Radio Button Spark control
Select this check box to display parameters on spark control
(SEREPS/SATEUS/SETEME).

Radio Button Saft Parameters
Select this check box to display parameters on control of SAFT integration.

Button OK
Click this button to shut down the dialog box. Changed inputs are read-in and stored.

Button Cancel
Click this button to shut down the dialog box. Changed inputs are not read-in and not stored.

Button Clear
Click this button to delete the inputs in the highlighted area.

Button Fill Area
Click this button to fill a highlighted area in the table automatically. The most upper inputs are used as filling content. The highlighted areas below are filled with the contents of the upper highlighted row.

Button Fill
Click this button in order to fill automatically a marked area in the table. The top marked settings are regarded as a filling content. The marked fields below are filled automatically with the content of the first marked line.

Button Delete Lines
Click this button in order to remove the selected lines.

Button Insert Lines
Click this button in order to insert an empty line above the marked line.

Button Print
Click this button in order to print out the excitation parameters.

SPECTROLAB Jr. CCD

In the case of the SPECTROLAB Jr. CCD, the dialog looks as follows:
Table field Excitation Parameters
In this table field, the excitation parameters for the different measuring cycles are adjusted. The table contains the following columns::

Column field Measuring Cycle
Select the measuring cycle in these combination fields. In addition to the measuring cycles for different excitation types, measuring cycles without excitation are also listed. The following measuring cycles can be selected:

---	Source not activ
Arc	Arc excitation, for low detection limits
Spark 1,2,3	Spark excitation, provides in general better reproducibility as arc excitation
Prespark1,2	Prespark for the remelting and homogenizing the focal spot
Flush	Source not active, spark stand is flushed with Ar
Wait	Retardation, source is turned off on a short-term basis
PIMS	Measuring cycle for PIMS - analysis
Calculation	Cycle in which concentrations are computed while the excitation unit is active

Column field Time (sec)
You enter the measuring time in these edit fields for the different measuring cycles.

Radio Button Spark control
Select this check box to display parameters on spark control
(SEREPS/SATEUS/SETEME).

Radio Button Saft Parameters
Select this check box to display parameters on control of SAFT integration.

Button OK
Click this button to shut down the dialog box. Changed inputs are read-in and stored.

Button Cancel
Click this button to shut down the dialog box. Changed inputs are not read-in and not stored.

Button Clear
Click this button to delete the inputs in the highlighted area.

Button Fill Area
Click this button to fill a highlighted area in the table automatically. The most upper inputs are used as filling content. The highlighted areas below are filled with the contents of the upper highlighted row.

Button Fill
Click this button in order to fill automatically a marked area in the table. The top marked settings are regarded as a filling content. The marked fields below are filled automatically with the content of the first marked line.
Button Delete Lines
Click this button in order to remove the selected lines.
Button Insert Lines
Click this button in order to insert an empty line above the marked line.

Button Print
Click this button in order to print out the excitation parameters.

SPECTROLAB Jr. CCD

In the case of the SPECTROLAB Jr. CCD, the dialog looks as follows:
Table field Excitation Parameters
In this table field, the excitation parameters for the different measuring cycles are adjusted. The table contains the following columns::
  Column field Measuring Cycle
  Select the measuring cycle in these combination fields. In addition to the measuring cycles for different excitation types, measuring cycles without excitation are also listed. The following measuring cycles can be selected:

---	Source not activ
Arc	Arc excitation, for low detection limits
Spark 1,2,3	Spark excitation, provides in general better reproducibility as arc excitation
Prespark1,2	Prespark for the remelting and homogenizing the focal spot
Flush	Source not active, spark stand is flushed with Ar
Wait	Retardation, source is turned off on a short-term basis
PIMS	Measuring cycle for PIMS - analysis
Calculation	Cycle in which concentrations are computed while the excitation unit is active

  Column field Time (sec)
  You enter the measuring time in these edit fields for the different measuring cycles.

The following column fields are only visible if the **selection field Excitation Parameters** is marked at the lower margin of the dialog.

With the used computer-controlled Source generator (also called source), the parameters pulse width, frequency and current graph can be selected from a list of different default values.

Column field Pulse Width
Select the pulse width for the different measuring cycles in microseconds.

Column field Freq (Hz)
Here you select the excitation frequency for the different measuring cycles.

Column field Interval (ms)
Select the interval length for the different measuring cycles.

The interval time is the time between two reading processes of the CCD unit. If a spectral line generates a high intensity, the interval time must be short so that it does not come for an electric overflow error of the photomultiplier.

> **HDS** (high dynamic scan) is used if the spectra shall be recorded. The spectrum images can only be evaluated with a specific service tool which is not delivered with the unit.

> With **dyn** (dynamic) the system recognizes the optimum interval time automatically. **1, 10, 100, 1000** specify fixed interval times in ms.

> You should not change settings which are already adjusted with startup of your spectrometer!

Column field Current Graph
The numbers to be selected identify parameter sets of current graphs. You as user cannot draw conclusions from the figures to related parameters. Leave these settings as they are adjusted with the startup of your spectrometer.

Column field Ar
You select in these column fields, whether one flushes with high (A = Analytical Flow) or low Ar-Fluss (C = Constant Flow) during the measuring cycle.

Column field Shutter
In these column fields you can define, whether the optical path into the UV optics (gas flushed optics) shall be interrupted for specific measuring cycles.

Column field Spei Scan
In these column fields you define whether the spectra (Scans) shall be stored. The spectrum images are only evaluable with a specific service tool which is not delivered with the spectrometer.

Column field SEREPS
Mark this field if the prespark time should not be a fixed unit but should adapt itself automatically depending on behavior of the sample.

Column field Erk. Schl. Probe
Mark this field if a bad sample shall be identified. This check box must be marked if you apply SATEUS or SETEME (specific applications).

The following column fields are only visible, if the **selection field Spark Control** is marked at the lower margin of the dialog.

Column field Good Sparks %
In this edit field you enter the desired percent rate of "good" sparks so that the presparking and the subsequent analytical sparking of the sample is recognized as usable. An entry of 80 mean that 80% must be the "good" sparks in one second so that the sparking process is continued. If the preset percentage of good sparks is not achieved, the system aborts the measuring cycle and a message is displayed in the measuring window.

Column field Max Time (sec)

In this edit field you specify the prespark time allowed at the most. Is the maximum time in which the number of good sparks must be achieved. As maximum prespark time, the double normal prespark time is usually specified, with 20 seconds prespark time the maximum of time is consequently 40 seconds.

Column field Line Index

In this edit field, you find reference for a line / wavelength which is used for the SEREPS function.

Column field Sample

In this combination field, you select the name of the standardization sample which is used for the standardization of the SEREPS channel. A pure sample is usually selected as a standardization sample for SEREPS.

Column field Deviation %

The deviation in% specifies by how many % the intensity of one individual spark may differ from the mean intensity, so that this spark is accepted as a "good" spark. The value for mean intensity is determined during standardization and updated during each new standardization.

Column field Stand. Int

In this edit field the intensity is displayed, which was determined during the standardization of the SEREPS channel as mean intensity. The standardization of the SEREPS - channel is carried out during each standardization automatically. The value of the standardization intensity is automatically entered by the system and must not be changed.

Selection field Excitation Parameters

Select this selection field so that general excitation parameters are displayed.

Selection field Sparc Control

Select this selection field, in order to display parameters for spark control (SEREPS/SATEUS/SETEME).

Button OK

Click this button to shut down the dialog box. Changed inputs are read-in and stored.

Button Cancel

Click this button to shut down the dialog box. Changed inputs are not read-in and not stored.

Button Clear

Click this button to delete the inputs in the highlighted area.

Button Fill Area

Click this button to fill a highlighted area in the table automatically. The most upper inputs are used as filling content. The highlighted areas below are filled with the contents of the upper highlighted row.

Button Fill

Click this button in order to fill automatically a marked area in the table. The top marked settings are regarded as a filling content. The marked fields below are filled automatically with the content of the first marked line.

Button Delete Lines

Click this button in order to remove the selected lines.

Button Insert Lines

Click this button in order to insert an empty line above the marked line.

Button Print

Click this button in order to print out the excitation parameters.

See:

Menu Edit
Program Development

11.2.3 Dialog Box Element Parameter

The dialog element parameters includes all the elements which belong to the Analytical Program loaded. Additionally the following data are recorded on each element: the name, the type of element, measurement yes/no, 100% calculation yes/no, element results editable yes/no. The dialog box contains the following dialog elements:

Table Field with Element-Data

Recording element data is performed in a Table Field. The table contains the following columns:

Column Field Element

The combo boxes are used to enter or edit elements which shall be measured or calculated by means of the Analytical Program loaded. The data input can either be done directly: editing the edit area of the combo box or selecting an entry of the list box of the combo box. The list box is filled with the element names of the lines installed in the simultaneous Optics. Sorting of elements in the list box corresponds to the photo multiplier number. To name the elements 9 characters are permitted. There are no further limitations, i.e. instead of the usually used element symbol the real element name can be entered, provided that the maximum length of the name does not exceed 9 characters. Additionally you are in the position to enter names of Pseudo Elements.

Blank rows are not permitted in the table. Enter further elements into the first blank row. Always start with row 1 to create a new Analytical Program. To disable entries, select the entry '--' in the list box. Please note: Element names have to be unambiguous. In case a chemical element should be in twice, they are to be distinguished by the names, e.g. add an index: Si(2). The row sequence which has to be used for filling-in the elements is the default of the element output to screen and printer. Compare Dialog Box Element Format.

Column Field Element Type

You can define the element type in these combo boxes. Element types are analytic element, Reference Element, Line Switch, Pseudo Element, Monitor Element and PIMS element. The analysis of analytic elements is performed by measurement of channel intensity and its transformation into concentration units by means of the affiliated Calibration Function. Most elements of a program are analytic elements. Based on the definition such elements belong to the analytic elements, which are characterized by a switchover between two lines with Line Switch. If there is a line switch the resp. type 'line switch' instead of type 'analytic element' shall be selected. If an element should be used as a monitor element, select the type 'monitor element'. Pseudo elements and PIMS elements are selected respectively.

Generally the reference element is the base element. Measuring channels for the base element are used as reference channels for most analytic lines; the measuring data of the analytic channels apply to the reference channels. Generally the concentration of the reference element is not determined by a calibration function. The way is to add up the concentrations of all analytic elements; the concentration of the reference element is given by subtracting this sum from 100.

Conc [RefEle] = 100% - Sum (Conc [Analyt. Ele])

Column Field Measure

The check boxes 'Measure' are used to define whether elements shall be measured. Pseudo elements will not be measured. Results on pseudo elements are calculated from other element results or entered manually into the Measure Window. The check boxes 'Measure' are also be used to prevent some elements to be measured temporary. Provided that these elements are elements in Sequence Optics (only SPECTROLAB-S), a faster analysis time will be achieved.

Column Field 100% Calculation

The check boxes '100% Calculation' are used to define which elements shall be included in the 100%-calculation. This box should be clicked for all analytic elements, including the line switch elements.

Note:

> In case a chemical element has a double output, e.g. because two different analysis channels shall be compared, this chemical element shall be included in the 100% calculation just once!

Column Field Editable

If this box is checked, you may enter or modify the value for the respective element in the measure window manually. Reference type elements cannot be edited. For more information about editing measurement results see Carry out a Measurement.

Button OK

Click this button to shut down the dialog box and to read-in the modified entries for the element parameters in the Analytical Program.

Button Cancel

Click this button to shut down the dialog box without reading-in any modified entries.

Button Pseudo

Click this button to select the Dialog Box Element Specific Formula Selection to select a formula for calculation of pseudo. This button is only enabled if you had selected a pseudo-type element in the table.

Button Line Switch

Click this button to set the values of the Dialog Box Line Switch which is used to switch the lines between two or more analytic channels (Line Switch). Enter at first the lines in the Dialog Box Channel Parameters which are subject to switch. This is necessary to set the values of the switch lines and concentrations. Then return to dialog box line switch to enter the switchover.

Button Clear

Click this button to delete a highlighted area in the table. You mark an area by moving the cursor from one field to another with the arrow keys or the mouse (keep the left mouse key pressed). The area selected is displayed dark.

Button Fill Area

Click this button to fill a highlighted area in the table automatically. The upper highlighted entries are regarded as filling content. Highlighted fields below are filled with the content of the upper highlighted row automatically. Highlight an area by moving the cursor from one field to another with the arrow keys or the mouse (keep the left mouse key pressed). The area selected is displayed dark.

Button Insert Row

Click this button to insert a row between two already filled rows. You may enter an element into this row which shall be displayed between the element of the upper row and the element of the lower row.

Button Delete Row

Click this button to delete a complete row. This row is deleted the cursor is on. Only rows can be deleted which contain elements without operation with measuring channels. In case such an operation exists, please cancel this connection in the Dialog Box Channel Parameters at first.

See:

Program Development
Menu Edit

Dialog Box Element Format
Dialog Box Channel Parameters

11.2.4 Dialog Box Line Switch

In the dialog box 'Line switch' the values are set for switchovers of elements between analytic lines if a single analytic line of an element does not cover the required concentration range (Line Switch). Instead of a switchover between two lines of different wavelengths it is possible to switch between different source parameters. Different channels are assigned to different Source Parameters; in this case it is a channel switch. The assignment of channels to lines and source parameters is effected in Dialog Box Channel Parameters. The dialog box 'Line switch' is called with the button in the Dialog Box Element Parameters.

The definition of channels to be switched is automatically accomplished after entry or modification of calibration ranges when you quit the Dialog Box Channel Parameters or the Dialog Box Calibration Ranges This is why this dialog is mainly used to display the line switch and to set the values for the switch mode (linear switch, average value switch). Here you may modify the switched lines as well the switch concentration. Please note that this modification will be overwritten by the automatic assignment in the moment you exit the dialog box 'Channel parameters' or 'Calibration ranges' with 'OK', when you have modified the calibration ranges.

The parameter setting of a new Line Switch is effected in the following sequence:

1. Make sure that there is an entry 'type line switch' in the Dialog Box Element Parameter on the respective element and that the Dialog Box Channel Parameters contains an entry of min. two channels.
2. Select the resp. element in the list box 'selected analytic elements' of the dialog box line switch.
3. Select a line/channel in the list box 'selected lines of element'. Click the button 'insert'. The selected line is copied into the list box 'selected lines for line switch'.
4. Select the just copied entry.
5. Fill in limit values 'low concentration' and 'high concentration'. Continue to select the next line in the list box 'selected lines of element'.

Note:

Make sure that undefined concentration ranges do not occur. All line concentration ranges shall overlap or at least touch each other. The sequence of entries in the list box 'selected lines for line switch' decides upon the sequence of the concentration check on switchover.

The dialog box contains the following elements:

List Box Selected analytic elements
In this list box you can see all elements with an adjustment for more than one lines/channels. Select the respective element for editing.

List Box Selected Lines of Element
In this list box you can see the available lines/channels of the element selected from the list box 'selected analytic elements'. Select here an entry for further editing.

Group Box Line Switch Mode
In this group box you define the line switch mode. Click the radio button 'linear line switch' if a switchover at the very end of the concentration range of the channel is desired. In case you want to work in an overlap area of two channels with a concentration average of both channels, please select the radio button 'average line switch'.

List Box Selected Lines for Line Switch

This list box displays the following: the channel names of the selected lines for line switch, the names of the Optics, where the lines are measured, the concentration ranges the lines are to be used. The sequence in the list box is the same sequence the evaluation of the lines is performed.

Note:

Some sensitive lines tend to self-absorption at high concentration levels. With increasing element concentration of the samples to be measured the intensity increases, comes to a maximum and decreases on very high concentration levels. As soon as the problem of self-absorption occurs a switch from the line of high concentrations to the line of low concentration is recommendable.

Edit Field Low-Concentration and High-Concentration

These edit fields are used to display and to enter concentration limits; within the limits the selected line is evaluated. The program checks whether the entry on high concentration is possibly lower than the entry on low concentration.

Button <- Include

With a click on the button you read-in the selected entry from the list box 'selected lines of element' into the list box 'selected lines for line switch'.

Button Remove ->

With a click on the button you remove the selected entry from list box 'selected lines for line switch'. The entry is displayed again in the list box 'selected lines of element'.

Button OK

Click the button to shut down the dialog box and to read-in the modified entries.

Button Cancel

Click the button to shut down the dialog box without reading-in the modified entries.

See:

Dialog Box Channel Parameters.
Dialog Box Element Parameters
Dialog Box Calibration Ranges
Menu Edit
Program Development

11.2.5 Dialog Box Element Specific Formula Selection

By means of this dialog box you select a formula which is calculated according to an analysis result and is displayed as Pseudo Element. Fields of application are e.g. approximation calculus on mechanical properties of a material (example: tensile strength, Brinell hardness) based on the chemical composition of the material determined with the spectrometer. Element specific formulas are entered separately on each Analytical Program and are saved. This dialog box is opened via the button 'Pseudo' in the Dialog Box Element Parameters. The dialog box is divided into two areas: a group box to display the selection and below a list box to display all formulas.

Group Box to display the selection

This group box displays the parameters on the selected formula of the respective pseudo element.

Display Area Element Name:

In this field the name of the pseudo element is displayed you are working on. This is the element the cursor was positioned in the front-end Dialog Box Element Parameter.

