. The plug-in is installed in subdirectory `Plugins\Readers` of the map where the Material Exchanger is installed.
- **A plug-in writer named AccessDBWriter.**  
This plug-in can read a CDS and add its contents to a LeachXS database. The plug-in is installed in subdirectory `Plugins\Writers` of the map where the Material Exchanger is installed.

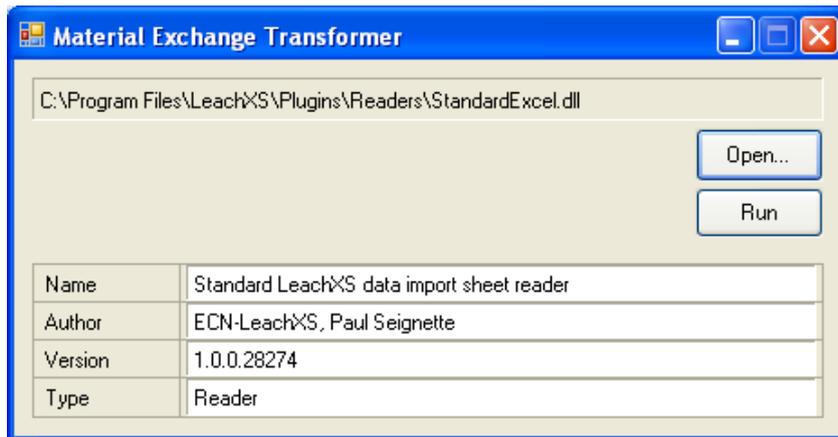
### Using the software

After you have installed the material exchange software, a shortcut with the name Material Exchanger has been placed in the **Start** menu. Double-click it to start the program. A small window appears that looks like this:



On the right there is the **Open...** button. Use this button to select a desired plug-in reader or writer.

As an example we'll open the `StandardExcel` plug-in reader in order to process an example workbook. Press the button. A dialog appears, assisting you in specifying the appropriate plug-in. Initially, the location that appears in the dialog is the map where the material exchange software is installed. Navigate to map `Plugins\Readers`, select `StandardExcel.dll` and press the **Open** button. The plug-in will be loaded and will present its details in the main window of the Material Exchanger:



Press the **Run** button to put the plug-in to work.

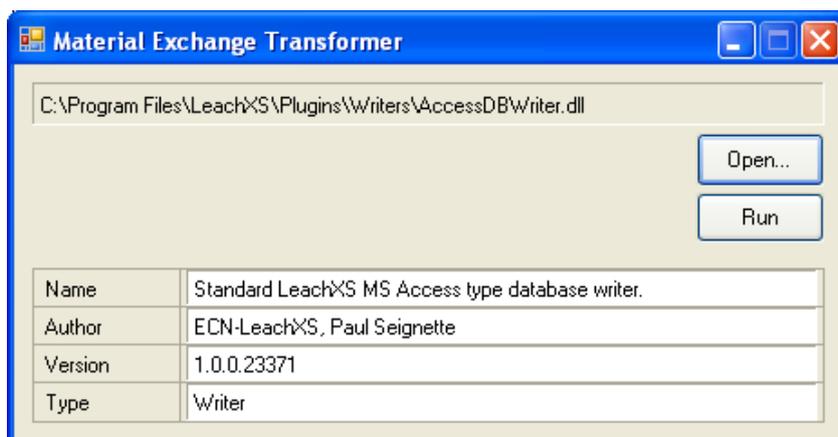
The first thing the plug-in must know is the Excel workbook to process and it will ask you to specify the name and location of the workbook. Navigate to the same location as where you have found this document. It should contain workbook `Example.xls`. Select this file and press the **Open** button.

Now, the plug-in will process the workbook and will report its progress and error messages in a separate window. If all went well and no errors were encountered, the Material Exchanger will ask you to specify a CDS where the read data should be put in. Select a name and location that suits you in the appearing dialog and press the **Save** button. The CDS has been created. Now, you can browse through the progress messages if you like.

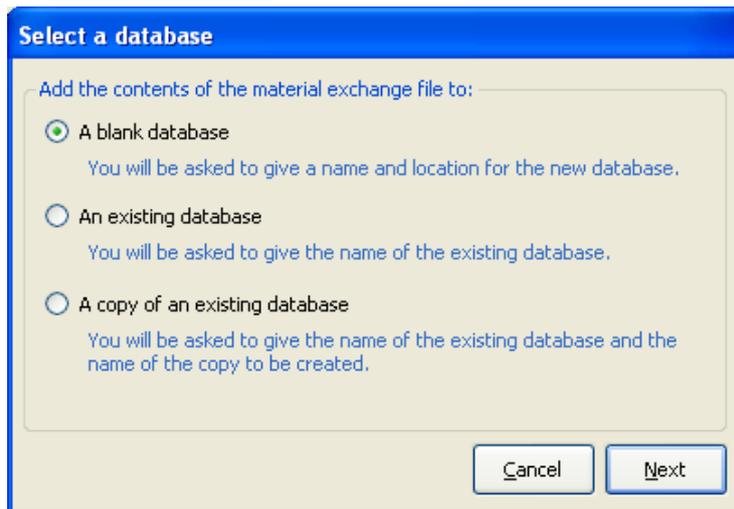
If you are interested in how the CDS is structured, double-click on the file you just saved. The file is opened in the Internet Explorer by default, but if you have another xml file viewer or editor installed the file will show up in that tool.

As a second example, we will create a new LeachXS database with the data that was stored in the CDS we just created.

