XRF Core Scanner

Getting Started Manual for

XRF Core Scanner Program

Version 3.0

AVAATECH
ANALYTICAL X-RAY TECHNOLOGY

Getting Started manual [1] for XRF Core Scanner Program [2]

Version 3.0   August 2006   Bob Koster

Contents:

---

[1] Contents of this manual is based on the Windows help files supplied with the XRF Core Scanner Software
[2] XRF Core Scanner was developed by the Royal Netherlands Institute for Sea Research and exclusively distributed and supported by AvaaTech Analytical X-Ray Technology

Part 1

Introduction to the XRF Core Scanner Software

Introduction:

The XRF Core Scanner Program is a multi-threaded application that runs on a personal computer with a WIN32 based operating system, like WinXP and Win2000, and connects to the XRF Core Scanner and to all of its scientific instruments.
The program controls all the instrument settings via the Instrument Settings window and can perform a XRF scan on a split sediment core. A core position description, the X-Ray excitation and measurement parameters are to be defined in the Measurement Setup window.

If a split sediment core has been put in the XRF Core Scanner the user needs to perform two things over which the program has no control.

1) Push the Helium switch to flush the measurement chamber with helium.
2) Push X-Ray ON switch to start the X-Ray tube.

From here the program can perform a fully automated scan over the core and store the measured XRF spectra in the chosen data directory.
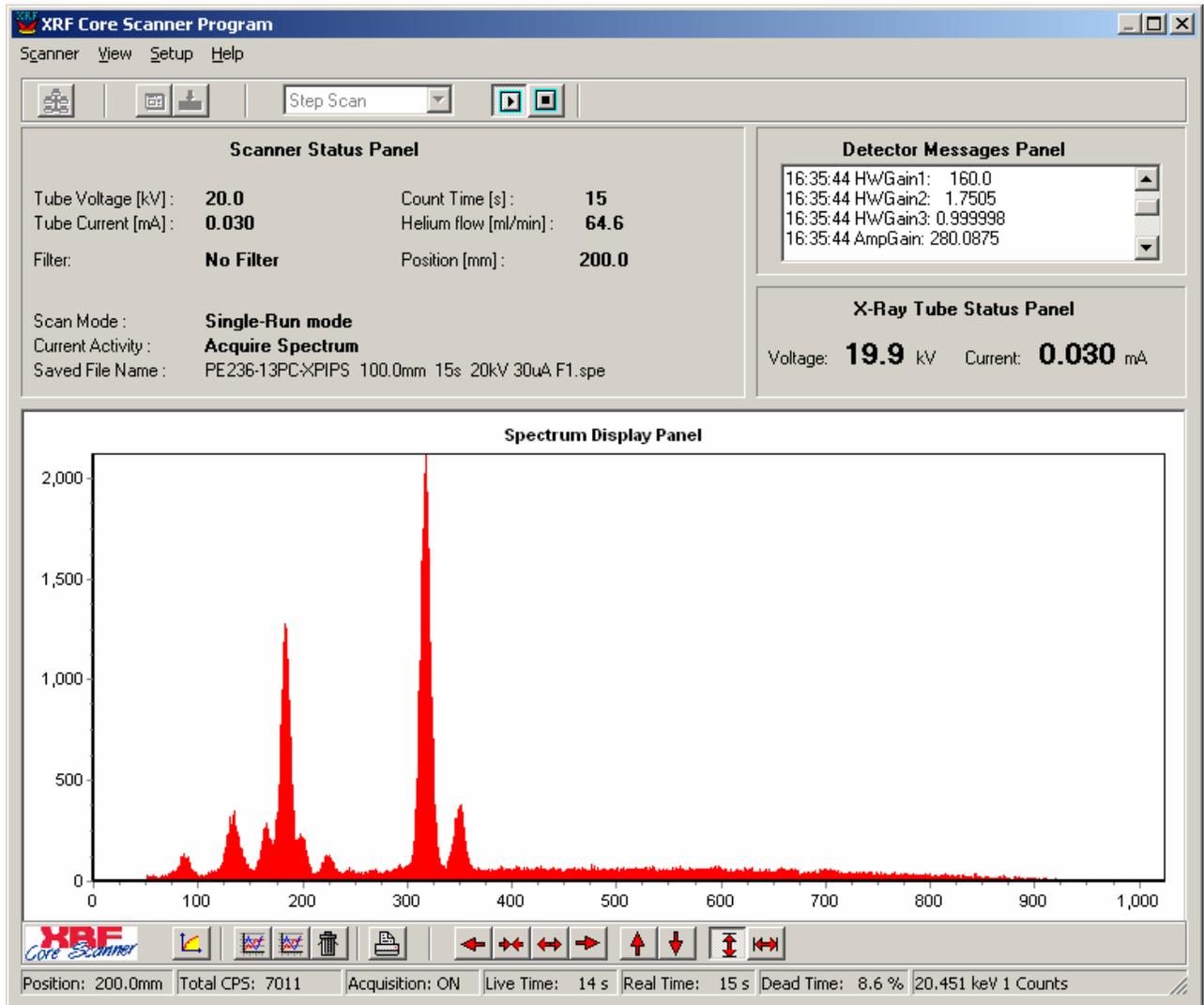At a later stage the acquired and saved spectra are to be processed with a separate processing package.