Display Area Formula-No.:
This display area displays an internal formula number. In case no formula is selected a '0' is displayed here.

Display Area Formula Text
This display area displays the formula text of the selected formula. This is about a reference text on predefined formulas (e.g. calculate PIMS Reference Intensity Ratio) or a calculation rule of the formula. In case no formula is selected the word 'none' is displayed.

List Box to display all formulas

This group box displays all implemented general formulas and the special formulas defined for the respective Analytical Program. The first entry is the word 'none', selected if you would not assign a formula to a pseudo element or cancel a selection. The definition of the formula is effected in the Dialog Box Edit Formula which is called with the buttons 'New' or 'Edit'.

The following formulas are predefined:

1. Calculate PIMS reference versus intensity ratio:
This calculation is necessary in connection with the parameter setting of PIMS, where you may find more information.

2. Calculate sum of all impurities:
Often the quality standards of alloys require a limit for the sum of some certain elements which must not be exceeded. thus the quality monitoring verifies not only whether a single element exceeds the limit, but also whether the sum of certain element concentration exceeds the default value. See Carry out a Quality Monitoring for more information.

Button OK
Click the button to shut down the dialog box. The selected formula, displayed in the upper display areas, is saved together with the element data of the Analytical Program.

Button Cancel
Click the button to shut down the dialog box. The selected formulas will not be saved.

Button Edit
This button opens the Dialog Box Edit Formula to change the formula highlighted in the list box. To highlight without mouse use the arrow keys.

Button New
This button opens the Dialog Box Edit Formula to define a further formula.

Button Delete
This button deletes the formula highlighted in the list box. To highlight without mouse use the arrow keys. The deletion cannot be undone. A formula selected for use cannot be deleted. To delete it, you have to call the dialog of the respective pseudo element and to undo the selection. Now the formula can be deleted. If necessary you should delete the corresponding pseudo element in the Dialog Box Element Parameters or link another formula to the pseudo element.

Button Select
This button selects a formula from the list box. Information about the formula are displayed in the upper part of the window. The formula result is displayed directly after the analysis.

See:

Dialog Box Element Parameters
Menu Edit
Program Development
Parameter Setting on PIMS

SPECTRO

11.2.6 Dialog Box Edit Formula

In this dialog box you edit a formula which is the calculation rule on a pseudo element or on a sample identification character. This dialog box can be called from the Dialog Box Element Specific Formula Selection or from Dialog Box Sample-ID-Format. When calling from dialog box 'Element specific formula selection' a list box with the elements of the Analytical Program is displayed additionally. The dialog box contains the following dialog elements:

Group Box Define Formula
This group box displays an edit field used for formula input and a list box with possible calculation and arithmetic operations.

Edit Field Formula
A suitable formula can be entered in this field directly. Note the formula syntax, e.g. opening brackets always have to be closed by closing brackets. Maximum 128 characters a formula may contain. Instead of a direct input a formula may be entered via list box 'Functions and operators'.

List Box Functions and Operators
This list box displays all functions and operators which can be used in connection with the formula calculation. A double click on the list entry moves this entry into the edit field formula where it may be completed with numerical values. Permitted functions and operators:

(,)	opening and closing brackets, several bracket levels possible
+,-,*,/	four elementary operations: addition, subtraction, multiplication, division
^	exponent, 2^3 corresponds to $2^3 = 8$
E	Euler's constant 2.71828
EXP	corresponds to e to the power of X
INP(X)	corresponds to the value of the x.st sample identification field
LN	natural logarithm
PI	constant 3.1415926
VAL(XY)	corresponds to the measure value of the element XY

Decimal numbers shall be entered with a . (point).

The following example shows a formula which displays a calculated Brinell hardness HB of a pseudo element, based on the analysis results C, Si, Mn, S:

444-71.2*VAL(C)-13.9*VAL(Si)+21*VAL(Mn)+170*VAL(S).

List Box Elements (only in case of entering a formula for a pseudo element)
This list box displays all elements which are defined on the Analytical Program. A double click on a list entry moves this element name into the edit field formula where it may be completed with numerical values. Instead of this a direct input into the edit field formula is possible.

Display Field Test Result
This display field shows the calculation result of the formula in the upper field of the window. The test calculation is carried out when the button 'test' is clicked. During the test calculation the numerical value 1 is used as numerical value for all variables of the formula. In case you use a complicated formula with several variables we recommend you to check the calculation result on the measure screen against a real analysis.

Button OK
Click this key to shut down the dialog box. The edited formula is displayed in the dialog started before editing the formula.

Button Cancel
Click this key to shut down the dialog box. The edited or new created formula is not read-in.

Note:

In case element results are used for calculation of formulas, the calculation is always performed with the results of the current output mode (concentration, intensity).

See:

Dialog Box Element Specific Formula Selection
Dialog Box Sample-ID-Format
Dialog Box Output Mode
Menu Edit
Menu Extras
Program Development

11.2.7 Dialog Box Channel Parameters

By means of the dialog box channel parameters the channels with its parameters are defined which shall be used in the loaded Analytical Program. The dialog box is opened with the menu item channel parameters in the Menu Edit of the Program Development. The record is effected in form of a Table. The dialog box contains the following elements:

Table Field with Channel Parameters
All table rows have to be filled in sequence. Start with the entry in column PM Wavelength! This is why this field is at first explained below. The fields PM Wavelength, SIM, Type, Reference, Excit. Para are visible if the radio button 'channel parameters' in the lower part of the dialog is enabled. Provided that the radio button 'calibration limits' is marked, you see the fields Matr. Corr., Type Intens., Low Limit, High Limit. In case where the check box 'SSE Parameter' is marked, the column with the check boxes 'use SSE' is displayed. The table contains the following columns:

Column Field PM Wavelength LAB CAST
At first select the electronic channel to be measured. This combo box is filled with the installation data of your Spectrometer. Each electronic channel is represented by the photo multiplier (PM), which measures the light of a definite wavelength. The further input in this field identifies the line connected to PM (element symbol + wavelength), the line type (I = atom line, II = ion line), and the optics which measure this line (e.g. [2], the simultaneous optic No. 2). At first define all reference channels and then the analytic channels.

Making a selection in this combo box the edit field 'channel' is automatically filled in. Using several channels for the same chemical element an index is annexed automatically, e.g. Si1. Additionally the marking field SIM is highlighted automatically and the line type (combo box Type) is pre-allocated with the entry A (analytic channel). It's not possible to skip a row. When you want to define a new channel, you have to make your inputs in the first blank row of the table or insert a new row between existing ones.

Note:

No PM number is displayed, if you don't use a channel from a simultaneous optic as reference line, but a line which shall be measured by an optionally available monochromator. The optic which measures the line, is marked with the letter M for monochromator. To get information which wavelengths may be selected, please read the items for the column field SIM.

Column field Wavelength ▊▊▊▊

This combination field is filled with the installation data of your spectrometer. The specifications in this field identify the line (element symbol + wavelength), the line type (I = atomic line, II = ion line, * = not defined) and the optics where this line is measured. First define all reference channels and then, the analytical channels.

The edit field Channel is filled automatically by your selection in this combination field. With several channels for a chemical element, an index is appended automatically by the program. Further, the check box SIM is marked automatically and the line type (combination field type) is pre-selected with the entry A for Analytical Channel. You cannot skip lines. If you would like to define a new channel, you must carry out your entries in the first free line of the table.

Column Field Channel

This edit field is pre-allocated after selecting an entry in combo box 'PM Wavelength'. However the channel name can be changed acc. to your demands. Please note that the channel name has a max. size of 9 characters and shall be unambiguously.

Column Field Element

By means of this combo box you select a reference element, which was defined in the Dialog Box Element Parameters. A check of your input is effected when you quit the dialog. In case you did not select a valid element, quitting the dialog and storing the edited data is not possible. The input '-' in the element field is regarded as invalid element.

Column Field SIM

In this marking fields all channels are marked which are located in a Simultaneous Optic. If you don't use a SPECTROLAB equipped with the optional monochromator, all channels are simultaneous channels. Then these fields are not accessible. If you want to measure a line with a monochromator, you have to unmark the check box. The combo box *PM Wavelength* is automatically filled with lines, which are marked as best lines (line proposal) in the line library. The entries in the combo box are sorted acc. to the sensitivity of the spectral lines.

Column Field Type

By means of this combo box you define the type of the channel selected. There is the choice between analytic channel (A), reference channel (R), monitor channel (M) and PIMS channel (P). An analytic channel is calibrated to determine concentrations, a reference channel belongs to the base element and is used as internal standard, a PIMS channel is used to determine metallic and undissolved concentrations of oxides forming elements. A monitor channel is not calibrated but used for intensity monitoring and is displayed on the measuring screen.

Column Field Reference

By means of the combo box reference a reference channel is assigned to the analytic channel. You see all reference channels in the combo box which were defined in this table. In case of a complete rerecording of the channels for an Analytical Program it is advantageous to define all reference channels at first. During recording the other channels a combo box is available which contains all possible reference channels. As a reference line for an analytic line, a line of the same optic and of the same source parameters should be chosen, if available.

Column Field Excit. Parameters

The Source Parameters for the selected channel are recorded in this combo box. Depending on application and desired concentration area different excitation parameters may be applicated on different elements.

Column Field Matr. Corr.

By means of the check box 'matrix correction' a definition is made whether a matrix correction is to carry out on this line. Most analytic channels are calibrated against a reference element (relative calibration). To be able to output these elements in absolute concentrations, i.e. not in concentration ratios, it is necessary to carry out a matrix correction.

Column Field Type Intens.

This edit field is enabled for reference channels exclusively. Enter a numeric value which is similar to the intensity of a blank sample of the reference element. The precision of the input does not effect the analysis precision. This entry takes only effect for the display of intensity ratios in the Measure Window. The display of intensity ratios is done on non-calibrated channels. Furthermore the display may be switched to intensity ratios for all channels to check the work routines of the spectrometer. As most channels are calibrated on intensity ratios, a display of relative channel intensities would result in small numbers. By multiplication with the numeric value 'typical intensity' values are displayed which correspond to the absolute channel intensity and are better readable.

Column Field low limit/high limit

You see the low limit and the high limit resp. of the calibration range in these edit fields in concentration units. These concentration units were used or will be used to calibrate the channel. The limits may be edited in the Dialog Box Calibration Data, which is called with the button 'calib. Data'. In case of reference type channels enter intensity values in the fields for low limit/high limit; when the current value drops below or exceeds a limit value, a warning is displayed on the Measure Window. E.g. a loss of light by contamination or misfitting can be easily recognized during the measurement process.

LAB CAST Column Field Use SSE

By means of the check box 'use SSE' you define whether you want to work with the single spark evaluation for the respective channel. These fields are only enabled for channels, where the box SSE in the Dialog Box Lines Installed is also marked. You enter in the dialog box Lines Installed whether the corresponding channel is equipped with SSE-Hardware. Here you define specifically for the entire analytical program whether this channel should operate with SSE.

Check Boxes Channel Parameters, Calibration Limits, LAB CAST SSE Parameters

Click these check boxes to switch between the display of channel parameters, the calibration limits, the SSE parameters.

Button OK

Click the button to shut down the dialog box and to read-in the modified entries on channel parameters in the Analytical Program.

In case you entered or modified calibration ranges, a table for line switching is automatically generated when you close the dialog: Based on the calibration range the most sensitive line is searched for each element. Based on this line, another channel of the same element is searched for, whose calibration range overlaps the current calibration range at the upper end. This channel is then used as starting point for a further search for another channel with overlapping calibration range. This search is performed separately for each element. The result of the line switch may be checked in the Dialog Box Line Switch, which is called-up in the 'Dialog Box Element Parameters'.

Button Cancel

Click the button to shut down the dialog box without reading-in the modified entries.

LAB Button Scanman.
Click this button to open the Dialog Box Select Lines for Scan. This button is only visible if your Spectrometer is equipped with an optional Monochromator, which is available for some models and if you have clicked into a field in the tabel. If you have marked a whole line or column, this button is not visible.

LAB CAST Button SSE Parameters
Click this button to open the Dialog Box PIMS-Parameter. This dialog is used to define the SSE-parameters for the channel which is selected in the table. The button initiates the check box only if for the selected channel the function SSE is activated.

Button PIMS Para.
Click the button to open the Dialog Box PIMS Parameters. This dialog is used to define PIMS-Parameters for the channel selected from the table. The button is enabled if the selected channel is a P (PIMS) type one, see Dialog Box Element Parameter.

Button Calib. Data
Click the button to open the Dialog Box Calibration Data. This dialog is used to display the data of the calibration function and limit values of the channel selected from the table.

Button Copy Line
Click this button to copy the channel data of a row. Not only the visible entry of the channel is copied, but also all data of the logic channel, including the measured calibration intensities etc. This function allows to split up a channel into several channels with e.g. divided calibration ranges.

Button Insert Row
Click the button to insert a row between two filled rows.

Button Scanman.
Click the button to open the Dialog Box Select Lines for Scanning. This button is only enabled if your Spectrometer is equipped with the optional monochromator and if you had clicked in a field of the table. If you have marked entire columns or rows, the button is not visible.

Button Del Row(s)
Click the button to delete a complete row. That row is deleted the cursor is positioned on. Please note that you change dependent data by deleting a definite channel. If you would delete e.g. a reference channel used by other channels, the pointer on the deleted reference channel will be removed for these elements too. Note additionally that you have to remove the corresponding element from the Dialog Box Element Parameters if necessary.

Button Fill Area
Click the button to fill a highlighted area in the table automatically. The upper highlighted entries are regarded as filling content. The highlighted field below are filled with the content of the upper row automatically. Highlight an area by moving the cursor from one field to another with either the arrow keys or the mouse (keep left mouse key down). The selected area is displayed dark.

Button Print
Click the button to print the table.

See:

> Program Development
> Scan Manager
> Menu Edit
> Dialog Box Element Parameters

11.2.8 Dialog Box Calibration Data

The dialog box displays the calibration data of one channel. The dialog box is called from the Dialog Box Channel Parameters. The active row of this front-end dialog defines the channel the dialog box 'calibration data' is opened for. The title row of the dialog box displays the name of the line the calibration data are shown. The dialog box contains the following data:

Display Field Line State
The entry in this field indicates whether the resp. channel is calibrated or not.

Display Field Weighting
The entry in this field indicates the weighting model used by the calibration samples addressed to the regression calculation of the calibration. Depending on the development stage of the program the following weightings may be selected in the regression program:

none:	all calibration standards are weighted equally
manual:	weighting factors were assigned to the calibration standards manually
concentration:	standards on high concentrations are less weighted
intensity:	standards showing high intensity values are less weighted
variance:	standards showing a low deviation on the calibration curve are weighted higher with the power of two

Group Box Calculated Calibration Data
This group box summarizes all calibration data which were calculated in the frame of the regression. Overwriting the entries is possible.

Note:

The calibration data are very critical data generating the relation between measured light amount and displayed concentration. By means of the calibration data the photometer device transforms into an analysis equipment. This is why we warn everybody to modify these data, especially a change of the polynomial coefficients A0-A3 of the calibration function.

Edit Fields A0, A1, A2, A3
These edit fields display the polynomial coefficients of the calibration function.

Edit Field Std. Err.
This edit field displays the standard error of the calibration function. The better the calibration spots meet the calibration function the lower is the standard error. Consequently the size of the standard error supplies a tendency about the quality of calibration.

Edit Fields Low Limit / High Limit
The concentration range of the calibrated area is displayed in the fields low limit / high limit. The low limit is equivalent to the detection limit if a detection limit was defined. Otherwise the low limit is the concentration of the lowest standard. The high limit corresponds to the concentration of the highest standard + 20%.

Edit Fields BEC/DL/Corr. Coef.
These fields display the size of the background equivalent concentration (BEC), the detection limit (DL), the correlation coefficient. Provided that all calibration samples lie on the calibration function, the correlation coefficient is 1. Similar to the standard error the correlation coefficient is a measure for the position of the calibration samples on the calibration curve.

Button OK
Click the button to shut down the dialog box and to read-in the modified entries on the channel parameters in the Analytical Program.

Button Cancel
Click the button to shut down the dialog box without reading-in the modified entries.

See:

Dialog Box Channel Parameters
Dialog Box Calibration Ranges
Menu Edit
Program Development

11.2.9 Dialog Box PIMS Parameters

This dialog box is used to display and edit PIMS parameters. The dialog box is called from Dialog Box Channel Parameters. A call is only possible for PIMS type channels. The active row in this front-end dialog defines for which channel the dialog box is opened. The title row of the dialog box displays the name of the channel the PIMS parameters are recorded for. The dialog box contains the following elements:

Group Box Edit Parameters
This group box displays and records PIMS-Parameters.

Check Box Soluble
This box is marked if the channel represents the soluble part of the total concentration on an (e.g. Al sol.) element. A chemical element which shall be characterized by its soluble and insoluble shares requires both, one PIMS channel with a marked check box 'soluble' and one channel with an **unmarked** check box 'soluble'.

Edit Field Background Intensity
This edit field displays the background intensity of the respective channel. The background intensity is determined by measuring a sample which does not contain the resp. element (e.g. a blank sample). The intensity ratio value achieved is entered here manually.