Press the **Open...** button again in the Material Exchanger and locate the AccessDBWriter plug-in. It is located in the map `Plugins\Writers`. Open it. The Material Exchanger window should look like this:



Press the **Run** button. You will be asked to specify the name and location of a CDS. Locate the file created with the StandardExcel reader and open it. Now, the plug-in will be put to work. It will need a LeachXS database to put the data from the CDS in and the following dialog is presented:



Let's put the data in a new, empty database. Select the first option and press the Next button. The plug-in will ask you to give a name and location to the new database that will be created. Select a location, type a name and press the **Save** button. The plug-in will process the data, writing messages to the appropriate message window.

## General data structure

Before going into details about the supplied plug-ins, this chapter contains information about how leaching data is laid out internally. If you have some knowledge about how data is structured, it is probably easier to prepare the input data for plug-in readers.

For the results of laboratory leaching tests, following entities are present in the data structure:

- Sites
- Materials
- Leaching tests
- Positions (or fractions)
- Analyses

The entities are connected in a hierarchical way:

A material undergoes one or more leaching tests. A leaching test usually contains one or more test positions or fractions. For instance, for a pH dependence test, the material is split up in a number of fractions, and each fraction will be brought to a certain pH value. After that, the eluate of each fraction is analyzed: a concentration or emission is measured for one or more constituents. Therefore, one or more analyses belong to a fraction.

Every entity contains information that belongs to that specific entity. Some values to an entity are mandatory and some are optional. Which entity values are mandatory and which are optional will be described in the chapter about the structure of the workbook templates that are read by the StandardExcel plug-in reader.

One entity is left undescribed, and that is the Site entity. This entity is optional. You can organize material entities as coming from certain sampling sites, if you like.

Site entities do play an important role in the specification of field data. The lay-out of field data is currently still under construction, and will be described in a later version of this document.

## Plug-in reader: StandardExcel

### **Introduction**

The StandardExcel plug-in reader is capable of creating a CDS from leaching data in an Excel workbook. Such a workbook needs to be structured in a way to be understandable by the reader. Currently, two workbook templates are shipped with the material exchange software. The first template, named `AllTests.xlt`, can be used to specify leaching data for the following main test types:

- Total Composition methods
- pH dependence tests
- Monolithic Leach tests
- Column tests
- Concise Leach tests
- Single and Parallel Batch tests
- Sequential Chemical Extraction tests
- Serial Batch tests

The second template, named `MainTests.xlt`, is a simplified version of the first template, and can be used if you have data for the following, mostly used tests:

- pH dependence tests
- Monolithic Leach tests
- Column tests

These workbook templates are installed in directory

`Plugins\Readers\StandardExcel` of the map where the Material Exchanger is installed. The easiest way to create a new workbook to fill is double-clicking one of the two templates. If you want to create new workbooks by using the **File->New...** menu entry in Excel, you must copy the two templates to the Excel template location. This is by default:

`C:\Documents and Settings\\Application Data\Microsoft\Templates`

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

### **The workbook structure**

The workbook contains two types of worksheets. Firstly, there are sheets where you can specify your data. The sheet tabs are colored according to their purpose:

- Green (  ) for specifying site information;
- Yellow (  ) for specifying material specific information;
- Light yellow (  ) for specifying leaching test specific and fraction specific information;
- Light blue (  ) for specifying analyses.

Secondly, there are sheets that contain lookup information. These sheets are colored light green (  ). Some of the sheets are used to fill lists that assist you in choosing an acceptable value in data entry sheets, while other sheets can be used as a reference. For instance, you can optionally specify a US waste code (EPA code) for a material. The sheet named *EPA codes* contains a list of a large number of EPA codes and their descriptions.

One sheet is colored orange (  ). This sheet is named *International*. This sheet is present on behalf of the plug-in reader. It contains the layout of the entire workbook and instructs the reader where to look for specific information. It can also be used to create workbooks in other languages. For now, do not touch this sheet. It is beyond

the scope of this manual to explain how to translate the workbook to another language. If you want to have a localized version of the workbook, please contact the LeachXS team.

### ***Lay-out of the data entry sheets***

All data entry sheets have the following lay-out:

The first 5 rows serve as identification and grouping of the data and must not be changed.

The first row has a dark grey color and groups columns into sections with a specific purpose.

The second and third rows contain column headings. They specify what kind of information is to be supplied in the cells below the headings, starting from the sixth row. Usually, the cells in the second row have a comment attached to them, giving details about the information to be supplied. Every column heading has a specific background and foreground color according to their purpose. The background color indicates to what entity the information belongs to:

Green	This column contains site-specific information.
Yellow	This column contains material-specific information.
Light yellow	This column contains leaching test-specific information.
Pink	This column contains position or fraction-specific information.
Light blue	This column contains analysis-specific information.

The foreground color is red or black. You must fill cells below a red-colored heading, while black-colored headings are optional: you can leave them blank.

The fourth and fifth rows contain the format or unit of measurement of the data to be supplied below them. You must not change the units of measurement.

The meaning of the most occurring phrases that are not units of measurements:

From <ref>	The supplied value must match a value that is present in another sheet. Which sheet is meant is indicated by <i>ref</i> .
[A-Z]	Enter a single capital. This format is used to define a material, test, position or analysis multiplicates. If you do not have measured multiplicates, just type "A".
\d+	Enter a positive integer number. This format is used to identify fractions or test positions. If fractions have a logical sequence, e.g. in time, like in a column or Monolithic Leach test, number them ascending.
from list	The supplied value must be one of a list. Usually, clicking on a cell that should contain a value from a list will reveal a small button next to it. Clicking that button will display the list and enables you to pick one of its entries.
text	The supplied value can be any text. If the information to be entered is mandatory, it cannot be left blank or filled with spaces. Note that trailing or leading spaces are always ignored.