Part 2

Launch Program

Launch Program:

The main screen looks like this:

At the top of the screen there is the main menu. Almost all the selectable items from the main menu are also accessible via the Application Toolbar buttons below it.

In the upper-left corner there is a **Scanner Status Panel** that shows various parameters as a scan proceeds. In the upper-right corner there is a **Messages Panel** that shows the various communication commands between computer, detector and scanner. This panel can be useful to locate the sources of possible errors.

Below there is an **X-Ray Tube Status Panel** that shows the actual X-Ray tube status. These values are only updated if the program is connected to the scanner.

The largest panel is the **Spectrum Display Panel**. The live acquired spectrum is always displayed in red. At any given moment an older spectrum can be read from disk and displayed as an overlay in the Spectrum Display Panel. The appearance of the spectra in the Spectrum Panel can be manipulated with the buttons from the Spectrum Toolbar.

At the bottom of the screen there is a Statusbar that shows spectrum related parameters as the scan proceeds.

Part 3

User Interface

Scanner Menu:

The Scanner Menu contains two items :

Connect   Connects program to scanner and its instruments
Hardware   Control Direct control of scanner, X-Ray tube and detector
Exit   Terminates the program

View Menu:

The View Menu contains three items :

Scanner Messages   Shows the logged messages from the scanner
Detector Messages   Shows the logged messages from the X-ray detector
None

**Setup Menu:**

The Setup Menu contains two items :

Instrument Settings   Contains settings related to scanner
Measurement Setup   Contains settings related to the measurement

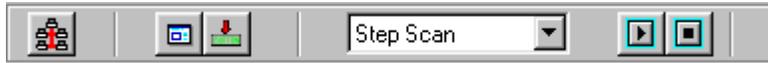See part 6 for detailed description of setup screens.

Help Menu:
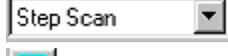
The Help Menu contains two items :

Help Contents   Start the Win Help program with the contents tab selected
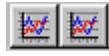About   Shows an about box with company information
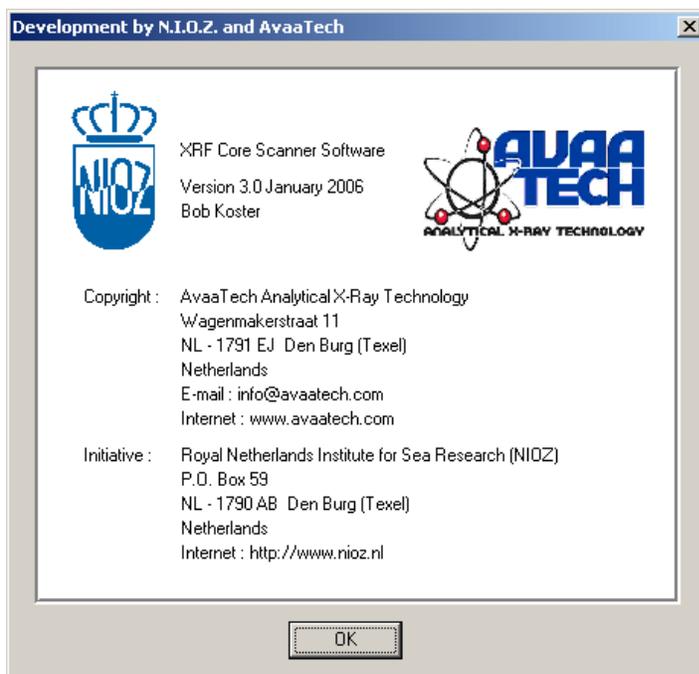
Application Toolbar:

	Connection button
	Instrument Settings button
	Measurement Setup button
Step Scan ▼	Scan Mode selector
▶	Start Scan button
■	Stop Scan button

Spectrum Toolbar:

	Select Linear or Logarithmic vertical scale
	Display a stored spectra with different colors
	Remove overlaid spectra from screen only
	Make a hard copy of the Spectrum Display Panel
← ←→ ↔ →	Move, Shrink and Expand spectrum horizontally
↑ ↓	Expand and Shrink spectrum vertically
↕ ↔	Auto-Scale spectrum vertically and horizontally

Statusbar:

Position: 200.0mm | Total CPS: 7011 | Acquisition: ON | Live Time: 14 s | Real Time: 15 s | Dead Time: 8.6 % | 20.451 keV 1 Counts

|	
Position:	Current X-position of the scanner in [mm]
Total CPS:	Total count per second counted by the multi channel analyzer
Acquisition:	Status of Multi-Channel Analyzer [On/Off]
Live Time:	Elapsed Live time of current measurement in [s]
Real Time :	Elapsed Real time of current measurement in [s]
Dead Time:	Percentage of Dead time in detection circuit in [%]
Energy Intensity(*):	Cursor values in [keV] and [Counts]

(*) See also Energy Calibration parameters on Instrument Settings window

Part 4

Instrument Settings
&
Measurement Setup

window description

Instrument Settings/Excitation:
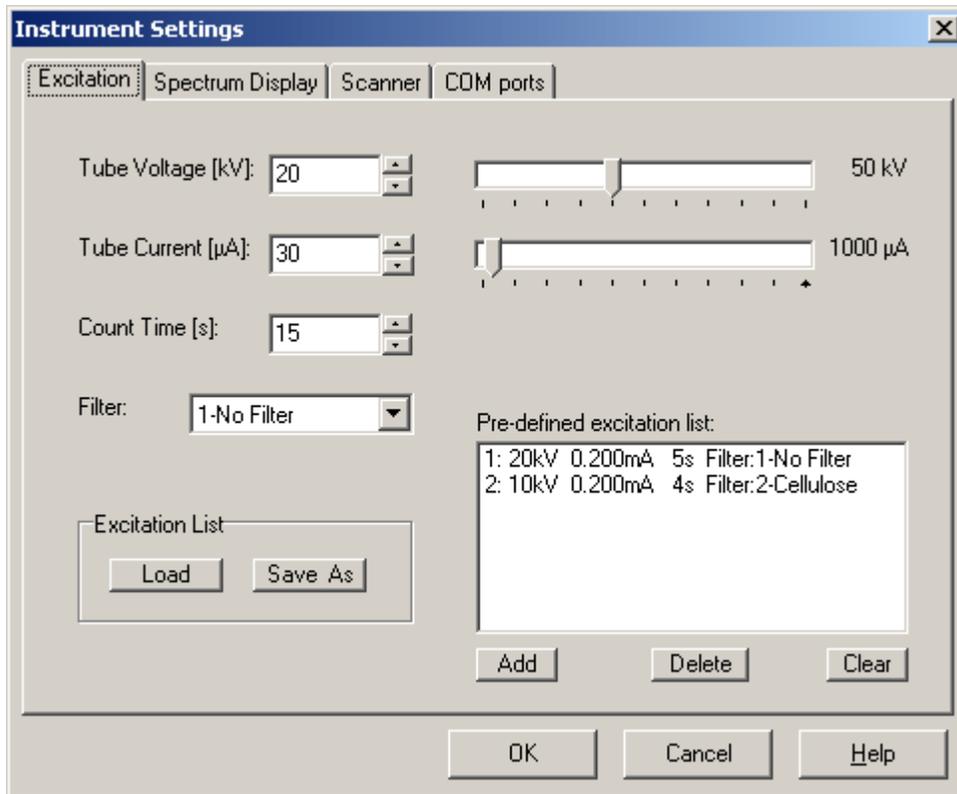
To set an X-Ray excitation condition adjust the **kV** and **mA** sliders with the left mouse button pressed at the correct value. Select the appropriate **CountTime(*)** and **Filter** between X-Ray tube and sample.
If the new excitation condition will often be used it could be added to the pre-defined excitation list. The contents of the pre-defined excitation list can be cleared with the corresponding buttons. An excitation list can be saved to or loaded from disk.
This pre-defined excitation list appears in the Measurement Setup window. There one can make a choice which excitation condition is to be used for a step-scan. Even all excitation conditions from the pre-defined excitation list can be chosen. That will result in a multi-run step scan that measures a specific sample with various excitation conditions.