Button OK
Click the button to shut down the dialog box and to read-in the modified entries of the channel parameters in the Analytical Program.

Button Cancel
Click the button to shut down the dialog box without reading-in the modified entries.

See:

Dialog Box Channel Parameters
Menu Edit
Program Development
Value Setting of PIMS

11.2.10 Parameter Setting for PIMS

This is a guide to set the values for PIMS for an already calibrated element which contains dissolved and undissolved components in the samples.

1. Dialog Box Excitation Parameter
Define a measure cycle PIMS with all necessary parameters in the dialog box **Excitation Parameter**. The PIMS - measure cycle has to be put in front of any other analytical measure cycle.

2. Dialog Box Element Parameter
Make sure that the element which contains dissolved and undissolved components, is entered in the table with the **Element Type Analytically**. If necessary rename this element to make clear that this element represents the the complete content: dissolved + undissolved. An example for the element Aluminum: Al compl.

Then define two more PIMS-elements for the dissolved and undissolved components. An example for the element Aluminium: Al diss. and Al undiss. Now assign these elements to the **Element Type PIMS**. Define a Pseudo Element e.g. called PIMS Ref. Click the button **Pseudo** to access the dialog box **Pseudo Element Selection**. Select the predefined formula **Calculate PIMS Ref. Intensity Ratio**. Please note that the button SELECT shall be pressed to make the selection; selecting the entry in the list box is not sufficient.
Please note that only one element with the type **Analytically** may be incorporated in the 100% calculation. Check the corresponding boxes.

3. Dialog Box Channel Parameter
Define two new channels and link them with two new generated elements. When you have renamed your analytical element, make sure that the connection between channel and element is correct. An example for the channel name of the element Aluminium: Al compl., Al diss., Al undiss.

Assign the channel type PIMS to these new two channels. Select the respective excitation parameters for the PIMS channels. Open for both channels the Dialog Box PIMS Parameter through a click on the button PIMS. Set the check box **Soluble** for the respective channel. Make sure that the check box is not set for the other channel.

4. Save Analytical Program
Select the Menu Item Save Program or open the Dialog Box New Program / Save as. Now the program is prepared for PIMS.

5. Measuring Samples with dissolved and undissolved Components
The measure window displays the overall content of the element, as well as the share of dissolved and undissolved components in concentration units. The pseudo element which was value set under item 2 for PIMS, views the intensity ratio of the reference line intensities for both PIMS elements. As the reference intensity should roughly be on the same level, the value for the pseudo element must be approximately 1. If not, the PIMS function may not work properly.

11.2.11 Dialog Box SSE-Parameters

This dialog box is used to display and edit SSE-Parameters. The dialog box is called-up from the Dialog Box Channel Parameters. You can call up the dialog only for channels which are flagged in the field 'use SSE'. The active line in this pre-dialog selects the channel in which the dialog box is opened. The header of the dialog box shows the name of the channel in which the SSE parameters are recorded. Depending on the software, the dialog box may contain the group box 'fitting Parameter'. You must not change any entries in this window. The dialog box contains the following dialog elements:

Group Box Calculation Parameters
The group box displays and records the calculation parameters. The calculation parameters specify the value retuned to the measure window of the Spark Analyzer.

Edit Field Number of Pre-Sparks
Enter the number of emitted sparks to be considered for a single spark evaluation.

Check Box Store Results
Mark this box to store the single spark intensities (ssefile.i00), a histogram (ssefile.h00) and the statistical results (ssefile.s00) of the current channel in a file. The file name ssefile is a default. You may also enter another name in the dialog box 'sample data'. This dialog box opens by pressing F9 or the respective button 'next sample'. But before you should have changed the name of the third field (sample-ID.) to 'file name' in the dialog box 'sample-ID-format'. The file is stored in the directory c:\winlab at the Spectrometer computer. You are not working with the interface of the SPARK ANALYZER in the PC-software is regarded as Spectrometer computer - but the built-in one-board PC inside the Spectrometer. Provided that the Spectrometer computer is connected to a network, you may change the directory if there is already a directory in the network. In this case ask the Spectro service for more information. If this item isn't checked for any SSE-channel of the Channel Parameter dialog, no file will be saved.

Use Check Box for Global Standardization
If this box is checked, the SSE results are used for global standardization.

Edit Field Warning for Standard Deviation
Enter a maximum relative standard deviation in % in order to mark exceeding intensity and standard deviation of the respective channel in the measuring window . The marking occurs in red paint in the measuring window at the corresponding channel, if the entered value for the relative standard deviation is exceeded. Standard deviation refers to the single spark intensities.

Check Box Total Mean
The mean intensity of all evaluated single sparks is shown in the measure window.

Check Box Gauss Mean
The Gaussian curve fits into the deviation of the single spark intensities and is shown in the Measure Window.

Check Box Total Area
All evaluated single spark intensities are summed up. The result will be shown in the Measure Window.

Check Box Gauss Area
A Gaussian curve fits automatically into the deviation of the measured single spark intensities. The area under this best Gaussian curve, i.e. the integral, is calculated and shown in the Measure Window.

Check Box Remaining Area
The difference between the no. of summed up single spark intensities (Total Area) and the Gaussian area is calculated and shown in the Measure Window.

Check Box Area with Discriminator
The single spark intensities summed up inside a specified interval around the mean single spark intensity are shown in the Measure Window. If you select a default calculation mode, two edit fields - the lower and the upper limit - will appear.

Edit Fields Lower Limit / Upper Limit

These edit fields only appear if you have marked the check box 'area with discriminator'. You can enter factors for the upper and lower limit. These factors are multiplied by standard deviation σ. Example: Lower limit = -127 and Upper limit = 3 means, that all single spark intensities will be summed up in the range m-127*s ... m+2*s (m = Gaussian mean). The highest possible values entered here are -127 and +127.

Group Box Prespark Parameters

You can make a choice between fixed and dynamic settings of a number of single sparks for the pre-sparking. We recommend a dynamic number of presparking-single sparks, until the process of reaching the steady state is completed. This necessary period could be obstructed by another element, especially by the Base element.

Check Box Dynam. Calc. of Pre-Sparks

Check this box to calculate dynamically the number of delay sparks, which depend on the time needed to reach the steady state of a reference channel. If this field is not enabled, you have to define a pre-spark reference channel first.

Edit Field Number of Pre-Sparks

Enter the number of emitted sparks until integration and evaluation of the single spark intensities starts. This parameter is only shown if the check box 'Dynamic calc. of pre-sparks' is switched off.

Edit Field Intensity Limit (%) of Pre-Spark Reference, Start SSE-Evaluation

Enter the relative intensity limit (%) to determine the break off criteria, i.e. the absolute intensity limit at which the movement of the average intensity should stop. The movement of the average intensity is described in the function description of SSE or in a future version of this help text.

The field only appears if the check box for dynamic calculation of pre-sparks is switched on.

Check Box Use current channel as reference for dynamic calc. of number of pre-sparks

This box must be checked to mark the current channel as a reference to calculate dynamically the no. of pre-sparks. This parameter is disabled, if another channel has already been marked as pre-spark reference. In this case, the name of the selected pre-spark reference is shown in the title of the pre-sparks group box. If dynamical calculation is requested, the box must be checked in at least one channel. Otherwise, the parameter 'Dynamic calc. of pre-sparks' is disabled.

Button OK

Click this button to close the dialog box and to store the modified channel parameter settings in the analytical program.

Button Cancel

Click this button to close the dialog box. No entries are stored.

Button Mult. Set.

Click this button to copy all entered SSE-Parameters in this channel into all SSE-channels. SSE-channels are marked with the check box 'SSE' in the Dialog Box Channel Parameter.

Button Default

Click this button to fill all SSE-fields of the current channel with default values.

See:

Dialog Box Channel Parameter
Menu Edit
Program Development
Parameter Setting for SSE

11.2.12 Parameter Setting for SSE

This information is still not available. Please used the operating manual in writing to be supplied by SPECTRO.

11.2.13 Dialog Box Element Format

The dialog 'element format' is used to display and edit the output sequence and to format elements and corresponding analysis results for several outputs. The dialog box is called from the menu item **Channel parameters** in the Menu Edit of the window Program Development. The record is effected in a table. The dialog box contains the following dialog elements:

Table Field with Element-Formatting-Data
The Table contains the following columns:

Column Field Element
In this display field you see the elements displayed with the output unit selected. The selected output unit can be identified by the marked check box on the bottom part of the screen.

Column Field Order
By means of these edit fields you define the order, the elements are displayed in the resp. output unit. Double order numbers cannot exist. In case an order number is entered twice, an error message will be displayed in the moment you try to quit the dialog with 'OK'. Additionally gaps cannot exist in the order. An error message will be displayed too.

Column Field Display
By means of these check boxes you define whether an element is displayed on the output unit. So you can adjust some elements not being displayed in the output unit.

Column Field Format
These combo boxes enable a formatting of the analysis results, individually for each element. The standard set is Dyn: dynamic formatting. In dynamic formatting the number of places behind the decimal point depend on the quantity of the value to be displayed. The dynamic formatting is defined by adjustments in a Parameter File. Experienced users may carry out adjustments here. Instead of the dynamic formatting a formatting with a fixed number of places behind the decimal point is possible. Click the combo box and select an entry between F0 and F7. E.g. F3 defines three places behind the decimal point. In case the necessary number of places behind the decimal point is not sufficient to display the value, the decimal value is cut. Please note that the analysis precision is not improved by increasing the number of places behind the decimal point. Below an example is given for dynamic formatting (Dyn) and fixed formatting (F3):

Dyn	F3
12.3	12.345
1.234	1.234
0.123	0.123
0.0123	0.012

Furthermore there is the entry 'Qual' in this combo box. When you click this entry and when a Alloy Grade term of the sample is recorded in the Measure Window, the formatting of the analysis results follows the formatting which is fixed in the alloy grade list.

Column Field Unit
By means of these combo boxes you define the output unit to be displayed. The list of the output units may be modified in Parameter File.

Column field Factor

This edit field is used to incorporate a conversion factor for the display of the analysis results. It is used to convert the unit, e.g. an element is calibrated in % but an output in ppm seems to be advantageous. In this case the conversion factor would be 10000.

Attention: If you want to proceed the results in the data evaluation program DIA, it is absolutely necessary that you save the results in the format "%" and factor = 1 is entered (applies only for the output unit 'File')!

Radio buttons on Output Units

A click on a radio button specifies the output unit, for which the element format is to be displayed and to be edited. There is a choice between monitor output, printer output locally and externally, saving and transmitting files.

Button OK

Click the button to shut down the dialog box and to read-in the modified entries in the Analytical Program.

Button Cancel

Click the button to shut down the dialog box without reading-in the modified entries.

Button All Devices

Click the button to validate the output settings for all output units(devices). This button is enabled if you have selected the output unit 'Monitor'.

Button Delete

Click the button to delete a highlighted area in the table. You mark an area by moving the cursor onto a field, press and hold down the left mouse key and move the cursor to the other fields. The selected area is highlighted dark.

Button Paste

Click this button to paste a highlighted area in the table automatically. The most upper marked entries are regarded as pasted content. The lines below are pasted automatically with the content of the first marked line. You mark an area by moving the cursor onto a field, press and hold down the left mouse key and move the cursor to the other fields. The selected area is highlighted dark.

Button Reorder

Click the button to undo the changes on the element order made by entries into the table column 'order'. The element in the first table column is assigned to the number 1 of the order and so on.

See:

Program Development
Menu Edit
Dialog Box Output Parameters
Dialog Box Output Setup

11.2.14 Dialog Box Output Format

This dialog box is used to define the output parameters. The output parameters fix which automatic outputs shall be effected on a definite output unit. The respective output units (e.g. printer, data file etc.) may be assigned to different parameters. The dialog box is called from the menu item 'output format' in the Menu Edit of Program Development. Entries are effected as marks into a matrix of check boxes.

Group Box Final Results
These rows are used to define the location, the final results shall be displayed. Final results are single measurements, average values, average values & relative standard deviations respectively. When you highlight the resp. fields these data are automatically transferred to the output unit.

The following output options are available:

Printer (local)
Printout on the local printer of the spectrometer.

External Printer
The printout is effected on a remote printer, e.g. at the furnace top platform or the process control room. This printer is connected to the spectrometer with a serial interface. Setting up an external printer is described under Tips &Tricks

Save
The results are stored in one or more files. File formats and file names are to be set with the button 'data file' which calls the Dialog Box Data File Parameter. To store results in files facilitates both, a convenient documentation and a later evaluation of data. When you store data in files take care that files do not become too big. Delete the processed data records in the memory files regularly.

Note:
The storage of analysis results is parametrized here and exclusively intended for ongoing processing with external programs. For operations with the window 'Sample manager' the storage of analysis results is controlled by a parameter file. Please read the text under the head word Sample Manager.

Transmit
Data are transmitted to another computer via a serial interface. Depending on the setting this is done in the Dialog Box Output Setup either directly after the analysis or with the Menu Item Transmit Buffered Data. The computer receiving the data is often used to document the results and enables a later evaluation of the data. Read the keyword 'data format' for the data format in use. Setting up a data transmission is described under Tips&Tricks.

Group box extended values
Here you define if and where you want to output further measuring data. You can select between "Save Data" and "Transmit", if a data transfer is installed. Raw intensities can be printed out at the local printer.
The data mentioned here are used for the calculation of the displayed analysis results. Based on row data and on knowledge of all program parameters the output final result can be determined again at any time.

Raw intensities: Raw intensities are measuring signals of the transducers (photo tube (PM) or CCD-unit). Raw intensities can be printed and stored.

Intensity ratios: Intensity ratios can be stored.

Reference intensity: Reference intensities can be stored.

SSE with RSD: Results of single spark evaluation can be stored with the associated standard deviations.

Stdz. coeff.: Results of a standardization (factor and offset) can be stored.

Button OK
Click the button to shut down the dialog box and to read-in the modified entries on output parameters in the Analytical Program.

Button Cancel
Click the button to shut down the dialog box without reading-in the modified entries.

Button Data File
Click the button to open the Dialog Box Data Parameter and to define file names and file formats on the data to be stored.

Button User Task
Click the button to open the Dialog Box User Task Parameter and to define the User Tasks to be called.

Tip: Several user tasks / several result files

If you want to call up several user tasks, you can write a small batch file which calls up your user tasks. Enter this batch file into the dialog box "User Task Parameter" (see above) as an program to be called up. During working with the batch file, your single user tasks are called. If all of your user tasks want to access an own file with stored analysis data, you can generate file copies with the program C:\SPECTRO\BIN\COPYFILE.EXE. At first call up this program and create the necessary copies. Then each user task can work with its own copy and then delete it. You save the selection of the files to be copied and the names of the target files in the Parameter File PS GEN.ASC.

See:

Program Development
Menu Edit (Program Development)
Menu File (Measure Window)
Menu Item Transmit Buffered Data
Dialog Box Output Setup
Dialog Box Element Format
Sample Manager
Tips&Tricks

11.2.15 Dialog Box Data File Parameter

By means of this dialog box you define the output format and the name of the result files of the analysis results. Up to four files with analysis results can be written simultaneously. These files use the same name but are equipped with different extensions. The dialog box is called from the Dialog Box Output Parameter.. The dialog box contains the following dialog elements:

Note (DIA):

If you intend to manage your element results by the external analysis management program DIA select **ANALYSEN** as file name. Check the box for the SPECTRO 4.3 format in the group window **Element Data** and type in the file extension **DAT**.

If want to manage your results only by means of the integrated sample manager you do not need this dialog.

Display Field Data File
This field displays the file name incl. its path but no file name extension. Selecting a file name is performed with the button 'file name'.

Group Box Channel Data File Extension
In this group box you define a storage of the channel measure results and the file name extension.

Check Box and Edit Field SPECTRO-4.3-Format
Mark the check box if you would like to store channel results in SPECTRO-4.3 format. The SPECTRO-internal SPECTRO-4.3 format generates an interface on the SPECTRO data management programs DIA and SDC. Of course you can evaluate a data file in that format by means of other programs, e.g. self-made programs. Information on the data format are available at SPECTRO service. The file extension of a SPECTRO-4.3 format is SFC generally. You may enter another extension in the edit field (3 characters) optionally.

Check Box and Edit Field ASCII-Delimited Format
Mark the check box if you would like to store channel results in a ASCII-Delimited file. The delimiter and the amount of the information to be stored (number of channels and sample identification concept) can be set with the Parameter File PS_STORE.ASC in the subdirectory SETS of the SPECTRO installation. Order of elements and formatting the output is defined in the Dialog Box Element Format. Tips on proper work with this parameter file are available at SPECTRO service. The extension of the file in ASCII-delimited format is ADC generally. You may enter another extension in the edit field (3 characters) optionally.

Group Box Element Data File Extension
In this group box you define a possible storage of element measure results and the file name extention.

Check Box and Edit Field SPECTRO-4.3-Format
Mark the check box if you would like to store element results in SPECTRO-4.3 format. The SPECTRO-internal SPECTRO-4.3 format generates an interface to the SPECTRO data management programs DIA and SDC. Of course you can evaluate a data file in that format by means of other programs, e.g. self-made programs. Information on the data format are available at SPECTRO service. The file extension of a SPECTRO-4.3 format is DAT generally. You may enter another extension in the edit field (3 characters) optionally.