## **Filling the sheets**

The reader processes the sheets in hierarchical order. First, it reads the sites. Then, the materials are read. After that, the reader walks through all sheets that contain information about leaching tests, accompanied by data on positions and fractions. Finally the analyses are read.

When data on a sheet is processed, the reader continues processing until the first column in a row of a sheet is empty. Therefore, be sure that you do not leave rows blank before the last data row.

The next sections of this chapter provide a detailed description of every sheet that can be filled. We start with the top level entities in the data hierarchy, sites and materials.

### **Sheet Field Sites (3a)**

If you have any materials that are taken from a site, you can use this sheet to define the sites. If not, you can leave this sheet blank. Every row defines one site.

The first 3 columns uniquely define a site:

<b>Column</b>	<b>Unit/format</b>	<b>Description</b>
Site name	text	This is the name of the site samples are collected from.
Site type	from list	This is the main type of the site or its category.
Site subtype	from list	This is a refinement of the type or category of the site.

The following columns are optional:

<b>Column</b>	<b>Unit/format</b>	<b>Description</b>
Site surface area	m <sup>2</sup>	This is the surface area of the entire site.
Site average height	m	This is the average site height in meters above sea level. Note that it can be negative if the site is below sea level.
Site density	kg/m <sup>3</sup>	This is the average density of the subject sample.
Average infiltration	mm/year	This is the average rate water is infiltrated on the site in millimeters per year.
Originator ID	text	This is the unique identification code for the site, as assigned by the organization governing the site.
Processor ID	text	This is the unique identification code for the site, as assigned by the organization using the site data.
Project or literature citation	text	This is the identifier or citation used to identify where the information was obtained from or project that the site is associated with. Ideally, this would be citation to a document that would provide further information on the site.
Remarks	text	This field is for any additional comments you may have regarding the site.
Attachments	file;file;...	Files attached to the Field location. Specify a list of file specifications, separated by semicolons.

### **Sheet Material Info (1a)**

Every row defines one material/multiplicate combination.

The first 2 columns uniquely define a material:

<b>Column</b>	<b>Unit/format</b>	<b>Description</b>
Short name	text	This is the common name of the material to be displayed as the material identity in the LeachXS database. The combination of Short name and Material replicate must be unique.
Material replicate	[A-Z] or \d+	The material replicate is used to differentiate between sub-samples of the same primary sample or a temporal sequence of samples. Use of a letter code (e.g. A, B, C, etc.) indicates different containers of the same sample, while use of a numeric code (e.g., 1, 2, 3, etc.) indicates the relative position in a sample sequence taken of the same material over a period of time. The combination of a numeric code and a letter code indicates a replicate of a sample sequence.

The following columns are mandatory:

<b>Column</b>	<b>Unit/format</b>	<b>Description</b>
Category	from list	This is the primary material category. This category is used for sorting data to ease data selection in LeachXS. See the <i>Categories</i> sheet for all categories and subcategories.
Subcategory	from list	This is the material sub-category within the primary material category selected from a list of existing sub-categories within the primary category selected. The material sub-category is used for sorting data within primary categories. See the <i>Categories</i> sheet for all categories and subcategories.

The following columns are optional:

Column	Unit/format	Description
Originator ID	text	This is the unique identification code for the specific material being tested, as assigned by the organization supplying the material. Example: BA21.
Processor ID	text	This is the unique identification code for the specific material being tested, as assigned by the organization receiving the material.
Full name	text	This is the full name of the material being evaluated.
Project or literature citation	text	This is the identifier or citation used to identify where the information was obtained from or project that the material is associated with. Ideally, this would be citation to a document that would provide further information on the material.
Reference date	dd-mm-yyyy	This date may be used in e.g. time series.
Date event	from list	Indicate the basis for the date in the date code, with preference to the following order of priority: Date sampled Date received at lab Date tested Your best guess
EU EWC code	see comment	This is the European Waste Code (EWC). See sheet <i>EWC codes</i> for a list of all codes. A single waste code has format: two digits - chapter only; four digits - chapter + section; six digits - chapter + section + detail; six digits, followed by an asterisk (indicating hazardous). Multiple waste codes can be entered. Separate them by semicolons.
US waste code	see comment	This is the United States waste code. See sheet <i>EPA codes</i> for a list of all codes. A single EPA code consists of a capital, followed by three digits. Multiple waste codes can be entered. Separate them by semicolons.
Place or installation of origin	text	This is the identifier of where the facility or site where the sample was obtained.
Country of origin	from list	This is the two letter country code indicating the country of origin for the material (see sheet <i>Country Codes</i> ).
Description (including sample preparation summary)	text	This is a summary of how the material was prepared prior to evaluation (e.g., "screened to < 5 mm", "size reduced to < 10 mm", "dried to constant weight at 60 C", etc.
Remarks	text	Add any remark to the site reference here.
Attachments	file;file;...	Files attached to the material. Specify a list of file specifications, separated by semicolons.