(*)CountTime is the time that the Multi-Channel Analyzer takes to acquire a spectrum. Since the MCA is programmed to measure in 'live-time' the actual time a measurement takes is calculated as [Count Time / (1- Dead Time/100%)], where Dead Time is a physical MCA phenomenon that is related to the total counts that enter the X-Ray detector. The Dead Time is displayed on the main screens statusbar. The Dead Time can be influenced by the X-Ray tube current.

Instrument Settings/Spectrum Display:
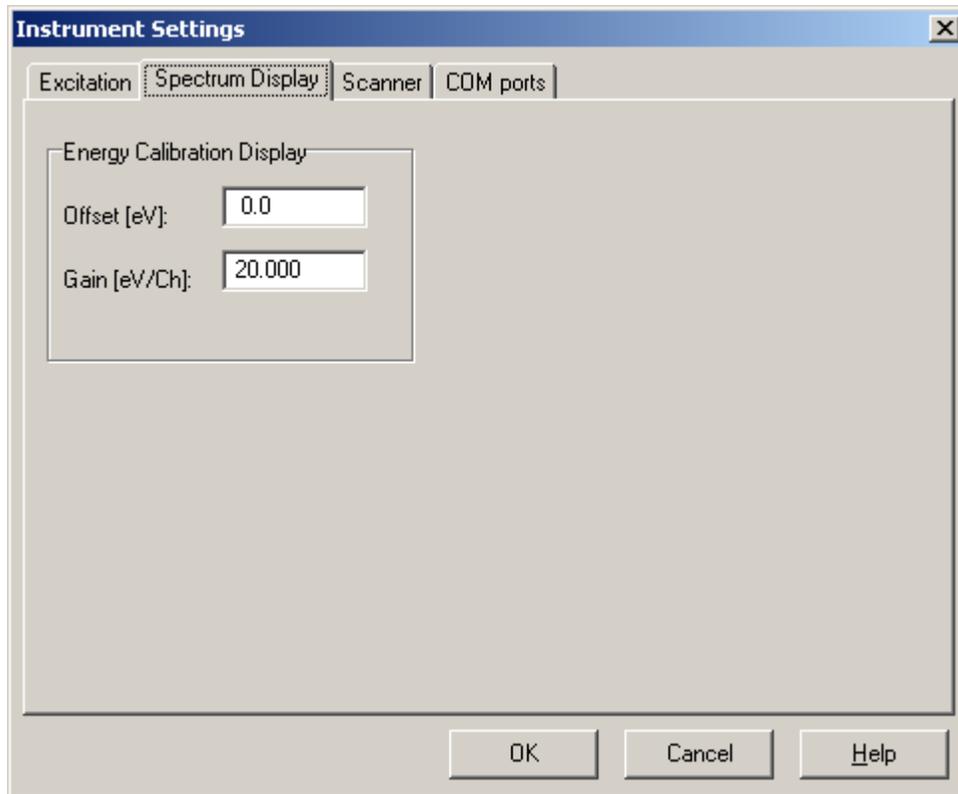
Both Energy Calibration settings **Offset** and **Gain** are implemented to transform the spectrum channel numbers, in the Spectrum Display Panel, into energy values. The settings on this screen are only to calculate the displayed energy value of the cursor in the Spectrum Display Panel. This energy value is displayed in the right corner of the statusbar.

The measured and stored raw-data spectra are not affected by this display energy calibration. Since the used spectrum post-processing package works with pre-defined processing models it is strongly advised to have the hardware detector gain always set to the same value. Recommended values are 20eV/Channel at 2048 channel spectra or 10eV/Channel at 4096 channel spectra.