Check Box and Edit Field ASCII-Delimited Format
Mark the check box if you would like to store channel results in a ASCII-Delimited file. The delimiter and the amount of the information to be stored (number of channels and sample identification concept) can be set with the parameter file PS_STORE.ASC in the subdirectory SETS of the SPECTRO installation. Tips on proper work with this parameter file are available at SPECTRO service. The extension of the file in ASCII-delimited format is ADE generally. You may enter another extension in the edit field (3 characters) optionally.

Button OK
Click the button to shut down the dialog box. The path and file name displayed in the upper edit field is used for storage of channel and element results. To effect the storage it is necessary to switch on storage in the front-end dialog and to highlight of at least one marking field in this dialog.

Button Cancel
Click the button to shut down the dialog box. Entries on file names and type of data to be stored are not read-in.

___

Button File Name
Click the button to define the standard-Windows-dialog box folder for definition of path and file names.

Note:

> Delete regularly either complete result files or single data records you no longer need. By means of this the files keep small and clear. You avoid a extensive growth of the files which cannot be stored on just one floppy disk. Additionally you save time. The duration of the storage process depends on the size of the file. The extreme case would be that the files become so large after a longer period that all space available on the hard disk is used.

See:

> Dialog Box Output Parameter
> Menu Edit
> Program Development
> Data Formats

11.2.16 Dialog Box User Task

By means of this dialog box you define the User Task which shall be called to process the analysis results before output on an output unit. A description of data interfaces for communication of user programs with the spectrometer program are available at the SPECTRO service. The dialog box is called from Dialog Box Output Parameter. The dialog box contains the following dialog elements:

Group Box File name for User Tasks
By means of this dialog box you define path and name of the called user tasks.

Check Boxes User Task for local Printer/Remote Printer/Store/Transmit
Mark the check boxes for output operations with a requested processing of data by a user task. When you mark the check box, the edit fields for path and file name as well as the button 'select' are enabled. Dialog elements on the remote printer are enabled if a remote printer as additional equipment was entered in the spectrometer program with the Dialog Box Install Additional Device.

Button Select
Click the button to open the standard-Windows-dialog box folder to select the path and file names of the user task.

Edit Fields on user tasks
This edit fields display the file names of the user tasks in that way as they are defined with the button 'select'. It is possible to enter directly into these fields without making a detour with the button 'select'. But please make sure that the name of the user task and the path name are typed correctly. You can do the input without path names, provided that the user task paths are entered in the operating system (see Handbook MS-DOS or WIN 95).

Button OK
Click the button to shut down the dialog box. The path and file names visible in the edit fields, are stored in the Analytical Program.

Button Cancel
Click the button to shut down the dialog box. Entries are not read-in.

See:

___

Dialog Box Output Parameter
Menu Edit
Program Development

11.2.17 Dialog Box Auto Aver. Parameters

In the dialog box 'Parameter Auto Average' you set the control of the automatic average calculation. Automatic average calculation means that in the measure window the automatic average calculation can be made automatically after a certain number of 'good' measurements. A test for freak values is integrated into this function. The automatic average calculation is only carried out, if the corresponding check box in the Dialog Box Global Parameter is marked. You access the dialog box via the corresponding menu item in the Menu Edit of the window for Program Development. All entries are only valid for the currently loaded analytical program. The dialog elements of the dialog box are described below. Please find at first a short description of the sequence of the automatic average calculation and the freak value test.

When you have carried out several measurements and the chosen number of measurements is exceeded, a freak value test is carried out. One of the procedures is used, which are described in the **Combo Box Auto Average Mode**. If a freak value is recognized, it is highlighted with the color cyan. If measuring is continued, the automatic average calculation is continued until the minimum number of 'good' measurements is obtained. The automatic average calculation may be switched off to display the freak values with no further processing.

Only 'good' values contribute to the automatic average calculation. You can decide in the Parameter File PS_GEN.ASC, whether only the freak value or the entire single measurement should be eliminated, i.e. the single results for all elements. Example: An analytical program contains the elements C, Si, Mn, P, S. The second measurement of the element Mn is a freak value. Now you may select by means of the parameter file, whether only the second single measurement of Mn should be excluded from average calculation or whether all values of the second single measurement for the elements C, Si, Mn, P, S should be eliminated. If a freak value had emerged, then the average value is displayed in the color cyan, if not enough god measurements were carried out.

When you print out the single results, all freak values will be marked with an exclamation mark (!) in front of the measured value. The exclamation mark is also printed in front of the average value. In case the reproduction is bad, the measurement sequence aborts and the automatic average calculation starts as soon as the maximum number of measurements is carried out.

Example for the screen output (left side: single value display, right side: average value display)

	C %			C %
1	0.0563			
2	0.3462		$\overline{x}$	0.3412
3	0.3361			
			s	0.0071
			s_r	2.092

Combination of the **Check Boxes Calc. Average** and **Freak Values only marking**

☑   Calc. Average

Freak values of the single value measurement are marked. If freak values are present, the average value is also marked, if not enough god measurements were carried out. The numerical value of the average **does not contain** the freak values. The average calculation is carried out automatically, if enough 'good' measurements are provided.

☐ Calc. Average

☐ Mark Freak Values

Freak values of single values are marked. If freak values are present, the average value is also marked, if not enough god measurements were carried out. The numerical value of the average **does not contain** the freak values. There is no automatic average calculation.

☐ Calc. Average

☑ Mark Freak Values

Freak values of single values are marked. If freak values are present, the average value is also marked, if not enough god measurements were carried out. The numerical value of the average **contains** the freak values! There is no automatic average calculation.

As you know, some functions of the Spark Analyzer program are graduated in a hierarchical user and password system. This graduation has also been chosen for the automatic average calculation. In user level 3 the possibility to carry out an average calculation is limited as long as the maximum number of measurements is not achieved, even if freak values are present. The dialog box contains the following dialog elements:

Group Box Spark Settings

Check Box Calc. Average

Mark this box if the average calculation is to be carried out automatically. Freak values are eliminated automatically.

Check Box Mark Freak Values

Mark this box if only the freak values should be displayed. There is no automatic average calculation. This box is not displayed if the check box 'Calc. Average' is marked.

Edit Field Minimum Number of Sparks

Fill in the number of sparks (single measurements) which have to be carried out in order to perform an average calculation. If you should try to calculate the average before the minimum number of sparks is carried out, a message will be displayed. Then you may either decide to go on with the average calculation or continue with the measurements.

Edit Field Maximum Number of Sparks

The maximum number of sparks is as follows: Number of measurements to be carried out for calculation of the average, even if the criteria for automatic average calculation are not fulfilled. The entry of this number is necessary to be able to terminate a measurement cycle, even if the reproducibility is bad.

Combo Box Mode Auto Average Calculation

Here you select the kind of check process for freak values and their elimination. The check starts with the completion of minimum number of sparks.
The following entries are available:

Min/Max-Mode

The difference between the smallest and the greatest measured value is calculated for each element. This value is compared with the element specific criteria in the table below. If the criteria for a 'good' measurement are not fulfilled, the value which is the furthest measured value, is eliminated and the system checked again. This procedure continues until a sufficient number of 'good' values is obtained.

Mode Standard Deviation

The standard deviation of a measurement sequence is checked for matching the element specific criteria of the table below. The elimination of measured values is carried out as described under Min/Max-Mode.

Table Field with Parameters for Automatic Average Calculation

Two different parameters may be assigned to each element for identification of freak values. In the lower concentration range the absolute deviations are investigated. In higher

concentration ranges, i.e. significantly higher than the detection limit, a check of the relative deviation is mostly recommended. The **Table** contains the following columns:

Column Field Element
These display fields show elements which are determined in the current analytical program.

Column Field Use
By means of these check boxes you define which of the listed criteria shall be used for the detection of freak values. If you enter something in the column, the box is marked automatically.

Column Field Unit
Here you see the output units for the single elements, e.g. % or ppm. The field entries correspond with the entries in the Dialog Box Element Format and can be changed only there.

Column Field Absol. Concentration Low Range / Deviation from Average Value
Min/Max-Mode: Enter here the maximum permissible difference between minimum value and maximum value.
Mode Standard Deviation: Enter here the maximum permissible absolute standard deviation.

Column Field Switch Concentr. Low -> High
Here you may enter the concentration threshold for the switch between the criteria for the lower concentration range and the criteria for the upper concentration range. If the entered concentration value is exceeded, the criteria for the upper concentration range are valid.

Column Field Relative Conc. Upper Range Deviation from average
Min/Max-Mode: Enter here the maximum permissible difference between minimum value and maximum value.
Mode Standard Deviation: Enter here the maximum permissible relative standard deviation.

Button OK
Click this button to close the dialog box and to import the modified entries to the analytical program.

Button Cancel
Click this button to close the dialog box. The modified entries are not read-in.

Button Delete
Click this button to delete a highlighted area in a table. You mark an area by moving the cursor on a field, keep down the left mouse key and move to next fields. The selected area is highlighted dark.

Button Paste
Click this button to paste a marked area automatically. The upper marked entries are regarded as paste content. The marked fields below are pasted automatically with the content of the first highlighted field. You mark an area by moving the cursor on a field, keep down the left mouse key and move to next fields. The selected area is highlighted dark.

Button Print
Click this button to print out the entries.

See:

Program Development
Menu Edit
Dialog Box Global Parameters
Measure Window
Carry out a Measurement
Dialog Box User List and Passwords

11.2.18 Dialog Box Calibration Ranges

The dialog box shows a survey on the calibration ranges of all analytic channels of the Analytical Program. The dialog box is opened with the menu item calibration ranges in the Menu Edit in the window of Program Development. The display is effected as a table. The dialog box contains the following dialog elements:

Table with Calibration Ranges
The Table contains the following columns:

Column Field Cannel
This table column displays all channels of the Analytical Program in successive rows. Changing channel numbers is not possible.

Column Fields Low Limit / High Limit
These edit fields display the low and high limits of the calibration range in concentration units. These limits may be modified here. The concentration units used are the same the channel was calibrated or should be calibrated. These limits may be also edited in the Dialog Box Cannel Parameters.

Button OK
Click the button to shut down the dialog box and to read-in the modified entries on channel parameters in the Analytical Program.
In case you entered or modified calibration ranges, a table for Line Switch is automatically generated when you close the dialog: Based on the calibration range the most sensitive line is searched for each element. Based on this line, another channel of the same element is searched for, whose calibration range overlaps the current calibration range at the upper end. This channel is then used as starting point for a further search for another channel with overlapping calibration range. This search is performed separately for each element. The result of the line switch may be checked in the Dialog Box Line Switch, which is called-up in the 'Dialog Box Element Parameters'.

Button Cancel
Click the button to shut down the dialog box without reading-in the modified entries.

Button Print
Click on this button to print the table.

Button Clear
Click the button to delete the entries in the highlighted area.

Button Fill Area
Click the button to fill automatically a highlighted area in the table. The upper highlighted entries are regarded as filling content. The highlighted fields below are filled with the contents of the first highlighted row automatically. You highlight an area moving the cursor to another field with the arrow keys or the mouse (keep left mouse key pressed). The selected area is displayed dark.

Note:

The calibration ranges are filled automatically during the calibration, based on the areas which are covered by the calibration samples. A subsequent modification of these data, especially an expansion of calibration ranges to lower or higher concentrations, should only be effected with greatest care and is to be checked and proved by measurements of suitable samples.

See:

Program Development

Menu Edit
Dialog Box Channel Parameter
Dialog Box Calibration Data
Dialog Box Element Parameter
Dialog Box Line Switch

11.2.19 Dialog Box Calibration Standards

This dialog is used to display and select standards which are called in for calibration of the Analytical Program. The dialog box is opened with the menu item 'calibration standards' in the Menu Edit of the window on Program Development. The right half of the dialog box displays all available Standard Samples of the respective Base, the left half contains the standard samples used for calibration. To take over standard samples into the calibration search for the respective standard sample in the right list box, mark it and click the button <-Insert. The selection of calibration standards has to be effected for each Analytical Program once again. Note the difference between calibration and standardization. This is explained in the glossary under Calibration and Standardization. The dialog box contains the following dialog elements:

List Box Selected Standards
The list box displays the already selected standards, either with a preceding reminder 'used' or '----'. Only entered standard samples are used for calibration which are marked with the reminder 'used'. To remove one or more standard samples, mark the samples to be deleted. To highlight more than one entry in a list box, click on the first field to be marked, press the <Ctrl> key on the keyboard and click further entries with the <Ctrl> key pressed down. In case you are working without mouse, a multi-highlighting is possible too: Use the arrow keys to search for the entries to be marked. To highlight the entries press the spacebar. The edit field above the list box is used for a fast search for a list entry. Enter the first characters of the name of the list element searched and the list will display the first list entry which corresponds to your entry.

Button Clear->
Pressing the button you delete **all** entries in the list box 'selected standards'. Click this key only in case you want to calibrate an Analytical Program with completely different standard samples. After exit the dialog the calibration intensities for the deleted standards of a prior calibration are lost irrevocably.

Button <- Incl. All
Pressing this button you take over **all** entries from the list box 'proposed standards' in the list box 'selected standards'. Click this switch only if you would like to use really all displayed standard samples for calibration. This operation makes better sense if you had previously enclosed the list of displayed standards with the button 'filter'. To select single standards for calibration work with the button <-Include.

Button <- Include
Pressing this button you take over one or more highlighted entries from the list box 'proposed standards' into the list box 'selected standards'. The button <- Include is enabled when min. one entry was highlighted in the list box 'proposed standards' before.

Button Remove ->
Pressing this button you remove permanently one or more highlighted entries from the list box 'selected standards'. During shut down the dialog the calibration intensities of the last calibration are deleted too. To exclude one or more standards from a calibration temporarily use the button 'Use/Not U.
The button Remove-> is enabled when min. one entry in the list box 'selected standards' was highlighted.

Button Use/Not U.

To exclude a calibration standard from a measurement on calibration temporarily, highlight one or more calibration standards in the list box 'selected standards' and press the button 'Use/Not U. In front of the name of the calibration standard in the list box the entry 'used' changes to '----'. Another click on the button the entry returns to 'used' again. Instead of the button you can effect a double click with the mouse on the respective entry in the list box 'selected standards'. In case a standard will not be measured for calibration acc. to the method described above, the intensity values are converted with the Standardization Factor/Offset to the current device state and displayed in the regression graph. The button Use/Not U. is enabled when min. one entry in the list box 'selected standards' was highlighted.

Button Cut / Paste Abo. / Paste Bel.

By means of these buttons the measure order of the calibration standards may be changed. The calibration standards are measured in the same order they are displayed in the list box 'selected standards'. To minimize a contamination of the spark stand and consequently a spreading of concentrations from one standard to another it is recommendable to measure the standards in the order of increasing concentration. This is why a change of order in the list box is often necessary. With the button 'cut' you remove a standard from the list box temporarily. The entry is stored in a clipboard. Now mark a standard in the list the cut standard shall be inserted below or above and click the button 'paste abo.' or paste bel.'. With this procedure you can position only one standard after the other to the new place. To mark and insert several standards at the same time results in a data loss. The button Cut/Paste Abo./Paste Bel. is enabled when min. one entry in the list box 'selected standards' was highlighted. The buttons Paste Abo./Paste Bel. become active after cutting.

List Box Proposed Standards

The list box displays the available standard samples of the base the currently processing Analytical Program is assigned to. These standards can be taken into the list box 'selected standards'. Highlight one or more standards to be selected for calibration. By means of the button <-Include you take over the selected standard(s) into the list box 'selected standards'. The way how to mark several entries in a list box is described under chapter 'list box selected standards'. Calling the dialog the list box 'proposed standards' displays all defined standard samples. Because this list may be very extensive there is another possibility to display only standard samples of special features. Use the button 'filter'. The edit field above the list box is used for a fast search for a list entry. Enter the first characters of the name of the list element searched and the list will display the first list entry which corresponds to your entry.

Button OK

Click this button to shut down the dialog box. The selected standard samples are stored as Calibration Samples of the Analytical Program.

Button Cancel

Click this button to shut down the dialog box. The modified settings are not read-in.

Button Print

Click this button to print the list on the calibration standard of the current Analytical Program.

Button Edit

This button opens the Dialog Box Edit Standard Samples. Here you can change the type of standard, the concentration values and written comments on the standard samples. Type of standard means the intended use of a standard sample: e.g. calibration sample, type-calibration sample, standardization sample, type-standardization sample, control sample. One standard may cover several types of samples. It is not possible to create new standards in this dialog box. Please use the button 'list'. This button is enabled when an entry in the list box 'proposed standards' was marked before. Multi-marking in the list box 'proposed standards' are not supported for this function. In case you marked several entries nevertheless, the dialog box 'edit standard samples' is displayed for the first highlighted standard.

Button List

The button opens the Dialog Box Standards Libary which displays a list of all standard samples similar to the list box 'proposed standards'. To edit standard data is here possible, similar to the button 'edit'. In contrast to 'edit' it is possible to define new standards with this dialog box. This dialog may also be called with the menu item 'sample list' in the Menu Extras.

Button Filter

The button opens the Dialog Box Filter Settings for Standard Libary. This dialog box is used to select definite standards to be displayed in the list box 'proposed standards'. So the display may be limited to e.g. all calibration type samples.