If you want the material to be attached to a site, you can use the following fields:

Column	Unit/format	Description
Site reference	text	This is a reference to a site where the material is taken from. See sheet <i>Sites</i> .
Sample location ID	text	This is a unique identification of a location where the sample has been taken from.
Sample latitude		This is the latitude of the location where the sample has been taken, in degrees and fractions of degrees. A negative value denotes the southern hemisphere.
Sample longitude		This is the longitude of the location where the sample has been taken, in degrees and fractions of degrees. A negative value denotes a location west of Greenwich.
Reference elevation	m	This is the elevation that is used as a reference for all other elevations given in this sheet, in meters above sea level.
Sample elevation	m	This is the sample elevation in meters relative to the Reference elevation.
Reference remarks		Add any remark to the site reference here.

### Leaching tests sheets, general

The light yellow-colored sheets are designed to supply data related to a leaching test, accompanied by test position or fraction information. The leaching test sheets are:

- pH Dependence (2a)
- Monolithic Leach (2b)
- Column (2c)
- Concise (2d)
- Single and Parallel Batch (2e)
- Sequential chem Extraction (2f)
- Serial Batch (2g)

All these sheets have the same structure, although there are differences in the data that is to be supplied. Another leaching test sheet, *Composition (1b)* has a structure that is different from the other test sheets, because this test does not have any fraction or test position information. This sheet is described later on.

Every row in a sheet from the list above defines data for a test and fraction combination, so if you have carried out a test containing 2 fractions or test positions, you have to specify 2 data rows. Since a test belongs to a material, the first two columns must be used to reference the material, defined in sheet 1a.

Below are lists of columns that occur in every sheet. Some columns contain test data, while others contain fraction data. Here are the lists that occur in every test sheet.

The following fields, common to every test, are mandatory:

Column	Unit/format	Description
Short name	(from 1a)	This field must refer to the subject material from the <i>Material Info</i> sheet.

Material replicate	(from 1a)	This is a reference to the subject material replicate.
Test replicate	[A-Z]	This is the code used to identify which replicate of the entire test method is being carried out on the sample. If only one replicate analysis is being carried out, then this value should be "A". Additional replicates should be B, C, etc.
Method or standard	from list	This is the test method reference. See sheet <i>Test types and methods</i> for appropriate methods of the test.
Moisture content	%	This is the solid material sample moisture content, typically measured on a separate sample aliquot. <i>Values are reported as percent of initial wet weight.</i>

The following fields, common to every test, are optional:

Column	Unit/format	Description
Test date	dd-mm-yyyy	This is the date the laboratory has carried out the test
Test originator ID	text	This is the unique identification code for the specific test, as assigned by the organization submitting the test.
Test processor ID	text	This is the unique identification code for the specific test, as assigned by the organization processing the test.
Lab name or ID	text	This is the name of the laboratory that has carried out the test.
Test remarks	text	This field is for any additional comments you may have regarding the test.

The following fields, common to every test position or fraction, are mandatory:

Column	Unit/format	Description
Fraction nr	\d+	This is the leachate number. It is a positive integer value. Every leachate within the test must have a unique leachate number.
Fraction replicate	[A-Z]	This is the code used to identify which replicate of the test position or fraction is being carried out on the sample. If only one replicate is being carried out, then this value should be "A". Additional replicates should be B, C, etc. <i>Note that not all test fractions contain this field; due to the nature of the test, it might be impossible to have fractions replicated. For instance, a column test can be replicated, but not its fractions.</i>
pH		This is the pH measured in the liquid extract at the end of the contact period.

The following fields, common to every test position or fraction, are optional.

Column	Unit/format	Description
Conductivity	mS/cm	This is the electrical conductivity measured in the liquid extract at the end of the contact period.
Eh	mV	This is the redox potential (Eh) measured in the liquid extract at the end of the contact period.
Temperature	°C	This is the temperature at which the extraction was carried out.
Fraction originator ID	text	This is the unique identification code for the specific test fraction, as assigned by the organization submitting the test fraction.
Fraction processor ID	text	This is the unique identification code for the specific test fraction, as assigned by the organization processing the test fraction.
Fraction remarks	text	This field is for any additional comments you may have regarding the leachate.

### How the reader processes a leaching test sheet

The reader processes the rows one by one, from top to bottom, until the first column of a row is empty. Firstly, the reference to the material is resolved. Secondly, the fields that uniquely identify a test are read. After that, the reader tries to resolve the test in the list of tests of the referenced material. If it is not found, the other fields of the test are read, and the test is added to the material. However, if the test was found in the test list, the reader assumes that the current row is used to specify another fraction of the test: the remaining fields that belong to the test are ignored.

This means that, when supplying tests and fractions, you only need to supply test data on the first row of that test. On the other rows that are used to add fraction data to the test, you only need to fill the first 4 fields.

### Sheet pH Dependence (2a)

Use this sheet for any pH dependence test you have carried out on a material. In addition to the general test and fraction fields that are common to all tests, this sheet contains columns that are specific to pH dependence test fractions. There are no test specific columns.

The following columns belong to a test fraction and are mandatory:

Column	Unit/format	Description
Sample weight (wet)	g	This is the measured mass (wet weight) of the sample used in this particular leachate.
Volume DI water	ml	This is the volume of deionized water added to the solid during the indicated extraction for the specified leachate. Depending on the test method, DI water, acid or base may be added separately or as a single solution.

The following columns belong to a test fraction and are optional:

Column	Unit/format	Description
Contact time	h	This is the contact time for the specific eluant.

The acid and base concentration and volume columns can be used to specify acid and base additions for a specific fraction. The fields are optional, but if you specify acid and/or base volumes, you will need to specify the concentration and acid or base name as well.