Instrument Settings/Scanner:
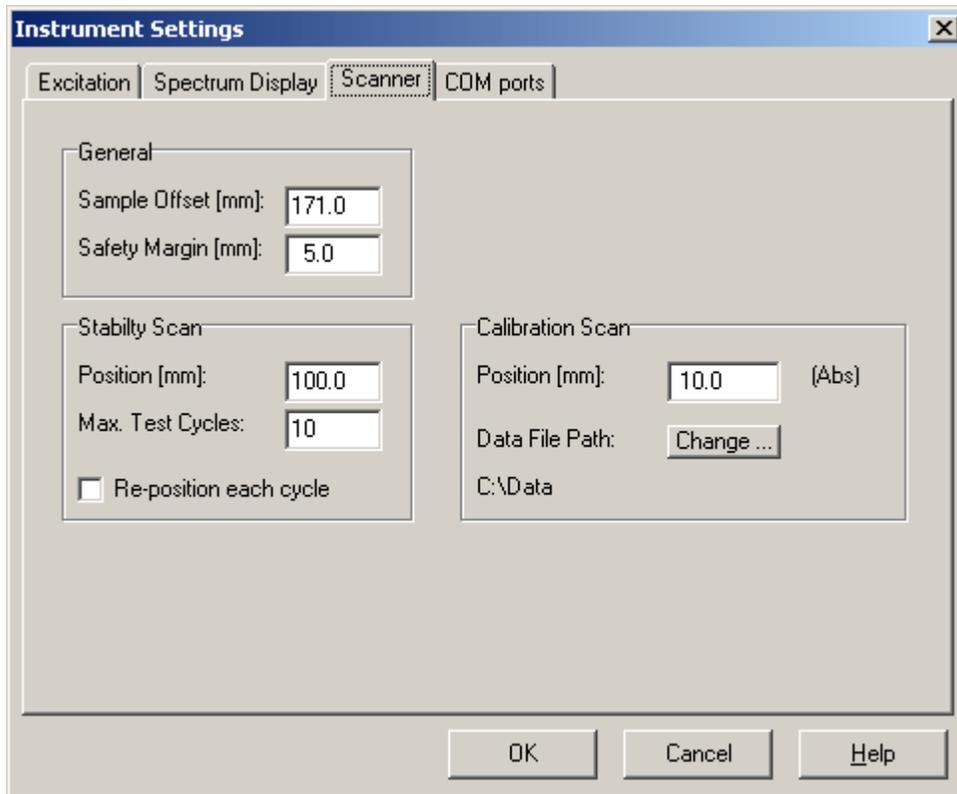
The General settings **Sample Offset** and **Safety Margin** are implemented to calibrate the scanners X-position and to prevent the scanner from measuring too close to the cores edges. The Sample Offset is the distance between the scanners homing-switch and the "0 cm" location of the core to be measured. Adjust this value if the mechanical "0 cm" position has been changed.

The Stability Scan settings **Position**, **Max.Test Cycles** and **Re-position** determine the behaviour of a stability scan. A stability scan repeatedly measures the same position on a core to check the systems (and samples) stability. A stability scan ends automatically after the number of cycles set at Max.Test Cycles. If the Reposition checkbox is checked the scanner re-positions before a measurement. If not checked the scanner positions only once before the first measurement and then repeats the measurements without any mechanical movements. The spectrum file name automatically contains a cycle number. The excitation condition and data file directory are to be set in the Measurement Setup window.

The Calibration Scan settings **Position** and **Data File Path** determine the behaviour of a calibration scan. A calibration scan is meant to monitor the systems long-term stability. At regular time intervals the user can measure a reference sample that usually is positioned at the left side of the scanners "0 cm" position. This position is entered as an absolute positive value in millimeters counted from the scanners homing-switch. The reference sample at such a location can be permanently available for monitoring.
The Data File Path is the directory were the spectra are stored and overrules the usual data directory path. This helps to collect all the long-term monitoring spectra at one central location. The spectrum file name automatically contains the time and date of the measurement.
The excitation condition is to be set in the Measurement Setup window and should always be the same !!!

Instrument Settings/Com Ports:
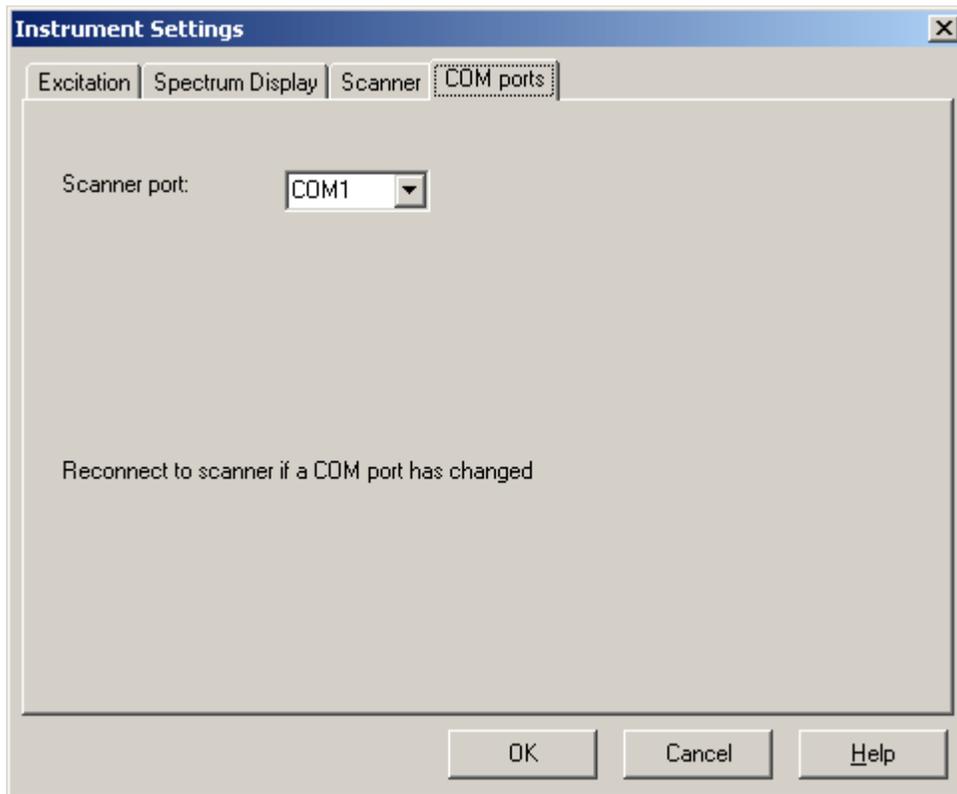
The scanner requires a serial COM port on the computer. The **Scanner port** setting determine which port number physically connects to the appropriate device. If a settings is changed the program should be re-connected to the scanner in order to activate the new settings.