See:

Menu Edit
Program Development

11.2.20 Dialog Box Intensities of Calibration Samples

In this dialog box you can see the determined intensities and intensity ratios of the calibration curves. The display is effected in a table. You may open the dialog box via the button 'Intens.' in the Dialog Box Standard Samples for Calibration. The dialog box contains the following dialog elements:

Table field Intensities

In this Table you see the measured intensities and intensity ratios of the selected calibration curve. The table contains the following columns:

Column field Channel

In this field the names of the analytical channels are displayed.

Column field Reference

In these display fields you see the names of the reference channels, which are assigned to the analytical channels.

Column field Average Intens.

In these display fields you see the average of the measured intensity of the respective channel. The fields are display fields for channels with an reference assignment and edit fields for channels with no reference assignment.

Column field Average Ratio

In these display fields you see the average of the measured intensity ratios for the respective channels. The fields are edit fields for channels with an reference assignment and display fields for channels with no reference assignment.

Button OK

Click on this button to close the dialog box. The modified entries are stored.

Button Cancel
Click on this button to close the dialog box. The modified entries are not stored.

Button Print
Click on this button to print the table.

See:

Menu Edit
Program Development
Carry out a Calibration
Dialog Box Standard Samples for Calibration

11.2.21 Dialog Box Global Interferences

This dialog box displays the Interferences which are recognized in the Analytical Program. New interferences can be entered here, existing interferences may be changed or removed. The dialog box is opened with the menu item **Global interferences** in the Menu Edit of the window on Program Development. The entry consists of the input of the interfered channel, the interfering element, the type of interference and the intensity.

The name of the interfered channel is displayed equivalent to the name which was entered in Dialog Box Channel Parameters. There are two types of interferences: additive Type (+) and multiplicative Type (*). Afterwards the intensity is listed. The intensity may have a linear or square factor. A linear correction factor is often sufficient to recognize the interference influence in a good way.

Example row:

interfered channel	interfering element	Type	Lin.Factor	Square Factor
SIM 3 Cd1	SIM 3 As	+	65.0	0.0

The channel Cd1 is interfered by As additively. 1 concentration unit Cd in the sample results in an intensity increase of 65 intensity units in channel Cd1. Generally the interferences are calculated in the regression program and should not be changed later.

The dialog box contains the following dialog elements:

Table Interference Data
In this Table interference data for the Analytical Program are displayed and edited. The table contains always one row more than interfered channels exist. This last row is used to enter another interfered channel. As soon as you have defined a new channel a new blank row is generated in the table to take up a new interfered channel. The table contains the following columns:

Column Field Interfered Channel
These combo boxes display the interfered channels. The name of the interfered channel is displayed equivalent to the name entered in the Dialog Box Channel Parameters. To replace a displayed channel by another channel open the combo box and select a channel from the list box of all channels of the Analytical Program. The entry '---' means the information in this row will not be evaluated.

Column Field Interfered Wavelength
These fields display the wavelengths which are measured with the interfered channels.

Column Field Interfering Element

These combo boxes display the names of the elements causing the interference. The name of the interfering element is displayed equivalent to the name entered in the Dialog Box Element Parameters. The entry '---' means the information in this row will not be used. Each channel is connected with one element. A interfered channel cannot be interfered by the element of its own. In case such an assignment is entered an error message will be displayed.

Column Field Type

This combo box displays the Type of interference. Additive types are marked with +, multiplicative types with *.

Column Field Intens./Conc.

The check boxes define the display of the interference: intensity per concentration unit or concentration per concentration unit. The last method is not jet implemented.

Column Field Linear Value/Square Value

In these fields the interference levels are displayed. The interferer may have a linear or square factor. Often a linear correction factor is sufficient.

Button OK

Click this button to shut down the dialog box and to read-in the changed entries in the global interference list of the Analytical Program.

Button Cancel

Click this button to shut down the dialog box without reading-in the changed entries.

Button Clear

Click this button to delete a highlighted area in the table. You mark an area by moving the cursor from one field to another with the arrow keys or the mouse (keep the left mouse key pressed). The area selected is displayed dark.

Button Fill Area

Click this button to fill a highlighted area in the table automatically. The upper highlighted entries are regarded as filling content. Highlighted fields below are filled with the content of the upper highlighted row automatically. Highlight an area by moving the cursor from one field to another with the arrow keys or the mouse (keep the left mouse key pressed). The area selected is displayed dark.

Button Delete

A click on the button removes the row the cursor is positioned irrevocably. The interferer is deleted irrevocably when you quit the dialog with OK.

See:

Menu Edit
Program Development

11.2.22 Dialog Box Standardization Samples

The dialog is used to display and to select samples which are called in for standardization of the Analytical Program. The dialog box is opened with the menu item **Standardization Samples** in the Menu Edit of the window on Program Development. The dialog box displays in the right half all available Standard Samples of the respective Base, in the left half the samples are displayed which are used for standardization. Another display informs about the date of the last standardization of the current program effected with these samples. To take over Standard Samples into the Standardization, search the respective standard on the right list box, mark it and click the button <-Include. Standardization samples are stored for each Analytical Program separately. Please note the difference between calibration and standardization. The difference is explained in the glossary under Calibration and Standardization. The dialog box contains the following dialog elements:

List Box Selected Samples
The list box displays the already selected samples together with a preceding mark + or -. Only samples are used for the standardization which are marked with +. To remove one or more samples highlight the respective samples. To highlight more than one entry in the list box click the first field to be marked, then press key Ctrl on the keyboard and click further entries with pressed Ctrl key. In case you are working without mouse, a multi-highlighting is possible too: Use the arrow keys to search for the entries to be marked. To highlight the entries press the spacebar. The edit field above the list box is used for a fast search for a list entry. Enter the first characters of the name of the list element searched and the list displays the first list entry which corresponds to your entry.

Button Clear->
Pressing the button you delete **all** entries in the list box 'selected samples'. Click this key only in case you want to standardize an Analytical Program with completely different samples. After exit the dialog the standardization intensities for the deleted samples of a prior standardization are lost irrevocably.

Button <- Incl. All
Pressing this button you copy **all** entries from the list box 'proposed samples' in the list box 'selected samples'. Click this switch only if you would like to use really all displayed standards for standardization. This operation makes better sense if you had previously enclosed the list of displayed standards with the button 'filter'. To select single standards for standardization work with the button <-Include.

Button <- Include
Pressing this button you copy one or more highlighted entries from the list box 'proposed samples' into the list box 'selected samples'. The button <- Include is enabled when min. one entry was highlighted in the list box 'proposed samples' before.

Button Remove ->
Pressing this button you remove permanently one or more highlighted entries from the list box 'selected samples'. During shut down the dialog the standardization intensities of the last standardization are deleted too. To exclude one or more samples from a standardization temporarily use the button 'Use/Not U'.
The button Remove-> is enabled when min. one entry in the list box 'selected samples' is highlighted.

Button Use/Not U.
To exclude a standardization sample from a measurement of standardization temporarily, highlight one or more standardization samples in the list box 'selected samples' and press the button Use/Not U. In front of the name of the standardization sample in the list box the entry '+' changes to ' - '. Another click on the button the entry returns to '+' again. Instead of the button you can effect a double click with the mouse on the respective entry in the list box 'selected samples'. In case a sample shall not be measured for standardization acc. to the method described above, the intensity values determined in the prior standardization are used to calculate the channel specific standardization factors and offsets. Please note: To achieve a reliable standardization all standardization samples have to be measured which are assigned as standardization samples to the channels of the Analytical Program. The button Use/Not U. is enabled when min. one entry in the list box 'selected samples' was highlighted.

Button Parameter
Click the button to open the Dialog Box Channel Parameter for Standardization Sample. In this box you can adjust the parameter on standardization for the sample which is highlighted in the list box 'Selected samples'. This button is enabled when an entry in the list box 'samples' was highlighted before. A multi-marking in the list box 'Selected samples' is not supported by the function. In case you marked several entries nonetheless, the Dialog Box Channel Parameter for Type Standardization Samples is displayed only for the first highlighted sample.

Button Cut / Paste Abo. / Paste Bel.
By means of these buttons the measure order of the standardization samples may be changed. The standardization samples are measured in the same order they are displayed in the list box 'selected samples'. To minimize a contamination of the spark stand and consequently a spreading of concentrations from one standard to another it is recommendable to measure the standards in the order of increasing concentration. This is why a change of order in the list box is often necessary. With the button 'cut' you remove a sample from the list box temporarily. The entry is stored in a clipboard. Now mark a sample in the list, the cut sample shall be inserted below or above and click the button 'paste abo.' or paste bel.'. With this procedure you can position only one sample after the other to the new place. To mark and insert several samples at the same time results in a data loss. The button 'Cut' is enabled when min. one entry in the list box 'selected samples' was highlighted. The buttons 'Paste Abo.' and 'Paste Bel.' are enabled after cutting.

List Box Proposed Samples
The list box displays the available Standard Samples of the Base, the currently processing Analytical Program is assigned to. These standard samples can be taken into the list box 'Selected samples'. Highlight one or more standards to be selected for Standardization. By means of the button <-Include you take over the selected standard(s) into the list box 'selected samples'. The way how to mark several entries in a list box is described under chapter 'list box selected samples'. Calling the dialog the list box 'proposed samples' displays all defined standards. Because this list may be very extensive there is another possibility to display only standards of special features. Use the button 'filter'.
The edit field above the list box is used for a fast search for a list entry. Enter the first characters of the name of the list element searched and the list will display the first list entry which corresponds to your entry.

Button OK
Click this button to shut down the dialog box. The selected samples are stored as standardization samples of the Analytical Program.

Button Cancel
Click this button to shut down the dialog box. The modified settings are not read-in.

Button Print
Click this button to print the list of all type calibration standards including date and time of the last modification; the list is on the right side of the screen.

Button Conc.
Click on this button to open the Dialog Box Standard Sample Concentration. Here you may record element-specifically the concentrations for the selected standards. The selected standard may be in the right or left list of the screen.

Button Edit
This button opens the Dialog Box Edit Standard Samples. Here you can change the type of standard, the concentration values and written comments on the standards. Type of standard means the intended use of a standard: e.g. calibration standard, type-calibration sample, standardization sample, type-standardization sample, control sample. A standard may cover several types of samples.
It is not possible to create new standards in this dialog box. Please use the button 'list'.
This button is enabled when an entry in the list box 'proposed samples' was marked before. Multi-marking in the list box 'proposed samples' are not supported by this function. In case you marked several entries nevertheless, the dialog box 'edit standard samples' is displayed for the first highlighted sample.

Button List
The button opens the Dialog Box Standards Library which displays a list of all standard samples similar to the list box 'proposed samples'. To edit standard data is here possible, similar to the button 'edit'. In contrast to 'edit' it is possible to define new standards with this dialog box. This dialog may also be called with the menu Extras / Standard Sample List.

Button Filter
The button opens the Dialog Box Filter Settings for Standards Library. This dialog box is used to select definite standards to be displayed in the list box 'Proposed samples'. So the display may be limited to e.g. all standardization-type samples.

See:

Dialog Box Standardization Data
Dialog Box New Standardization Sample
Carry out a Standardization
Spectrometer Standardization

11.2.23 Dialog Box Channel Parameter for Standardization Sample

This dialog box displays channel parameter for standardization samples, which are selected in the front-end Dialog Box Standardization Samples or in the front-end Dialog Box New Standardization Sample. These parameters are listed in a table. The dialog box contains the following dialog elements:

Group Box Average Conditions

Edit Field Minimum No. of Measurements
In this field the number of individual measurements is defined which are to be carried out before calculating the average of the type-standardization sample. In case the minimum number of measurements is not carried out, a warning is displayed during averaging. In an automated system without operator the averaging is carried out not before the adjusted number of individual measurements is reached.

Table Field Edit Channel Parameter
In this Table channel specific parameter are recorded. The table contains the following columns:

Column Field Channel

In these fields the channels of the Analytical Program are displayed which are subject to a standardization. These channels are of type analytic, line switch and PIMS.

Column Field Low/High

The fields display whether a standardization sample on the respective channel is a low sample or a high sample. Provided that the sample is not used for standardization of the channel, a ---- is displayed.

Column Field Max. RSD

The edit fields display the maximum standard deviation % of single measurements which are accepted in automatic processing without operator. In case the limit will be exceeded, no type-standardization is effected. This field is not evaluated in manual mode.

Button OK

Click this button to shut down the dialog box and to read-in the modified entries of the channel parameters for standardization samples in the Analytical Program.

Button Cancel

Click this button to shut down the dialog box without reading-in the modified entries.

Button Source Para.

Click the button to define source parameters for the standardization sample. Each standardization sample may have individual source parameters. So a shorter pre-spark time can often be set for standardization samples than for production samples.

Button Clear

Click this button to delete a highlighted area in the table. You mark an area by moving the cursor from one field to another with the arrow keys or the mouse (keep the left mouse key pressed). The area selected is displayed dark.

Button Fill Area

Click this button to fill a highlighted area in the table automatically. The upper highlighted entries are regarded as filling content. Highlighted fields below are filled with the content of the upper highlighted row automatically. Highlight an area by moving the cursor from one field to another with the arrow keys or the mouse (keep the left mouse key pressed). The area selected is displayed dark.

See:

Dialog Box Standardization Samples
Dialog Box New Standardization Sample
Menu Edit
Menu Extras
Program Development

11.2.24 Dialog Box Standardization Parameter

The dialog box standardization parameter is used to display and edit the samples used for the Standardization and the assigned standardization intensities. The dialog box is opened with the menu item standardization parameter in the Menu Edit of the window for the Program Development. The dialog is build up as a table which displays all parameters of a channel in one row. The dialog box contains the following dialog elements:

Table Edit Standardization Parameter
The Table incorporates two boxes, a sample display and a intensity display to be switched over with two radio buttons. The table contains the following columns:

Column Field Channel
The table 'Column' displays a list of all the channels a standardization is possible for. Reference channels and monitor channels are not displayed. For channels with a reference channel parameter setting, the intensity ratios are standardized, consequently a separate standardization of the reference channels is not necessary.

Column fields **Standardization Low Sample, Standardization High Sample, Standardization Type** are only visible if the check box 'Select sample' on the button of the screen is clicked.

Column Field Standardization Low Sample
The combo boxes display the low samples of standardization for the respective channel. In case a 1-point standardization is set in the field standardization-type, no standardization low sample is required. The list box of the combo box is filled with all standardization samples which are selected from the Dialog Box Standardization Samples.

Column Field Standardization High Sample
The combo boxes display the high samples of standardization for the respective channel. The list box of the combo box is filled with all standardization samples which are selected from the Dialog Box Standardization Samples.

Column Field Standardization Type
The combo boxes define whether a1-point or a 2-point Standardization shall be carried out.

Column fields **Intensities Low Sample, High Sample** are only visible if the check box 'Edit intensities' on the button of the screen is clicked.

Column Field Low Sample Nominal Value
The edit fields display the nominal values of the channel intensities for the low samples. The nominal value is the intensity value which was determined during the calibration of the channel for the respective sample. The field is enabled in case a 1-point standardization was chosen in the field standardization type.

Column Field Low Sample Last Value
The edit fields display the intensity values of the low sample which were determined during the last standardization. The intensity value of the current standardization is displayed in the next column. A comparison between the current standardization intensity values and the last values facilitate an identification of possible jerky changes. This field is disabled in case a 1-point standardization was chosen in the field standardization type.

Column Field Low Sample Actual Value
The edit fields display the intensity values of the low samples which are used for standardization currently. This field is disabled in case a 1-point standardization was chosen in the field standardization type.

Column Field High Sample Nominal Value
The edit fields display the nominal values of the channel intensities for the high samples. The nominal value is the intensity value which was determined during the calibration of the channel for the respective sample.

Column Field High Sample Last Value

The edit fields display the intensity values of the high sample which were determined during the last standardization. The intensity value of the current standardization is displayed in the next column. A comparison between the current standardization intensity values and the last values facilitates an identification of possible jerky changes.

Column Field High Sample Actual Value

The edit fields display the intensity values of the high samples which are used for standardization currently.

Radio Buttons Select Sample/Edit Intensity

The two radio buttons facilitate switching over between the display of samples used for standardization and the display of standardization intensities.

Button OK

Click this button to shut down the dialog box and to read-in the modified standardization parameters in the Analytical Program.

Button Cancel

Click this button to shut down the dialog box without reading-in the modified standardization parameters.

Button Clear

Click this button to delete a highlighted area in the table. You mark an area by moving the cursor from one field to another with the arrow keys or the mouse (keep the left mouse key pressed). The area selected is displayed dark.

Button Fill Area

Click this button to fill a highlighted area in the table automatically. The upper highlighted entries are regarded as filling content. Highlighted fields below are filled with the content of the upper highlighted row automatically. Highlight an area by moving the cursor from one field to another with the arrow keys or the mouse (keep the left mouse key pressed). The area selected is displayed dark.

Button Print

Click the button to print a list of the standardization samples used for the channels of the current Analytical Program incl. the intensity values.