Column	Unit/format	Description
Acid <sub>i</sub> or Base <sub>i</sub>	from list	Use these columns to specify details about acid and base additions at the subject fraction. The cell next to this field contains a list from which the acid or base name can be picked. <i>Note that if there are different tests on this sheet and these tests use different acids or bases, you can use alternative columns that can contain acid and base information.</i>
Volume	ml	This is the volume of the acid or base that is added.
Conc.	N	This is the molar concentration of the acid or base used for the addition.

## Sheet Monolithic Leach (2b)

Use this sheet for any Monolithic Leach test you have carried out on a material. In addition to the general test and fraction fields that are common to all tests, this sheet contains columns that are specific to Monolithic Leach tests and their fractions.

The following columns belong to a test and are mandatory:

Column	Unit/format	Description
Sample weight as prepared	g	This is the mass of the subject material for the Monolithic Leach test.
Sample geometry	from list	This is the geometry or shape of the sample.
Sample dimension 1	cm	If the sample geometry is a block, this is the block height. If the sample geometry is a cylinder, this is the cylinder height. Leave it empty if the sample has an irregular shape.
Sample dimension 2	cm	If the sample geometry is a block, this is the block width. If the sample geometry is a cylinder, this is the cylinder radius. Leave it empty if the sample has an irregular shape.
Sample dimension 3	cm	If the sample geometry is a block, this is the block length. Leave it empty if the sample is cylindrical or has an irregular shape.
Sample volume	cm <sup>3</sup>	This is the volume of the sample if it is irregularly shaped. Can be empty if the sample is a block or cylinder, because it can be calculated from the sample dimensions.
Leaching surface	cm <sup>2</sup>	This is the effective leaching surface. If the leaching surface can be calculated from the previous fields, you can leave this field empty.
Eluant	from list	This is a brief description of the eluant being used in the test. See the <i>Misc</i> sheet for a list of all predefined eluants for this test.

The following columns belong to a test and are optional:

Column	Unit/format	Description
Bulk density	kg/m <sup>3</sup>	This is the bulk density of the subject material for the Monolithic Leach test.
Porosity		This is the fraction of void space in the subject material for the Monolithic Leach test.

The following columns belong to a fraction and are mandatory:

Column	Unit/format	Description
Contact time	h	This is the time the eluate has been into contact with the sample in the subject fraction.
Resting time	h	This is the time the sample has not been into contact with an eluate, after the fraction has been collected. This can be zero.
Eluate volume	ml	This is the total amount of eluant that has eluted in this eluate fraction.

The following columns belong to a fraction and are optional:

Column	Unit/format	Description
Flow rate	ml/h	Specify a flow rate if subject fraction eluant was continuously renewed.
Vessel volume	ml	Specify this volume if fraction eluant was continuously renewed.

### Sheet Column (2c)

Use this sheet for any column test you have carried out on a material. In addition to the general test and fraction fields that are common to all tests, this sheet contains columns that are specific to column tests and their fractions.

The following columns belong to a test and are mandatory:

Column	Unit/format	Description
Sample mass (wet)	g	This is the mass of material (wet weight) packed into the column for the test.
Length	cm	This is the length (height) of the material being tested packed into the column.
Column diameter	cm	This is the inner diameter of the column being used for the test.
Eluant	from list	This is a brief description of the eluant being used in the test. See the <i>Misc</i> sheet for a list of all predefined eluants for this test.

The following columns belong to a test and are optional:

Column	Unit/format	Description
Column dry bulk density	kg/m <sup>3</sup>	This is the dry bulk density of the material as packed into the column.
Porosity		This is the the fraction of void space in the material as packed into the column.

The following columns belong to a fraction and are mandatory:

Column	Unit/format	Description
Flow rate	ml/h	This is the flow rate of the eluant into the column.
Cumulative eluate at start of fraction	ml	This is the total amount of eluant that has eluted from the column at the start of preserving this eluate fraction.
Cumulative eluate at end of fraction	ml	This is the total amount of eluant that has eluted from the column at the end of preserving this eluate fraction.
Recycling	from list	Specify here if the eluant is recycled. If so, then include the description in the 'Remarks' field.

### Sheet Concise (2d)

Use this sheet for any concise leaching test you have carried out on a material. In addition to the general test and fraction fields that are common to all tests, this sheet contains columns that are specific to concise leaching tests and their fractions.

The following column belongs to a test and is mandatory:

Column	Unit/format	Description
Eluant	from list	This is a brief description of the eluant being used in the test. See the <i>Misc</i> sheet for a list of all predefined eluants for this test.

The following columns belong to a fraction and are mandatory:

Column	Unit/format	Description
Contact time	h	This is the contact time for the specific eluant.
Sample weight (wet)	g	This is the measured mass (wet weight) of the sample used in this particular leachate.
Volume DI water	ml	This is the volume of deionized water added to the solid during the indicated extraction for the specified leachate. Depending on the test method, DI water, acid or base may be added separately or as a single solution.

The acid and base concentration and volume columns can be used to specify acid and base additions for a specific fraction. The fields are optional, but if you specify acid and/or base volumes, you will need to specify the concentration and acid or base name as well.

Column	Unit/format	Description
Acid <sub>i</sub> or Base <sub>i</sub>	from list	Use these columns to specify details about acid and base additions at the subject fraction. The cell next to this field contains a list from which the acid or base name can be picked. <i>Note that if there are different tests on this sheet and these tests use different acids or bases, you can use alternative columns that can contain acid and base information.</i>
Volume	ml	This is the volume of the acid or base that is added.
Conc.	N	This is the molar concentration of the acid or base used for the addition.