Measurement Setup/Basic:

The **Data Directory** is the directory where the spectrum files, acquired during a scan, are saved in. By pressing the **Change …** button an existing directory can be chosen or a new directory can be created. **Sample Name** is the name of the core that is to be measured. Do **not** use any of the following characters since they could give problems in Windows file names: [. , / \ * ' " : ;] Sample Length is the exact length of the core. **Step Size** is the distance between each measurement during a step scan. A [Special positions apply] sign next to the Step Size parameter indicates that special positions apply for this scan. See Special tab topic for an explanation. The **Excitation** condition to be applied can be chosen from the Instrument Settings / Excitation tab or from the pre-defined excitation list. Even all excitation conditions from the pre-defined excitation list can be chosen. That will result in a multi-run step scan that measures a specific sample with various excitation conditions.

For loading and saving **Measurement Scripts** see Special tab topic for an explanation.

Measurement Setup/Special:
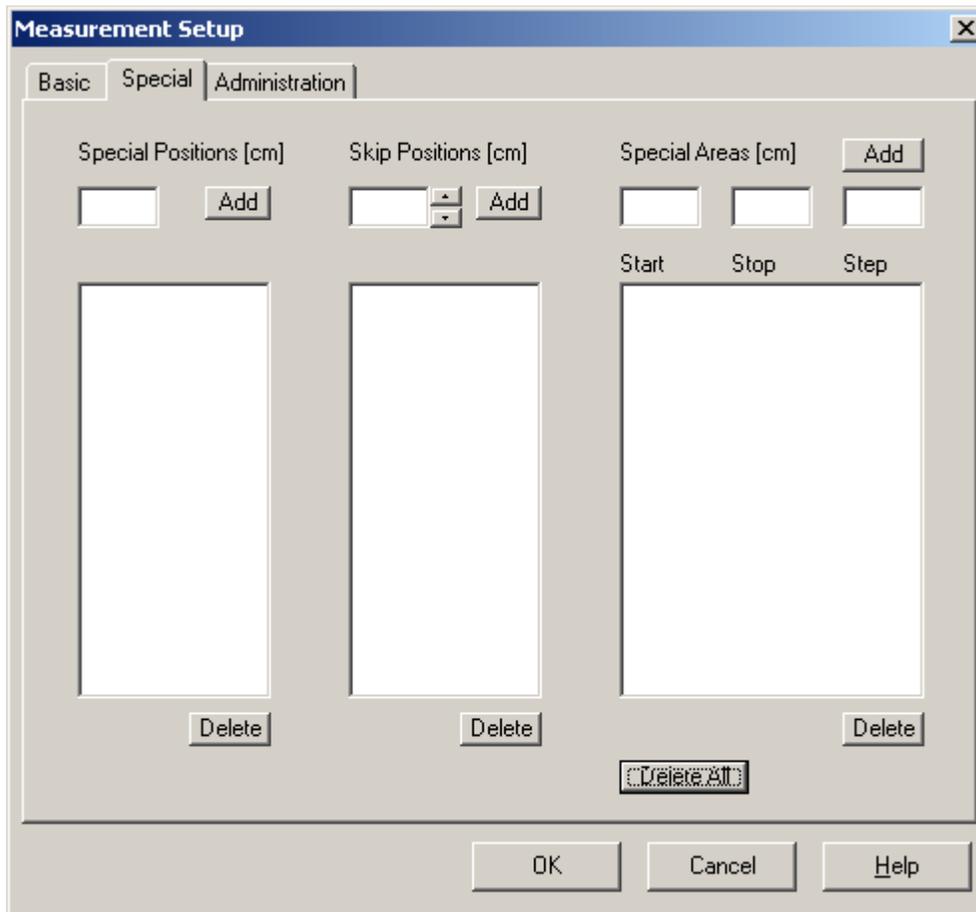
During a step scan the scanner jumps with Step Size steps over the core. To anticipate better on possible interesting core positions or huge gaps in the sediment surface it is possible to define **Special Positions** (e.g. in between a normal step), **Skip Positions** (a normal step that should be skipped) and **Special Areas** (a possible interesting area where one would like to step with a smaller step size).
The entries in each list are sorted ascendant.
To delete a single entry from any of the three lists: select the entry and click a **Delete** button. To delete the contents of all the lists press the **Delete All** button.