See:

Menu Edit
Program Development
Spectrometer Standardization

11.2.25 Dialog Box Control Samples

This dialog is used to display and to select control samples. The dialog box opens with the menu item **Control samples** in the Menu Edit of the window on Program Development. On the right side the dialog box exhibits all available Control Samples of the respective Base, on the left side samples, which are used as control samples. To take over samples as control samples, search one or more respective samples, mark these samples and click on the button <insert>. In case on the right side no proposed control samples are displayed or you want to use other samples than the displayed ones for control samples, you have to define control samples at first. You also may extend the display to samples, which are not of the type 'Control sample'. For details please read the items button 'List' and 'Filter' below. You have to carry out once again the selection of control samples for each Analytic Program, which uses control samples. For a definite control sample, different limits may be entered for each analytic program. This may be carried out with the button 'Limits'. Carrying out the control sample test is performed in the Measure Window through the menu **Measure**, menu item 'control sample test'. Please read Carry out a Control Sample Test.

➡ Tip:
In case identical limit values for several programs should be used for a certain control sample, we recommend to enter the limits through the dialog box 'Standard samples - concentrations'. These entries are considered to be default values, which may be separately adapted to each analytical program. You may call-up the dialog box 'Standard sample - concentrations' by means of the button 'Edit'.

The dialog box contains the following dialog elements:

List box Selected Samples
The list box exhibits the already selected control samples for the loaded analytical program. To remove one or more entry from the list box, click on the first field to be marked, then press the key <Ctrl> on your keyboard and click on further entries holding down the <Ctrl> key. In case you are working without mouse, a multi-marking is possible too. In this case use the arrow keys to search for the entries to be marked. To mark them, press the space bar to mark it. The edit field above the list box is used for a fast search for a list entry in large lists. Enter the start or any other part of the name on the list element to be searched for. The start of the list is moved to the first entry which complies with your entry.

Button Remove All >
Click this button to remove **all** entries form the list box 'Selected samples'. After clicking the button and quitting the dialog through the button 'OK' the stored control sample limits are lost for the selected control samples in the list box!

Button <- Insert All
Click this button to copy **all** entries form the list box 'Proposed samples' into the list box 'Selected samples'. Operate this button only in case you really want to applicate all displayed control samples. To select individual standards, please operate with the button <-Insert.

Button <- Insert
Click this button to copy one or more highlighted entries from the list box 'Proposed standard samples' into the list box 'Selected standard samples'. The button 'Insert' is only enabled, if you had marked at least one entry in the list 'Proposed standard samples'.

Button Remove Select. ->
Click this button to remove finally one or more selected (highlighted) entries from the list box 'Selected samples'. When you click the button and quit the dialog with the button 'OK', the stored control sample limits for selected control samples in the list box are lost! Even in case that removed samples may immediately be inserted again, the program specifically stored

control sample limits are lost. The button 'Remove select.' is only enabled, if you had marked at least one entry in the list Selected standard samples'.

Button Limits
By means of this button you open the Dialog box Limits for Control Samples. Here you enter specifically the control sample limits for the loaded analytical program.

Button Cut / Paste above / below
By means of this button you may vary the measure sequence of the control samples. During the control sample tests, the control samples are called-up in that sequence, which is displayed in the list box 'Selected samples'. To minimize contaminating the spark stand and to avoid transmitting contents from one standard to another we recommend you to measure the control samples in the order of increasing concentration. This is why a change of the sequence in the list box gets often necessary. You temporarily remove a sample from the list by means of the button 'Cut', and the entry is stored on the switchboard. Now mark the sample in the list, where above or below the cut sample should be fit in. Click the button 'Paste above' or 'Paste below'. To reorganize the position of several control samples, you have to proceed one after the other. If you mark several samples and try to paste them, all data will be lost! The button 'Cut' is enabled, if minimum one entry is marked in the list 'Selected standard samples' before. After cutting out the entry the buttons 'Paste above' and 'Paste below' are enabled.

List box Proposed Samples
In this list box you see the available control samples of the Base, the currently edited analytical program is assigned to. These samples may be imported into the list box 'Selected samples'. Highlight one or more samples you want to select for calibration. Through the button '<- paste' you import the sample(s) into the list 'Selected samples'. How to mark several entries in the list box, is described under the list 'Selected samples'. Calling-up the dialog, the list 'Proposed standard samples' displays all defined control samples of the base. When you want to use a sample as a control sample, but the sample is not the type 'Control sample', you may extend the display criteria by means of the button 'Filter'. This list may be very extensive: this is why the edit field above the list boy may be used for a fast search. Enter into this field the first part or any other part of the name of the sample to be searched. The start of the list moves to the first list entry, which corresponds to your entry.

Button OK
Click this button to shut down the dialog box. The selected samples are stored as Control Samples of the analytic program.

Button Cancel
Click this button to shut down the dialog box. The modified settings are not imported.

Button Print
Click this button to print out a list of all calibration samples on the right side including date and time of the last modification.

Button Conc.
Click on this button to open the Dialog Box Standard Sample Concentration. Here you record element specifically the concentrations for the selected standard. The selected standard may be positioned on the right or left list.

Button Edit.
Click this button to open the Dialog Box Edit Standard Sample. In this dialog box you may change the standard type, the concentration limits, helptexts for standard samples. The standard type is defined as the intended use of the standard sample, e.g. calibration sample, type-calibration sample, standardization sample, type-standardization sample, control sample. One standard may contain several types. It is not possible to generate new

standards by means of this dialog box. If you want to create a new standard, please use the button 'List'. The entry of program-comprehensive control sample limits is done through the Dialog Box Standard Sample Concentrations, which is called-up from the Dialog Box Edit Standard Samples.

This button is only enabled, when an entry had been marked in the list 'Proposed samples'. A multi-marking in the list 'Proposed samples' is not supported for this function. In case you have still marked several entries, the dialog box 'Edit standard samples' opens for the sample, which is displayed in the upper edit field.

Button List

The button opens the Dialog Box Standard Sample List, which displays a list of all standard samples, similar to the list box 'Proposed samples'. From this position you may edit standard data, similar to a click on the button 'Edit'. In contrast to this you may define new standards by means of this dialog box. Additionally this dialog may be called-up through the menu item **Standard sample list** in the Menu Extras.

Button Filter

This button opens the Dialog Box Display Mode Standard Sample File. The dialog box is used to select definite standards, which should be displayed in the list box 'Proposed standards'. Calling-up the dialog, all samples of the type 'Control sample' are displayed. This selection criterion may be modified, so that different samples may be displayed too. Additionally the display may be limited, e.g. to all standards which belong to a certain alloy group.

See:

Menu Edit
Program Development
Carry out a Control Sample Test

11.2.26 Dialog Box Control Sample Limits

By means of this dialog box you work on the concentration limit values of a Control Sample. The dialog is called-up with the button 'Limits' in the Dialog Box Control Samples in the Menü Edit in the window on Program Development. Limit values are specifically stored for the actual Analytic Program.

If you want to record the control limits for samples program-comprehensivly, another method has to be applied. We recommend to record the limits through the Menu Extras in the program development, menu item standard samples. Here you may open the Dialog box Edit Standard Samples, and you may enter concentration limits independent from analytical programs. Entries made there are displayed as default values in this dialog 'Control sample limits'. The default limit values may here be fitted program-specifically.
The dialog box contains the following dialog elements:

Group Box Average Conditions
Edit field Minimum Number of Measurements

Enter the minimum number of measurements to be carried out during measuring the control sample. In case during the control sample test this number of measurements is not carried out, a warning message is displayed. To calculate the average and to continue the process is still possible.

Table field Concentration limits

In this Table you may record the concentration limits for the single elements of the control sample. The table contains the following columns:

Column field Element
This column exhibits in its display fields the analytic elements of the actual analytic program. There is no possibility to edit elements. In case you want to enter concentration limits for elements, which are not measured in the actual analytic program, enter these values through the Dialog box Edit Standard Samples (see above).

Column field Cert. Conc.
In this display field you see the certified concentrations for the elements, provided entries are made in the dialog 'Edit standard samples'. The display fields are only informative and do not influence the course of the control sample measurement.

Column field Unit
This column views in its display fields the concentration units used e.g. %, ppm. In case the display field 'Unit' is blank, no corresponding entry for the element exists in the dialog 'Edit standard samples'.

Column fields Outer Min., Inner Min., Inner Max., Outer Max.
Enter in the edit fields the limits, which are still accepted for the control sample result. In the Measure Window only inner and outer limits are checked. The values of the limits are stored in the Parameter File. These column fields are possibly pre-allocated. The pre-allocation corresponds to the entra in the dialog 'Edit standard samples'.

Column field Max. RSD
Enter into this edit field the maximum standard deviation, which is allowed to occur. In case the standard deviation is exceeded, a warning message is displayed. If you do not enter anything into these fields, the check of the standard deviation does not take place.

Button OK
Click this button to shut down the dialog box. The modified entries are stored.

Button Cancel
Click this button to shut down the dialog box. The modified entries are not imported.

Button Fill
Mark an area with several rows in the table field and click the button to copy data from the first highlighted row into the other marked rows. Entries in the column fields 'Element', 'Cert. Conc.', 'Unit' are not copied.

Button Delete
Click this button to delete the highlighted area in the table field.

See:

Dialog box Edit Standard Samples
Dialog box Standard Sample List
Menu Edit
Program Development

11.2.27 Dialog Box Type Calibration Samples

This dialog box displays and select samples which are used for Type Calibration on the Analytical Program. The dialog box is opened with the menu item **Type calibration samples** in the Menu Edit of the window for Program Development. In the right half the dialog box displays all available Standard Samples of the respective Base, in the left half the samples which are used for type calibration. Additionally the date of the last type calibration of the current program, carried out with these samples, is displayed. To select standards for type calibration, search for the respective standard in the right list box, mark it and click the button <-Include. The measurement of the type calibration samples is effected in this dialog box too. Type calibration samples are stored on each Analytical Program separately. Please note the difference between type calibration and type standardization. The difference is explained in the glossary under Type Calibration and Type Standardization. The dialog box contains the following dialog elements:

List Box Selected Samples
The list box displays the already selected samples. To remove one or more samples highlight the respective samples. To highlight more than one entry in the list box click the first field to be marked, then press key Ctrl on the keyboard and click further entries with pressed Ctrl key. In case you are working without mouse, a multi-highlighting is possible too: Use the arrow keys to search for the entries to be marked. To highlight the entries press the spacebar. The edit field above the list box is used for a fast search for a list entry. Enter the first characters of the name of the list element searched and the list displays the first list entry which corresponds to your entry.

Button Clear->
Pressing the button you delete **all** entries in the list box 'selected samples'. Click this key only in case you want to type standardize an Analytical Program with completely different samples. After exit the dialog the type calibration data for the deleted samples of a prior type calibration are lost irrevocably.

Button <- Incl. All
Pressing this button you copy **all** entries from the list box 'proposed samples' in the list box 'selected samples'. Click this switch only if you really want to use all displayed standards for type calibration. This operation makes better sense if you had previously enclosed the list of displayed standards with the button 'filter'. To select single standards for type calibration work with the button <-Include.

Button <- Include
Pressing this button you copy one or more highlighted entries from the list box 'proposed samples' into the list box 'selected samples'. The button <- Include is enabled when min. one entry was highlighted in the list box 'proposed samples' before.

Button Remove ->
Pressing this button you remove permanently one or more highlighted entries from the list box 'selected samples'. During shut down the dialog the type calibration data of the last type calibration are deleted too. To exclude one or more samples from a standardization temporarily use the button 'Use/Not U'. The button Remove-> is enabled when min. one entry in the list box 'selected samples' is highlighted.

Button Measure
You start measuring the first highlighted type calibration samples with a click on this button. The button is only enabled when an entry in the list box 'selected samples' is highlighted.

Button Parameter

A click on this button opens the Dialog Box Element Parameter for Type Calibration Sample. Here you can set values on the sample selected form the list box 'Selected samples'. The values control the run of type calibration. E.g. you can set the number of individual measurements necessary for measurement of the type calibration sample. Furthermore you can define the limit values: exceeding the limits the type calibration is regarded as non-successful. The button is enabled when an entry in the list box 'selected samples' was highlighted before. A multi-marking in the list box 'Selected samples' is not supported by the function. In case you marked several entries nonetheless, the Dialog Box Element Parameter for Type Calibration Sample is displayed only for the first highlighted sample.

List Box Proposed Samples

The list box displays the available Standard Samples of the Base, the currently processing Analytical Program is assigned to. These standard samples can be taken into the list box 'Selected samples'. Highlight one or more standards to be selected for type calibration. By means of the button <-Include you copy the selected standard(s) into the list box 'selected samples'. The way how to mark several entries in a list box is described under chapter 'list box selected samples'. Calling the dialog the list box 'proposed samples' displays all defined standards. Because this list may be very extensive there is another possibility to display only standards of special features. Use the button 'filter'. The edit field above the list box is used for a fast search on a list entry. Enter the first characters of the name of the list element searched and the list will display the first list entry which corresponds to your entry.

Button OK

Click this button to shut down the dialog box. The selected samples are stored as type calibration samples of the Analytical Program.

Button Cancel

Click this button to shut down the dialog box. The modified settings are not read-in.

Button Print

Click this button to print the list of all type calibration standards including date and time of the last modification; the list is on the right side of the screen.

Button Conc.

Click on this button to open the Dialog Box Standard Sample Concentration. Here you may record element-specifically the concentrations for the selected standards. The selected standard may be in the right or left list of the screen.

Button Edit

This button opens the Dialog Box Edit Standard Samples. Here you can change the type of standard, the concentration values and written comments for the standards. Type of standard means the intended use of a standard: e.g. calibration standard, type-calibration sample, standardization sample, type-standardization sample, control sample. A standard may cover several types of samples.

It is not possible to create new standards in this dialog box. Please use the button 'list'. This button is enabled when an entry in the list box 'proposed samples' was marked before. Multi-marking in the list box 'proposed samples' are not supported by this function. In case you marked several entries nevertheless, the Dialog Box Edit Standard Samples is displayed for the first highlighted sample.

Button List

The button opens the Dialog Box Standards Library which displays a list of all standard samples similar to the list box 'proposed samples'. To edit standard data is here possible, similar to the button 'edit'. In contrast to 'edit' it is possible to define new standards with this dialog box. This called dialog may also be called with the Menu Extras / Standard Sample List.

Button Filter
The button opens the Dialog Box Filter Settings for Standards Library. This dialog box is used to select definite standards to be displayed in the list box 'proposed samples'. So the display may be limited to e.g. all type calibration-type samples.

See:

> Menu Edit
> Program Development
> Carry out a Type Calibration

11.2.28 Dialog Box Survey on Type Calibration

This dialog box is used to display and to check the results of the measurement of a type calibration sample. The dialog box is automatically displayed after a measurement of the type calibration sample. The measurement of the type calibration sample is effected from the Dialog Box Type Calibration Samples. The dialog box contains the following dialog elements:

Table field Element Data
In this field the type standardization data of the respective elements are temporarily displayed. The following columns are displayed:

Column field Element
Element symbols are displayed in this column. The display is limited to elements which are incorporated in the type calibration sample.

Column field Check
The check boxes in this column prompt you to check carefully the results of the line element. The line element is only marked if this dialog box was opened automatically after a measurement and one of the three error conditions occurred.
Error conditions are:
- measure value out of limits Min. / Max. Con. (Measurement is red highlighted)
- relative standard deviation RSD is bigger than allowed (measured RSD is red highlighted)
- offset is too big

The status of the box 'Check' has no influence on the measurement of the production sample. When you quit the dialog through OK, the type correction is carried out, independent from a mark in the check box. Because the type calibration is carried out only once per type calibration sample and the measured values are firmly incorporated into the determination of the analysis results of production samples, you should accept only measurements with no mark in the box 'Check'.

Column field Cert. Conc.
This column displays the certified concentration for the respective element.

Column field Min. Conc.
This column displays the used minimum concentration which is used for the check of the respective element.

Column field Measurement
This column displays the calculated concentration of the respective element, which was effected with no type standardization.

Column field Max. Conc.
This column displays the used maximum concentration which is used for the check of the respective element.

Column field By Factor
If this field is marked, the calculated factor is used for the respective field. If it is not marked, the offset is used.

Column field Factor
This column displays the calculated corrective factor.

Column field Offset
This column displays the calculated offset.

Column field Meas. RSD
This column displays the measured relative standard deviation.

Column field Max. RSD
This column displays the maximum relative standard deviation which is used for the check.

Button OK
Click on this button to close the dialog box and to accept the displayed values.

Button Cancel
Click on this button to close the dialog box. The process related to the display in the dialog box is interrupted.

Button Print
Click on this button to print the values displayed in the table.

See:

Dialog Box Samples for Type Calibration
Menu Measure
Measure Window
Dialog Box Element Parameter for Type Calibration

11.2.29 Dialog Box Element Parameter for Type Calibration Sample

This dialog box displays element parameters on the type calibration sample, which was selected in the front-end Dialog Box Type Calibration. These element specific parameters are listed in a table. The dialog box contains the following dialog elements:

Group Box Average Conditions

Edit Field Minimum No. of Measurements
In this field the number of individual measurements is defined which are to be carried out before calculating the average of the type calibration sample. In case the minimum number of measurements is not carried out, a warning is displayed during averaging. In an automated system without operator the averaging is carried out not before the adjusted number of individual measurements is reached.

Table Field Edit Element Parameter
In this Table element specific parameters are recorded. The table contains the following columns:

Column Field Element
In these fields the channels of the Analytical Program are displayed which are subject to a type calibration. These elements are of type analytic, line switch and PIMS.