### Sheet Single and Parallel Batch (2e)

Use this sheet for any single batch or parallel batch test you have carried out on a material. In addition to the general test and fraction fields that are common to all tests, this sheet contains columns that are specific to single batch or parallel batch fractions. There are no extra test specific columns.

The following columns belong to a fraction and are mandatory:

Column	Unit/format	Description
Eluant	from list	This is a brief description of the eluant being used in the test. See the <i>Misc</i> sheet for a list of all predefined eluants for this test.
Eluant volume	ml	This is the volume of the eluate that is separated for analysis.
Sample weight (wet)	g	This is the measured mass (wet weight) of the sample used in this particular leachate.

The acid and base concentration and volume columns can be used to specify acid and base additions for a specific fraction. The fields are optional, but if you specify acid and/or base volumes, you will need to specify the concentration and acid or base name as well.

Column	Unit/format	Description
Acid <sub>i</sub> or Base <sub>i</sub>	from list	Use these columns to specify details about acid and base additions at the subject fraction. The cell next to this field contains a list from which the acid or base name can be picked. <i>Note that if there are different tests on this sheet and these tests use different acids or bases, you can use alternative columns that can contain acid and base information.</i>
Volume	ml	This is the volume of the acid or base that is added.
Conc.	N	This is the molar concentration of the acid or base used for the addition.

The following column belongs to a fraction and is optional:

Column	Unit/format	Description
Contact time	h	This is the contact time for the specific eluant.

### Sheet Sequential chemical extraction (2f)

Use this sheet for any sequential chemical extraction test you have carried out on a material. In addition to the general test and fraction fields that are common to all tests,

this sheet contains columns that are specific to sequential chemical extraction fractions. There are no extra test specific columns.

The following columns belong to a fraction and are mandatory:

Column	Unit/format	Description
Contact time	h	This is the contact time for the specific eluant.
Sample weight (wet)	g	This is the measured mass (wet weight) of the sample used in this particular leachate.
Eluant	from list	This is a brief description of the eluant being used in the test. See the <i>Misc</i> sheet for a list of all predefined eluants for this test.
Eluant concentration	N	This is the concentration of the eluant used in this step of the test.
Eluant volume	ml	This is the volume of the eluant used in this step of the test.
Recovered volume	ml	This is the volume of the eluate that is separated for analysis.

### Sheet Serial Batch (2g)

Use this sheet for any serial batch test you have carried out on a material. In addition to the general test and fraction fields that are common to all tests, this sheet contains columns that are specific to serial batch fractions. There are no extra test specific columns.

The following columns belong to a fraction and are mandatory:

Column	Unit/format	Description
Contact time	h	This is the contact time for the specific eluant.
Eluant	from list	This is a brief description of the eluant being used in the test. See the <i>Misc</i> sheet for a list of all predefined eluants for this test.
Eluant volume	ml	This is the volume of the eluant used in this step of the test.
Recovered volume	ml	This is the volume of the eluate that is separated for analysis. <i>Note: the recovered volume in the last fraction must have a value of zero.</i>
Sample weight (wet)	g	This is the measured mass (wet weight) of the sample used in this particular leachate.

### Sheet Eluate Analysis (4a)

In the *Eluate Analysis* sheet, you can specify data of the analyses that have been carried out on the leachate of a test fraction. In principle, you can specify all analysis data belonging to a fraction leachate on a single row. In special cases, for instance if not all analysis have been carried out by the same lab, or some or all analyses have been carried out in duplicate, you can use additional rows for a single fraction leachate.

Because analyses belong to a fraction leachate, the first six columns are used to reference the subject material, test, and fraction. These columns are mandatory:

Column	Unit/format	Description
Short name	(from 1a)	This field must refer to the subject material from the <i>Material Info</i> sheet.
Material replicate	(from 1a)	This is a reference to the subject material replicate.
Method or standard	(from 2)	This is the test method reference. See sheet <i>Test types and methods</i> for appropriate methods.
Test replicate	(from 2)	This is a reference to the subject test replicate.
Fraction nr	(from 2)	This is the leachate number. It is a positive integer value. Every leachate within the test must have a unique leachate number.
Fraction replicate	(from 2)	This is the code used to identify which replicate of the test position or fraction is being carried out on the sample. If only one replicate is being carried out, then this value should be "A". Additional replicates should be B, C, etc.

In columns 7 to 12, you can specify information common to all analyses after these columns. The fields and their meanings are:

Analysis replicate	[A-Z]	This is the code used to identify which replicate of the analyses is being carried out on the sample. If only one replicate analysis is being carried out, then this value should be "A". Additional replicates should be B, C, etc.
Analysis date	dd-mm-yyyy	This is the date the laboratory has been carried out the analyses.
Lab name or ID	text	This is the name of the laboratory that has carried out the analyses.
Analysis originator ID	text	This is the identification code of the analysis used when the sample is submitted by the sample provider to the laboratory for analyses.
Analysis processor ID	text	This is the identification code of the analyses as been given to the analyses by the laboratory that carried out the analysis.
Analysis remarks	text	This field is for any additional comments you may have regarding the analyses.