To avoid re-entering core parameters such like Special Positions, Skip Positions and Special Areas in case a particular core must be measured more then once **Measurement Scripts** are introduced. A measurement script can be saved or loaded from disk and contains the following parameters:

Sample Name / Sample Length / Step Size
Special Positions / Skip Positions / Special Areas

Parameters that are **not** included in a measurement script are:

Data Directory / Excitation condition

Measurement Setup/Administration:

This program keeps track of the number of measurements done and the length of the samples that have been scanned.
The counters can be reset to zero for a specific project. Another pair of counters can be used to register the systems total usage.

Part 5

Spectrum Processing

Spectrum File Format:

The spectrum files are saved with a *.SPE file extension. SPE files are Block Structured Ascii (BSA) files that can be viewed or modified with any available text editor.
A BSA-file is divided into blocks. Each block is identified by a string that starts with a dollar sign ($) and ends with a colon (:), thus, $BLOCK_NAME:. The structure of the data in each block is uniquely defined; the order in which blocks appear in the file is, however, not defined.

NECESSARY BLOCK

```
$DATA:                          (spectral data)
first_chan last_chan
chan_cont[first_chan] ...
...chan_cont[last_chan]
```

OPTIONAL BLOCKS

```
$SPEC_ID:                       (core position in [mm])
spectrum_id
```

```
$MEAS_TIM:                      (spectrum measurement time in seconds)
livetime truetime
```

```
$DATE_MEA:                      (start date of measurement)
month day year  hour min sec
```

Using WinAxil for Spectrum Processing:

Canberra's WinAxil can be used for spectrum processing. WinAxil is based on the international well known AXIL (**A**nalysis of **X**-ray spectra by **I**terative **L**east squares) fitting routines. The WinAxil software package contains various components :

WinAxil   - Basic X-ray spectrum analysis with graphical interface
WinAxilBatch   - Program for unattended batch operation of WinAxil on
                  multiple X-ray spectra and export facility to Microsoft Excel
WaxLibManager - Program to organise the WinAxil parameter file in a database
                  environment
WinFund   - Quantitative analysis program based on fundamental parameter
                  method

In order to achieve good processing results it is important to set up a correct parameter database that contains all the relevant XRF parameters such as: tube type, detector type, filter materials, excitation settings and measurement atmospheres. This can be done with the **WaxLibManager** component.

Before **WinAxil** can start processing a measured spectrum file (*.SPE) it needs to know a lot of information about the measurement condition of the spectrum (e.g. X-ray tube type and settings, X-ray detector type, excitation filter, chamber atmosphere, tube-sample-detector geometry). Also a proper energy calibration is to be performed and proper peak- and continuum fit parameters are to be chosen. Finally the Region Of Interest and the elements of interest are to be specified.

If the fitting results for all the elements of interest are acceptable the processed spectrum can be saved as a *.WAX file. This file type includes the original spectrum, measurement- calibration- and fitting parameters and the fitting results. All these settings can also be saved as a *.AFM file. This file type is called a 'Model File'. Such a Model File can be used in WinAxil to accelerate the processing of other spectra that are measured under the same conditions.

WinAxilBatch is a batch processing program without a graphical interface that uses the same mathematical core as WinAxil. It is able to process large amounts of spectra that are measured under the same condition and can export the fitting results 'on the run' to Microsoft Excel. WinAxilBatch needs a Model File that contains al the proper measurement-, calibration- and fitting parameters.