Column Field Cert. Conc
This field displays the respective element concentrations in the same way as displayed in Dialog Box Standard Sample Concentrations. This dialog box is accessible from the Dialog Box Samples for Type Calibration with the buttons 'Edit' or 'List'.

Column Field Use Fact

In the check boxes you define whether the type calibration shall be effected with a factor or an offset. In case of higher concentrations a correction with a factor is recommended. Low concentrations may be corrected with an offset in a better way.

Column Field Min. Conc/Max. Conc

The edit fields display the minimum and maximum concentration, which are subject to a correction via a type calibration. In case the determined value for a production sample is out of the min/max window, no type calibration will be effected. In this case the non-corrected element concentration is output, which results from the calibration curve. If you work with Type Standardization in other analytical programs (in contrast to the type calibration just discussed), please note the difference in this field. Additionaly the measurement of the type calibration curve in these fields is checked automatically to discover a possible sample mix-up. If min/max values are exceeded during a measurement of the type calibration sample, the elements which are out of the min/max concentrations, are red highlighted in the Dialog Box Survey on Type Calibration.

Column Field Factor

These edit fields display the corrective factors of the type calibration. The factors are determined in the Measure Window during a type calibration. These fields are enabled for the rows with a marked check box 'Use Fact'.

Column Field Offset

These edit fields display the corrective offsets of the type calibration. An offset is defined as a constant deviation. The offsets are determined in the Measure Window during a type calibration. These offsets are active for the rows **without** a marked check box 'Use Fact'.

Column Field Max. RSD

The edit fields display the maximum standard deviation % of single measurements. In case the limit will be exceeded. no type calibration is effected. When you work with the type calibration in the Measure Window, the elements which are out of the max. standard deviation, are marked.

Column Field Smp. Sel.

The check boxes define the elements which are called-in to select a suitable type calibration sample. Provided that the first individual measurement of each marked sample show values which are within the min/max concentrations, the current type calibration parameter are used for analysis correction.

Button OK

Click this button to shut down the dialog box and to read-in the changed entries of element parameter for type calibration samples in the Analytical Program.

Button Cancel

Click this button to shut down the dialog box without reading-in the changed entries of element parameter for type calibration samples in the Analytical Program.

Button Clear

Click this button to delete a highlighted area in the table. You mark an area by moving the cursor from one field to another with the arrow keys or the mouse (keep the left mouse key pressed). The area selected is displayed dark.

Button Fill Area

Click this button to fill a highlighted area in the table automatically. The upper highlighted entries are regarded as filling content. Highlighted fields below are filled with the content of the upper highlighted row automatically. Highlight an area by moving the cursor from one field to another with the arrow keys or the mouse (keep the left mouse key pressed). The area selected is displayed dark.

See:

Dialog Box Type Calibration Samples
Menu Edit

Program Development
Carry out a Type Calibration

11.2.30 Dialog Box Type Standardization Samples

This dialog box is used to display and to select samples which are called-in for Type Standardization of the Analytical Program. The dialog box is opened with the menu item **Type standardization samples** in the Menu Edit of the window on Program Development. The dialog box displays in the right half all available Standard Samples of the respective Base, in the left half the samples are displayed which are used for type standardization. Another display informs about the date of the last type standardization of the current program effected with these samples. To take over standards into the type standardization search the respective standard in the right list box, mark it and click the button <-Include.

The measurement of the type standardization samples to carry out a type standardization is started in the Measure Window. Type standardization samples are stored for each Analytical Program separately. Each Alloy Grade may be assigned to a type standardization sample. This assignment is effected in the dialog box for editing alloy grades. The type standardization samples as well as the correction factors determined during the last type standardization are loaded in the Measure Window when you select a alloy grade. The period between current date and last type standardization is compared with the maximum period allowed: if necessary a remeasurement of the type standardization is requested. In case no alloy grade name of a production sample is given in the Measure Window, no automatic type standardization is possible but a manual type standardization may be effected at all times. Please note the difference between type calibration and type standardization. The difference is explained in the glossary under Type Calibration and Type Standardization. The dialog box contains the following dialog elements:

List Box Selected Samples
The list box displays the already selected samples. To remove one or more samples highlight the respective samples. To highlight more than one entry in the list box click the first field to be marked, then press key Ctrl on the keyboard and click further entries with pressed Ctrl key. In case you are working without mouse, a multi-highlighting is possible too: Use the arrow keys to search for the entries to be marked. To highlight the entries press the spacebar. The edit field above the list box is used for a fast search for a list entry. Enter the first characters of the name of the list element searched and the list displays the first list entry which corresponds to your entry.

Button Clear->
Pressing the button you delete **all** entries in the list box 'selected samples'. Click this key only in case you want to type standardize an Analytical Program with completely different samples. After exit the dialog the standardization data for the deleted samples of a prior type standardization are lost irrevocably.

Button <- Incl. All
Pressing this button you copy **all** entries from the list box 'proposed samples' in the list box 'selected samples'. Click this switch only if you want to use really all displayed standards for type standardization. This operation makes better sense if you had previously enclosed the list of displayed standards with the button 'filter'. To select single standards for standardization work with the button <-Include.

Button <- Include
Pressing this button you copy one or more highlighted entries from the list box 'proposed samples' into the list box 'selected samples'. The button <- Include is enabled when min. one entry was highlighted in the list box 'proposed samples' before.

Button Remove ->
Pressing this button you remove permanently one or more highlighted entries from the list box 'selected samples'. During shut down the dialog the type standardization data of the last type standardization are deleted too. The button Remove-> is enabled when min. one entry in the list box 'selected samples' is highlighted.

Button Parameter
A click on this button opens the Dialog Box Element Parameter for Type Standardization Sample. Here you can set values on the sample selected form the list box 'Selected samples'. The values control the run of type standardization. E.g. you can set the number of individual measurements necessary for measurement of the type standardization sample. Furthermore you can define the limit values: exceeding the limits the type standardization is regarded as non-successful. The button is enabled when an entry in the list box 'selected samples' was highlighted before. A multi-marking in the list box 'Selected samples' is not supported by the function. In case you marked several entries nonetheless, the Dialog Box Element Parameter for Type Standardization Sample is displayed only for the first highlighted sample.

List Box Proposed Samples
The list box displays the available Standard Samples of the Base, the currently processing Analytical Program is assigned to. These standard samples can be copied into the list box 'Selected samples'. Highlight one or more standards to be selected for type standardization. By means of the button <-Include you copy the selected standard(s) into the list box 'selected samples'. The way how to mark several entries in a list box is described under chapter 'list box selected samples'. Calling the dialog the list box 'proposed samples' displays all defined standards. Because this list may be very extensive there is another possibility to display only standards of special features. Use the button 'filter'. The edit field above the list box is used for a fast search for a list entry. Enter the first characters of the name of the list element searched and the list will display the first list entry which corresponds to your entry.

Button OK
Click this button to shut down the dialog box. The selected samples are stored as type standardization samples of the Analytical Program.

Button Cancel
Click this button to shut down the dialog box. The modified settings are not read-in.

Button Print
Click this button to print the list of all type calibration standards including date and time of the last modification; the list is on the right side of the screen.

Button Conc.
Click on this button to open the Dialog Box Standard Sample Concentration. Here you may record element-specifically the concentrations for the selected standards. The selected standard may be in the right or left list of the screen.

Button Edit
This button opens the Dialog Box Edit Standard Samples. Here you can change the type of standard, the concentration values and written comments for the standards. Type of standard means the intended use of a standard: e.g. calibration standard, type-calibration sample, standardization sample, type-standardization sample, control sample. A standard may cover several types of samples.
It is not possible to create new standards in this dialog box. Please use the button 'list'. This button is enabled when an entry in the list box 'proposed samples' was marked before. Multi-marking in the list box 'proposed samples' are not supported by this function. In case you marked several entries nevertheless, the Dialog Box Edit Standard Samples is displayed for the first highlighted sample.

Button List

The button opens the Dialog Box Standards Library which displays a list of all standard samples similar to the list box 'proposed samples'. To edit standard data is here possible, similar to the button 'edit'. In contrast to 'edit' it is possible to define new standards with this dialog box. This called dialog may also be called with the Menu Extras.

Button Filter

The button opens the Dialog Box Filter Settings for Standards Library. This dialog box is used to select definite standards to be displayed in the list box 'proposed samples'. So the display may be limited to e.g. all type standardization-type samples.

See:

> Menu Edit
> Program Development
> Carry out a Type Standardization

11.2.31 Dialog Box Element Parameter for Type Standardization Sample

This dialog box displays element parameter for the type standardization sample, which was selected in the front-end Dialog Box Type Standardization. These element specific parameters are listed in a table. The dialog box contains the following dialog elements:

Group Box Average Conditions

Edit Field Minimum No. of Measurements

In this field the number of individual measurements is defined which are to be carried out before calculating the average of the type standardization sample. In case the minimum number of measurements is not carried out, a warning is displayed during averaging. In an automated system without operator the averaging is not carried out before the requested number of individual measurements is reached.

Table Field Edit Element Parameter

In this Table element specific parameter are recorded. The table contains the following columns:

Column Field Element

In these fields the channels of the Analytical Program are displayed which are subject to a type standardization. These elements are of type analytic, line switch and PIMS.

Column Field Cert. Conc

This field displays the respective element concentrations in the same way as displayed in Dialog Box Standard Sample Concentrations. This dialog box is accessible from the Dialog Box Samples for Type Standardization with the buttons 'Edit' or 'List'.

Column Field Use Fact

In the check boxes you define whether the type standardization shall be effected with a factor or an offset. In case of higher concentrations a correction with a factor is recommended. Low concentrations may be corrected with an offset in a better way.

Column Field Min. Conc/Max. Conc

The edit fields are used to supervise the measurement of the type standardization sample. In case the determined value is out of the limits,the measure result is highlighted red in the Dialog Box Results of Type Standardization. The measurement and type correction of the 'production sample' is not influenced. If you work with 'Type calibration' (in contrast to the type standardization just discussed), please note the difference in this field.

Column Field Factor

These edit fields display the corrective factors of the type standardization. The factors are determined in the Measure Window during a type standardization. These fields are enabled for the rows with a marked check box 'Use Fact'.

Column Field Offset

These edit fields display the corrective offsets of the type standardization. An offset is defined as a constant deviation. The offsets are determined in the Measure Window during a type standardization. These offsets are active for the rows **without** a marked check box 'Use Fact'.

Column Field Max. RSD

The edit fields display the maximum standard deviation % of single measurements. In case the limit will be exceeded, no type standardization is effected. When you work with the type standardization in the Measure Window, the elements which are out of the max. standard deviation, are marked.

Button OK

Click this button to shut down the dialog box and to read-in the changed entries of element parameters for type standardization samples in the Analytical Program.

Button Cancel

Click this button to shut down the dialog box without reading-in the changed entries of element parameters for type standardization samples in the Analytical Program.

Button Clear

Click this button to delete a highlighted area in the table. You mark an area by moving the cursor from one field to another with the arrow keys or the mouse (keep the left mouse key pressed). The area selected is displayed dark.

Button Fill Area

Click this button to fill a highlighted area in the table automatically. The upper highlighted entries are regarded as filling content. Highlighted fields below are filled with the content of the upper highlighted row automatically. Highlight an area by moving the cursor from one field to another with the arrow keys or the mouse (keep the left mouse key pressed). The area selected is displayed dark.

See:

Dialog Box Samples for Type Standardization
Menu Edit
Program Development
Carry out a Type Standardization
Dialog Box Results of Type Standardization

11.3 Menu Instrument (Program Developement)

The menu **Instrument** contains menu items to view and change parameters of the analytic device and to start definite test routines on the device. The menu contains the following menu items:

➡ **Installation**

Select this menu item to install and configure the system as well as to open several test functions. The following sub-menu items are available:

✦ **Devices**

This menu item opens the Dialog Box List of Devices to define the additional devices connected to your analysis machine.

+ **Mode & Interval**
  This menu item opens the Dialog Box Mod & Intervals to define the way of mode and various intervals on the operation of the spectrometer.Sprache

+ **Language**
  By means of this menu item you change the dialog language of your program. Commonly available are an english and a german version. Select your language and exit the program SPARK ANALYZER.After the restart of the program the user interface presents the selected language.
  Further languages: Ask SPECTRO for a version of your language. Subject to availability you will be supplied with files named SP01_LNG.DLL, SP01A_LN.DLL, LAB_LNG.HLP, and DFMETSID.LNG, which you have to copy into the subdirectory 'Language'. Then select 'other' in the menu 'language' to activate your language.

+ **Parameter Files**
  Her you can edit parameter files. A standard editor of Windows is used as user interface. Please read the Help of Parameter Files about the content of the single files and how to edit them.

+ **External Programs**
  Two submenu items are available:
  The submenu item **Data Conversion** opens the Dialog Box Data Conversion, to call-up an external program for converting old spectrometer data.
  The submenu item **Performance Test** is used to check the spectrometer during production. This menu item is without any meaning to the operator.

+ **UV-Transm. Test**
  This menu item opens the Dialog Box UV-Transmission Check Measure to define the parameter for a UV-check.

+ **SIM-Profile Test**
  This menu item starts a scan across the whole scanning range of the simultaneous optics.
 This menu item is not available for SPECTROLAB Jr. CCD.

+ **Dark Current Test**
  This menu item opens the Dialog Box Dark Current Test to define the parameters for the Dark Current Test.
  This menu item is not available for SPECTROLAB Jr. CCD.

+ **Const. Light Test**
  This menu item opens the Dialog Box Const. Light Test to define the parameters for the Const. Light Test.
  This menu item is not available for SPECTROLAB Jr. CCD.

➡ **Optics**
  Select this menu item to open a sub-menu to install and configure the optics. The following sub-menu items are available:

+ **Installed Optics**
  This menu item opens the Dialog Box Installed Optics to check or change the parameters of the optics installed.

+ **Installed Lines**
  This menu item opens the Dialog Box Installed Lines to check or change the parameters of the lines installed.

♦ **SIM-Parameter**

This menu item opens the Dialog Box SIM Parameter check or change the parameters of the SIM parameter.

▓▓▓ This menu item is not available for SPECTROLAB Jr. CCD.

♦ ▓▓▓ **SEQ-Parameter**

This menu item opens the Dialog Box SEQ Parameter check or change the parameters of the sequential optics.

⇒ **Diagnostics**

Select this menu item to open a sub-menu for diagnosis of communication with the instrument controller. The following sub-menu items are available:

♦ **Logbook**

The Menu Item Logbook displays the content of the journal file for communication with the instrument controller.

♦ **ICS Access**

The Menu Item ICS Access starts a program to check directly definite functions of the instrument controller.

♦ **ICS Spy**

The Menu Item ICS Spy starts an additional program to monitor the communication between PC and instrument controller.

⇒ **Initialize**

The Menu Item Initialize initializes the analysis device again.

⇒ **UV-Transm. Check**

The Menu Item UV-Transm. Check starts a UV-check.

⇒ **Reprofile Optics**

Select this menu item to carry out a Reprofiling. First information about this topic is described in section Profile Check.

See:

Program Development

11.3.1 Dialog Box List of Devices

This dialog box defines the additional devices connected to your spectrometer. It is not allowed to change the settings without particular demand from SPECTRO. If you enter non existing devices the measure routines of the spectrometer may be affected. The dialog box contains the following elements:

Check Box SPECTROLUX

This check box is marked in case a fully automatic analysis laboratory type SPECTROLUX is incorporated.

Check Box Manipulator

This check box is marked in case the sample supply to your spectrometer is effected with a manipulator.

Check Box SAFT

This check box is marked if your spectrometer is equipped with additional hardware for measure signal integration by SAFT. By means of the SAFT technique the detection limits of a lot of elements can be decreased significantly.

LAB CAST **Check Box SSE**
This check box is marked if your Spectrometer is equipped with additional hardware for the single spark evaluation, SSE.

Check Box Ar/ArH2
This check box is marked in case your spectrometer may be switched over between pure argon mode and argon/hydrogen mode. In case the box is not marked your spectrometer is operated with either pure Ar or ArH2. There is no change possible.

LAB **Check Box LASER excitation**
This check box is marked if your Spectrometer is equipped with an additional laser excitation.

Check Box SSE
This check box is marked if your Spectrometer is equipped with additional hardware for single spark evaluation, SSE.

Check Box Remote Printer
This check box is marked in case your spectrometer addresses both, the local printer of the spectrometer and a remote printer. All analysis results may be printed in the same way on the remote printer as on the local printer. Depending on the adjustments in the dialog box the output on the remote printer may contain less elements or have another formatting. Remote printers are often positioned e.g. on furnace top platforms or in process control rooms to have analysis results directly available.

Check Box Data Multiplexer
This check box is marked in case your spectrometer is equipped with a data multiplexer. A data multiplexer distributes the output of analysis results to several printers or terminals. Depending on the Type of the data multiplexer and the software necessary all output units display either a identical output simultaneously or the output unit are addressed selectively and display data specially addressed.

Check Box Serial Data Transmission
This check box is marked in case your spectrometer is connected to another computer with a serial data line. The serial data line is used to transmit analysis results to another computer for storage and evaluation.