From column 14 onward, the actual measured concentrations of constituents can be given. The mostly used constituents are already defined. Their names appear in the second row. There are 4 attributes to every analyzed constituent:

Analysis method	This is the method or instrument used to measure the concentration. Note that only one method can be given for a specific constituent in the entire sheet.								
Detection limit, in µg/l	This is the smallest value the method or instrument can measure. Note that only one detection limit can be given for a specific constituent in the entire sheet. There are some exceptions. See the information at "Measurement flag".								
Concentration, in µg/l	This is the measured or estimated concentration. See the information at "Measurement flag".								
Measurement flag	<p>This flag indicates the reliability of the value, given in the Concentration column. The values of the flag can be picked from a list:</p> <table> <tr> <td>(no flag)</td> <td>Measured</td> </tr> <tr> <td>U</td> <td>Undetected - Detection limit shown</td> </tr> <tr> <td>U½</td> <td>Undetected - Half detection limit shown</td> </tr> <tr> <td>E</td> <td>Estimated</td> </tr> </table> <p>If you use one of the <i>Undetected</i> flags, you can leave the concentration column blank. The reader will calculate the concentration value from the detection limit field, given in the fourth row of the concentration column.</p> <p>If one of the <i>Undetected</i> flags is used and you specify a concentration anyway, the reader will assume that the detection limit or half detection limit is given and will deduce both concentration and detection limit from this value, ignoring the global detection limit for this specific analysis in the fourth row.</p>	(no flag)	Measured	U	Undetected - Detection limit shown	U½	Undetected - Half detection limit shown	E	Estimated
(no flag)	Measured								
U	Undetected - Detection limit shown								
U½	Undetected - Half detection limit shown								
E	Estimated								

### Changing the constituent list

A large number of mostly used constituents have been defined for your convenience. If you have measured other constituents than those are listed in this sheet, you can add them: just copy a column tuple containing a predefined constituent, paste it at the end of the list and change the name of the constituent you have analyzed. Currently only constituent names are supported that appear in the lists on workbook sheet named *Constituents*.

If the list contains constituents you never use, you can safely remove the corresponding columns.

If you like to change the order of appearance of the constituents, you can safely do so: cut and paste column tuples or, even easier, rename the constituents.

### Dealing with bulk data

If you have a lot of analyses, it may be awkward to get the data below the correct column header. Here is an example how you might paste your data into the sheet, if you have the analyses arranged in columns.

Suppose you have your data arranged like this:

Al	43398.4	14793	250	115.5	9204.7
Cd	0.2	1	2.6	46.1	132.9
Mn	1.5	2.1	134	1218	3568.6

In this example, there are three analyses (Al, Cd and Mn) and four fractions in some other workbook.

First, add a column for the analyses methods, one for the detection limits and one blank column after the constituent names:

Al	ICP-AES	5		43398	14793	250	115.5	9204.7
Cd	ICP-AES	2		0.2	1	2.6	46.1	132.9
Mn	ICP-AES	1		1.5	2.1	133.7	1218.1	3568.6

Now, add a blank row after every row:

Al	ICP-AES	5		43398	14793	250	115.5	9204.7
Cd	ICP-AES	2		0.2	1	2.6	46.1	132.9
Mn	ICP-AES	1		1.5	2.1	133.7	1218.1	3568.6

Add any measurement flags below the concentrations, if necessary. In this example, we add “E” flags to some values for Cd:

Al	ICP-AES	5		43398	14793	250	115.5	9204.7
Cd	ICP-AES	2		0.2	1	2.6	46.1	132.9
				E	E			
Mn	ICP-AES	1		1.5	2.1	133.7	1218.1	3568.6

Now, select this data block and copy it to the clipboard (**Edit->Copy**). Go to the destination *Eluate Analysis* sheet and select the first blue cell of the block containing a constituent name. This will probably be *Al*.

Use the Excel context menu by pressing the right mouse button and select **Paste Special...** In the appearing dialog, choose **Values** in the **Paste** section, choose **None** in the **Operations** section and mark the **Transpose** and **Skip Blanks** checkboxes. Leave the dialog by pressing the **OK** button.

Remove excess unfilled columns beyond the last column containing data.

### Sheet Composition (1b)

This sheet can be used to specify total composition data. The structure of this sheet is different from other sheets containing leaching tests, because this test does not contain fraction specific information. The analyses results of this test must be entered directly in this sheet and not in the *Eluate Analysis* sheet. Fill the test specific data analogous to the other test sheets. The specification of analyses is the same as on the *Eluate Analysis* sheet, but the units of measurements of the analyses and detection limits are in mg/kg instead of µg/l.

### Appending data to existing materials

Sometimes you might want to add new data to materials, tests or fractions that have already been imported in a LeachXS database.

Suppose that you want to add results of a Column test that has been performed on a material and that this material is already present in your LeachXS database.

Because adding data to a database is a two-step process, the first step (transferring an Excel workbook to an xml file) has no knowledge of the contents of the database that you want to use to add the data to in the second step. It is therefore necessary that you repeat the material data again if you want add a new test to it.

Likewise, if you want to add a fraction to an existing test, you need to repeat both material and test data. If you want to add analyses to an existing fraction, you need to repeat the data specific to a fraction as well.

This might be cumbersome, but the basic idea behind the central data structure is that can be used to exchange leaching data with others.

If you are not planning to distribute the xml file with additions to others, you'll only have to fill in the mandatory (red) columns for the entities that are supposed to be present in the LeachXS database.

In the next chapter you can read how data in an xml file is added to a LeachXS database and how is dealt with additions to existing entities.