WinFund is a program that can perform quantitative analysis of XRF spectra based on the fundamental parameter approach. It can work in three different modes: Standardless fundamental parameters mode, Standard-based fundamental parameter mode and Compare mode. This program is still in development and can only be used with extreme care.

Part 6

How Do I …

How Do I … Connect to Scanner

Before starting an actual scan be sure that the XRF Core Scanner is switched on and operates in Remote mode. Only when the program was just started it needs to be connected to the scanner and its instruments.

Press the ![button] button to connect the program to the scanner and its instruments.

If the connection is established the ![buttons] buttons become visible as a sign that a scan can be started. However before starting a scan the Instrument Settings and the Measurement Setup parameters should be properly set.
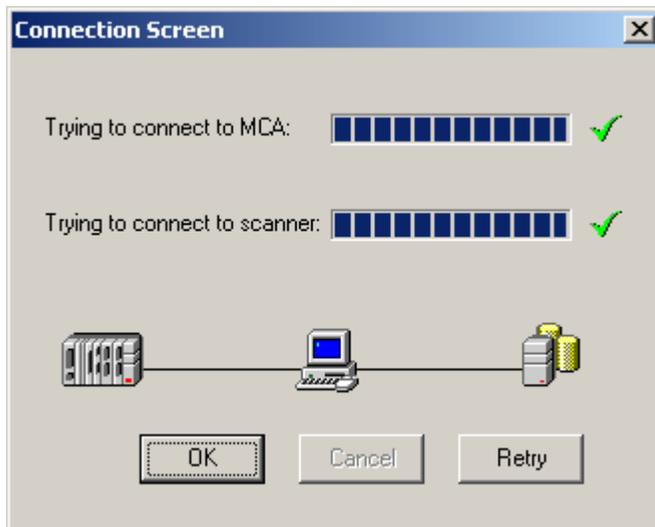
How Do I … Start a Step Scan:

Make sure that the program is connected to the scanner.
Click the Measurement Setup button on the Application Toolbar.
Fill in **Data Directory**, **Sample Name**, **Sample Length**, **Step Size** and choose an appropriate X-Ray **excitation**.
Close the Measurement Setup window by pressing the Ok button.
Select the Step Scan mode with the Scan Mode selector.
Be sure that the Helium and X-Rays are switched 'ON' at the scanner.
Press the Start button to start scan.

How Do I … Start a Calibration Scan:

A calibration scan is meant to monitor the systems long-term stability. At regular time intervals the user can measure a reference sample that usually is positioned at the left side of the scanners "0 cm" position.
The spectrum file name automatically contains the time and date of the measurement.
The excitation condition is to be set in the Measurement Setup window and should always be the same !!!

Make sure that the program is connected to the scanner.
Click the Measurement Setup button on the Application Toolbar.
Choose an appropriate X-Ray **excitation**.
The other parameters are ignored.
Close the Measurement Setup window by pressing the Ok button.
The **Data File Path** and measurement **Position** are taken from the Instrument Settings window Scanner-tab. Check if they still apply.
Select the Calibration Scan mode with the Scan Mode selector.
Be sure that the Helium and X-Rays are switched 'ON' at the scanner.
Press the Start button to start scan.

How Do I … Start a Stability Scan:

A stability scan repeatedly measures at the same position on a core to check the systems (and samples) stability. A stability scan ends automatically after the number of cycles set at Max.Test Cycles. If the Reposition checkbox is checked the scanner re-positions before a measurement. The spectrum file name automatically contains a cycle number.

Make sure that the program is connected to the scanner.
Click the Measurement Setup button on the Application Toolbar.
Fill in **Data Directory**, **Sample Name** and choose an
appropriate X-Ray **excitation**.
The other parameters are ignored.
Close the Measurement Setup window by pressing the Ok button.
The measurement **Position**, **Max.Test Cycles** and **Re-position** are taken
from the Instrument Settings window Scanner-tab. Check if they still apply.
Select the Stability Scan mode with the Scan Mode selector.
Be sure that the Helium and X-Rays are switched 'ON' at the scanner.
Press the Start button to start scan.

How Do I …   Reset a scanner error on the touch screen

If any serious failure in the scanner is detected like emergency stop, low air-pressure etc. the system stopped and an error symbol at the top of the touch screen will appear.
When the cause of the error has been found and eliminated the system should be re-activated again.
To recover from an emergency stop pull the red emergency stop button out and press the blue RESET EMERGENCY STOP button.

In any case press always the RESET ERROR and RESET CYCLE buttons at the touch screen. These buttons are available on the Main Menu Screen.