## **Plug-in writer: AccessDBWriter**

The plug-in module that is capable of adding the contents of a CDS to a LeachXS database is called AccessDBWriter.

Adding data to a database is performed in an “All or Nothing” process: if some kind of error occurs during the data addition transaction, the entire transaction will be rolled back and nothing will be changed in the database.

The chapter named “The software” already described how to use this module. This chapter gives details about the process of adding data to a LeachXS database.

### ***The LeachXS database structure***

The LeachXS database structure has been designed back in 2003. The design provided for storage of the most essential leaching data. In 2007 we have redesigned the entities containing leaching data, resulting in a structure that is capable of holding much more details about entities. For compatibility, LeachXS still uses the databases with the design from 2003. This means that the plug-in module to write a CDS to a LeachXS database only adds data from a CDS that fits to this design, ignoring all added features. This ensures that you can work with your new data in LeachXS, but also that you won't find back some details that you specified in your workbooks.

A new database structure for LeachXS is planned for 2008, capable of storing all fields of the current Excel workbook template, and probably even more for future use. We therefore advise you to keep the generated xml files or your workbooks with leaching data, so that you will be able to add your data quickly if a new LeachXS database structure is used.

### **General field mapping remarks**

- There is no equivalent entity to sites in a LeachXS databases. However, the materials on a site will be processed as if it were “siteless” materials.
- All entities have the fields Originator ID, Processor ID and some entities have attachments. These fields do not have a corresponding database storage location and their contents will therefore not be stored in LeachXS databases.
- Materials and test carry a date field denoting sampling date or date tested. There are no corresponding fields in LeachXS databases, so they won't be stored.
- All entities can have replicates. They are denoted by a capital. In the LeachXS database, replicates are denoted by a positive integer value. In the LeachXS database, material replicate number is called BatchNumber and a test replicate is called MeasurementNumber. An analysis replicate is called AnalysisNumber. The mapping from capitals to numbers will be performed by the plug-in: a replicate denoted by “A” will be mapped to 1, a “B” to 2, and so on.
- Although fractions of some test can be replicated, the LeachXS database does not have any provisions for fraction replicates. If you have fraction replicates, use test replicates instead.
- Concentrations or emissions in analysis data in LeachXS databases do not carry a flag. This means that the indication of a measured value to be an estimated value will be lost.
- A material can carry a list of EPA codes and a list of EWC codes. In the LeachXS database there is room for a single EPA code and a single EWC code. Only the first codes you have specified will be inserted into the database.

## Reference lists in LeachXS databases

For efficiency, the LeachXS database contains a number of lists to hold recurring information. Instead of storing information in a database object, a reference to the entry in such a list is stored. Among other lists, there is a list named Suppliers that contains all referenced suppliers of samples, and a list named Labs that contains all referenced laboratories that have carried out tests.

If you have used the columns *Place or installation of origin* on sheet *Material Info* or column *Lab name or ID* on any test sheet, the plug-in first tries to match the information to the Suppliers list or Labs list, respectively. If a match is found, the corresponding object will get a reference to that entry. If not, a pop-up dialog will appear, asking you whether it is ok to add the unmatched item to the appropriate list or not. If you don't want the item to be added, the import process is aborted, rolling back any additions made so far. If you acknowledge the addition, the entry will be added to the list and the corresponding object will get the correct reference.

In a LeachXS database, a material must belong to a material group. There is no corresponding entity in the CDS. Therefore, the plug-in will ask you to specify a group name where all materials from the CDS will be part of. You can pick an existing group name or specify a new name.

## Adding or updating data from a CDS

As you might have read at the end of the chapter about the StandardExcel plug-in, it is possible to append new data to a material, test or fraction that already exists in a LeachXS database. However, updating in the sense that some property of an entity can be given a different value is not possible.

This section briefly describes the process of adding and updating data.

For every material that is present in the CDS, the plug-in takes the following steps:

1. It checks if the material already exists in the database. The material exists if its unique identification, being the combination of its Short name and its Replicate, exists. If it does exist, the material from the CDS is considered to be a reference, and other fields that belong to the material are ignored. However, if it doesn't exist, it is added, and fields relevant to the material are filled.
2. From this point on, a reference to the material is present, be it a reference to the newly added material or a reference to a material that was already in the database. Now, the same procedure is followed for every test to the material that was taken from the CDS: the unique identification of a test, being its type, replicate and method, is looked up, and the test with its fields is added if it was not present in the database.
3. The fraction information to a test is treated likewise.

An analysis is an end node in the hierarchy of sites, materials, tests and fractions and does not carry any lists of dependent entities. Therefore, any analysis in the CDS cannot exist already in a LeachXS database.

## Inspecting the steps taken by the plug-in

During the processing of the CDS, the plug-in reports its progress in a window. You should inspect this report carefully to see if the decisions made by the plug-in are correct. Consider the following scenario:

Suppose that you have analyzed a material by performing a column test. Now,

you want to add this data to a LeachXS database. You do not know exactly what materials are in the database and you haven't added any materials to it yet. You have created a workbook and transformed the workbook into a CDS with the StandardExcel plug-in. Now, you run the AccessDBWriter plug-in to add the CDS with your material and test to a database.

You have given a nice name to your material, but probably don't realize that there might be a small chance that there already is a material in the destination database that carries the same name. If so, the plug-in will try to append the test data to the found material, which would be wrong, because your intention was to add a new material. The only way to find out is by inspecting the progress report of the AccessDBWriter plug-in: it will report the fact that it found a material with the same name and replicate in the database.