Check Box Network
This check box is marked in case your spectrometer computer is integrated into a computer network.

Check Box Big Data Display
This check box is marked in case your spectrometer addresses a big data display. A big data display is a multi-segment window the analysis results are large-area displayed. This may be applied in large sheds the analysis results shall be read out of several positions.

Check Box Stepper Controller
This check box is marked if your Spectrometer is equipped with motors to support reprofiling the simultaneous optics.

Group Box Other Devices
Entries in this group box are assigned to additional hardware cards of the spectrometer peripheral control and shall not be changed.

Button OK
Click this button to shut down the dialog box and to read-in the changed entries on the additional devices. The storage is effected globally and is not assigned to a Analytical Program.

Button Cancel
Click this button to shut down the dialog box without reading-in the changed entries.

See:

> Dialog Box Output Parameters
> Dialog Box Output Setup
> Menu Edit
> Program Development

11.3.2 Dialog Box Mode & Interval

This dialog box is used to select the spectrometer operation mode and to set intervals on regularly routines to be carried out. The dialog box contains the following dialog elements:

Group Box Mode
This group box displays general settings of the spectrometer configuration and operation mode.

Display Field Instrument Type:
This field displays the instrument type, optics equipment and computer concept. The entry **extern** means that the computer, which you use to operate the spectrometer, controls an external microcomputer which is built-in the instrument and drives independently the measurements. Consequently the computer with its user interface is partly available to carry out other tasks even if longer measurements are performed.

Radio Buttons Real Mode/Demo Mode
By means of the two radio buttons you decide whether the computer accesses the spectrometer hardware or simulates the spectrometer hardware during measurement. The Demo Mode is intended to make a demonstration of the spectrometer software. Never switch over to Demo Mode when your computer is connected to the spectrometer. You cannot distinguish between a simulation based analysis and a measurement analysis. The experienced operator realizes the demo mode due to missing noise of the source unit and some other hardware controls.

Group box Interval
This group box displays intervals: after running-out the spectrometer program prompts to carry out definite check measurements or set check. Other checks without prompt are effected in the background, e.g. Hg-check or system check.

Edit Field Reprofile SEQ every n hours
You can enter in this field the time interval the program shall prompt you for Reprofiling of the SEQ Optic (Monochromator). The entry in this field is only significant if your spectrometer is equipped with a monochromator.

Edit Field Reprofile SIM every n hours
You can enter in this field the time interval the program shall prompt you for Reprofiling of the SIM Optics (simultaneous optics).

Edit Field Reprofile Hg-check every n minutes
You can enter in this field the time interval for the Hg-check. The entry in this field is only significant if your spectrometer is equipped with a monochromator (SEQ optic). The radiation of a mercury discharge lamp (Hg-lamp) is used for SPECTRO monochromators to check the calibration of the monochromator regularly. This operation is very fast and is effected in the background.

Edit Field System check every n seconds
You can enter in this field the time interval the PC communicates with the built-in micro computer even if no measure operations should be performed. By means of this time interval status changes of the hardware are recognized. Standard value is 1 second.

Edit Field UV-Transmission check every n days

You can enter in this field the time interval the program shall prompt you to check the transmission of the UV-optic. The entry in this field is only significant if your spectrometer is equipped with a optical system filled with nitrogen. The nitrogen filling prevents the absorption of spectral lines of short wavelengths as it is noticeable in an air environment. You should not change the presetting!

The following edit fields display the time or sample interval the system prompts you to carry out definite check measurements, set measurements and cleaning operations. You can define time intervals **and** sample intervals, or one of the intervals or even no entries. In case you define both, a time **and** a sample interval, you will be prompted for the respective operation, when the first of the intervals has expired. Without interval no prompt will be effected. Then you have to ensure on your own that all necessary measurements are always effected in time.

Edit Field Check every n hours / Sparking:

Standardization
Prompt to carry out the standardization after expiration of the interval.

Control sample test
Prompt to carry out the control sample test after expiration of the interval.

Type standardization
Prompt to carry out the type standardization after expiration of the interval.

Clean spark stand
Prompt to clean the spark stand after expiration of the interval.

Button OK

Click this button to shut down the dialog box and to read-in the changed entries on mode & intervals. The storage is effected globally and is not assigned to an Analytical Program.

Button Cancel

Click this button to shut down the dialog box without reading-in the changed entries.

Button Argon Saver

Click on this button to open the dialog box for Argon saving. If you do not use the switched-on Spectrometer for a definite period, Argon will bew wasted. It is possible to reduce the Argon consumption during these periods by means of an automatic function. This function switches down the Argon flow to a lower flow level, when a definite time has gone by with no sparking. If you want to carry out another sparking and you press the start key F2, the Argon flow goes back to its initial level. After a short time for flushing the Argon system, your Spectrometer is ready for operation again.

See:

Menu Instrument
Program Development

11.3.3 Dialog Box Argon Saver

This dialog box is called-up by means of the button 'Argon saver' in the Dialog Box Mode & Interval. If you do not use the switched-on Spectrometer for about half an hour, lot of Argon will be consumed unnecessary. You can reduce the Argon consumption during these downtimes by through an automation. The automatic system switches down the Argon flow to a lower level (low flow), after a defined period without sparking process. When you want to carry out a new sparking and you press the start key F2, the Argon flow goes back to its higher level. After a short flush period your Spectrometer is ready again to operate. The dialog box contains the following dialog elements:

Edit field activate Argon saver after n minutes
Enter into this edit field the period at rest, when the save function shall be switched on. A typical entry is 30 minutes. If you enter 0 or nothing, the save function is disabled.

Edit field reactivation period in seconds
Here you enter the reactivation period in seconds. A typical entry is 30 minutes.

Button OK
Click on this button to close the dialog box and to store the modified entries for the Argon saver. The storage is done globally and does not apply to a special analytical program.

Button Cancel
Click on this button to close the dialog box with no storage of the modified entries.

See:

Dialog Box Mode & Interval
Menu Instrument
Program Development

11.3.4 Dialog Box Data Conversion

This dialog is used to convert spectrometer data which were determined by means of a non-Windows-based spectrometer program under MS-DOS. To open the dialog box select the menu item **Installation**, submenu item **External programs**, submenu item **Data conversion** in the Menu Instrument in the window for Program Development. The data conversion becomes necessary when updating your SPECTRO-spectrometer from MS-DOS to MS-Windows. The data conversion has to be carried out by a SPECTRO-technician in the frame of an adaptation to MS-Windows. Please note that a pure data conversion is not enough to convert your MS-DOS spectrometer to a MS-Windows spectrometer. Additional replacement of some electronic components is necessary. This conversion can only be effected by SPECTRO. If a conversion had been carried out, a repetition of this conversion should be avoided. Otherwise adjustments of analytic programs and data processed in the period since the conversion will be lost. The dialog box contains the following dialog elements:

Group Box Select data type
In this group box you find check boxes for all data to be converted. The old data shall be in the directory CONVDATA below your main directory for the spectrometer software. Generally all data shall be converted.

  Check box Instrument Data
  Tick this check box to convert general device data like configuration of optic, lines installed etc..

  Check box Standard Samples
  Tick this check box to convert data of the Standard Samples.

  Check box Program Data
  Tick this check box to convert data of the analytic programs.

Check box Use Global Stand.
Tick this check box to use the global standardization for the converted analytical programs.

Check box Standard Intensities
Tick this check box to convert the intensities which were determined for the standards. The data are badly needed to display and - if necessary - to recalculate calibration curves in the regression program.

Check box Alloy Grade Library
Tick this check box to convert the alloy grade library.

Group Box Production Data
In this group box you find check boxes for production data to be converted. The conversion of production data is with no meaning for the Spectrometer user and is left to employees of SPECTRO.

Check box QC Programs
Tick this check box to convert analytical programs of the quality control.

Check box Base List
Tick this check box to convert the list of installed bases.

Edit field Device Number

Before a conversion of production data, enter here the device number in the format NNNN/YY, NNNN represents the device number, YY the year of production. In case of a conversion of production data, the device number shall be entered.

Button Close
Click this button to shut down the dialog box.

Button Conversion
Click on this button to convert the data which are marked in the check boxes.

See:

Menu Instrument
Program Development

11.3.5 Menu item UV-Transmission Test

By means of the menu item UV-transmission test you may start the measurement of the UV-test standard, to obtain a basic value for later checks of the UV-Optic, which shall be repeated regularly. The menu item is called-up from the window on Program Development with the Menu Instrument. This menu item is only important if your spectrometer is equipped with a UV-optic which is filled with nitrogen. To carry out the UV-transmission test, the Measure Window is automatically placed in the foreground. Automatically an analytic program is loaded, which was prepared for this purpose by SPECTRO. Generally it contains 2 Monitor Lines with different wavelengths. One wavelength is as much as possible in the UV range with short wavelength, the other monitor line is in the long-wave end of the wave length range of the UV-optic.

You are prompted to measure the UV-test standard. After single measurements and average calculation please press F9, **Next Sample**. Now the calculation of the intensity relation of the two lines is carried out. This relation is stored as a set value. The analytic program, which was called-up before the UV-transmission test, is reloaded again.

The measurement started from here is allowed to be performed **only once** at the occasion of the delivery of the spectrometer. The comparison between the determined set value and the actual value indicates whether the Oxiclear Cartridge shall be changed. The actual value is determined with the Menu item UV-Check.

See:

Change Oxiclear Cartridge
Menu item UV-Check
Menu Instrument
Program Development

11.3.6 Dialog Box Optics Installed

This dialog displays information about the Optics installed. The dialog box is opened via the menu item **Optics** in the Menu Instrument in the window on Program Development. In the course of the spectrometer manufacturing, information about the optics installed are entered here. The entries show which optics belong to the hardware equipment of the Spektrometer. The relevant information is transferred to the Spectrometer computer during initialization. **Unauthorized changes of these data cause malfunction!** The Spectrometer would receive information about another hardware equipment than installed. The dialog box contains the following dialog elements:

Table field Optics installed
This table field contains in its columns the possibly installed optics SEQ1, SIM1-SIM 5. In case another optic is installed, the respective check box is ticked. Provided that a sequential optic SEQ1 is installed, an entry from the combo box 'Additional control board Mono' is selected. Please note that an optional monochromator is only available with SPECTROLAB-S. This entry informs the Spektrometer computer about the hardware board, which controls the monochromator.
Further text fields are of just informative type like grating, focus, slit width, production id-no., comment. Currently these data are not used by the Spektrometer program. The entries are pre-allocated in the moment an optic like SEQ1, SIM, is selected.

⬛ With SPECTROLAB jr. CCD the columns are named CCD1 to CCD5.
Button OK
Click the button to shut down the dialog box. Changed entries are stored. To get the Spektrometer computer informed about the new data, you should select the Menu item Initialize in the Menu Instrument.
Button Cancel
Click the button to shut down the dialog box without reading-in the modified entries.
Button Print
Click the button to print the content of the dialog box.

See:

Menu Instrument
Program Development

11.3.7 Dialog Box Lines Installed

This dialog displays the electronic evaluation channels which are used to measure the intensity of spectral lines. You may open the dialog box via the menu item Optics in the Menu Instrument in the window on Program Development. Each electronic evaluation channel corresponds to one spectral line, provided that the lines are measured through the simultaneous optics SIM1 - SIM5. Using a monochromator (Sequential Optic), all spectral lines within a defined wavelength range can be measured by just a few channels. This option is only available with SPECTROLAB-S. This dialog is used to set the spectrometer during production. **Unauthorized changes of these data cause malfunction!** The dialog box contains the following dialog elements:

`LAB` `CAST` **Table field Lines Installed**

Here you see details on the assigned wavelength for each evaluation channel.

Column PM

That's the list of possible hardware channels from 1 to 128. The term 'PM' derives from 'photomultiplier'.

`CAST` With SPECTROCAST, this column must only be interpreted as consecutive numbers.

Column Channel

This edit field displays channel names which are predefined depending on the element to be measured. In case an element can be measured with several channels, an index may be annexed, e.g. Al1. The entry comprises 4 characters maximally. The channel name will not give any information about the element to be measured, if the hardware channel is used as evaluation channel for a monochromator.

`CAST` Each reference line for SPECTROCAST must have assigned several entries in the column 'channel'. This is the only way to ensure that the reference signal is determined simultaneously for each analysis line (see column 'cycle').

For example:

PM: 7	channel: Fe4	Phy. PM: 4	cycle 1
PM: 8	channel: Fe5	Phy. PM: 4	cycle 2
PM: 9	channel: Fe6	Phy. PM: 4	cycle 3

Column Wavelength

Here you may see the wavelength of the line which is evaluated via this channel. In a wavelength library more than 15000 wavelengths are stored. By means of a click on the button 'Library', the Dialog box Line Library opens, where lines for the respective elements are proposed.

Column Type

There is a difference between lines radiated by atoms, mark I, and lines radiated by ions, mark II. In case no type assignment was carried out, a '*' is displayed in this combo box.

Column field Order

The order, the line is measured. Usually measurements are carried out in first order.

Column field Optic

Here you may identify the optic, the channel is measured with. Possible entries are SIM1-SIM5, SEQ1 for monochromator measurements and ----- resp., if no entry is selected.

Column field Emerge

In this column field the slit width of the photomultiplier might be entered. This entry is just informative and does not influence the spectrometer program.

Column field PM-Type

In this column field the type of the photomultiplier might be entered. This entry is just informative and does not influence the spectrometer program.

Column field PM-rec.
In this column field the relative sensitivity of the photomultiplier might be entered. This entry is just informative and does not influence the spectrometer program.

Column field SAFT
This check box is ticked, if the evaluation channel is equipped with an optional SAFT-electronic device for most sensitive detection limits.

Column Field SSE
This field is marked if the evaluation channel is equipped with additional SSE-electronics for single spark evaluation.

CAST Column Field Phy.PM
This column field indicates which signal receiver is connected to the channel. Several channels may share a signal receiver with SPECTROCAST.

CAST Column field Cycle
This column indicates the shutter position for the measuring procedure with SPECTROCAST. This column entry shows also the temporal sequence of the line measurement, because several lines are measured consecutively with one measuring receiver. The entries 1, 2, 3 apply.

Column field PM-type
The type of the light detector may be entered in this field. This entry is only informative and does not influence the Spectrometer program.

Column field Comment
This field can contain comments up to 20 characters.

Button OK
Click the button to shut down the dialog box. All modified entries are imported.
Button Cancel
Click the button to shut down the dialog box without reading-in the modified entries.
Button Delete
Click this button to delete the content of the marked table fields.
Button Library
Click this button to select a line from the line library and to incorporate it into the table.
Button Print
Click this button to print the table.

With **SPECTROLAB jr. CCD**, the fields have the meaning as described above: **channel, wave length, type, order**. The entry Chip identifies a CCD chip. Several chips are combined to a controller. With the **button Info** further information is accessible for the channel which is selected by the cursor.
The entries can not be varied with the SPECTROLAB jr.CCd.

See:

Menu Instrument
Program Development
Dialog Box Optics Installed

11.3.8 Dialog Box SIM-Parameters

The dialog displays parameters of the SIM-Optics, which are needed for the automated Reprofiliation. It is called from the menu Instrument Optics of the Program Development. The dialog box contains the following dialog elements:

Text fields Optic Number
Her you may see the internal number of each optic. The first simultaneous optic gets the internal number 2, the next optic gets the 3 and so on. Data of optics, which are not installed, are displayed grey.

Text field Optics
The names of the optics are displayed here (SIM1 to SIM5).

Check boxes Reprofiling
These fields are tagged, if the optics are reprofiled with program support. That does not mean that these optics are also equipped with an automatic stepper motor. In the case that no stepper motor is built-in, the reprofiliation is carried out by manual turning of selection knobs.

Edit fields Stepper Profile Position
In these edit fields, you see the profile positions of individual optics. These entries are the result of the first profile adjustment in the factory or of a past reprofiliation. After each new reprofiliation the respective profile value is entered here. The entry is done automatically if the reprofiliation is executed computer-assisted. When a too great deviation is found in the case of a reprofiliation compared with the previous profile position, the new value will nor be entered. Read the chapter 'Carry out a SIM-Reprofiliation.

Edit fields Profile Offset
If the profile position should differ from the entry in the above field by a specific step number, the value can be entered as a negative number (deviation to smaller steps) or positive number (deviation upwards). That can be reasonable in very special cases of application.

Combination field Available Lines
Here you see the line names of each optics with the numbers of associated electronic channels. First select a line per optics which should be analyzed in the case of reprofiliation. By clicking the **button Delete**, this line is taken over into the list of lines to be analyzed. By repeated selection of another line in the same optics, further lines can be considered for a reprofiliation of an optics.

List field of lines included into reprofiliation
In these list fields, the lines are displayed which are analyzed with a reprofiliation. A double-click on an entry opens a dialog with further specifications for reprofiliation process with the selected line.

Button Entf
Click this button in order to remove a line from the selection of lines to be analyzed for reprofiliation.

Button OK
Click on this button to shut down the dialog box. All modified entries are stored.

Button Cancel
Click on this button to shut down the dialog box without reading-in the modified entries.

Button Source Para.
Activate this button in order to open the dialog box Source Parameters. Through the call of the dialog box from the current dialog SIM Parameters, you parametrize the excitation parameters for the measurements for the reprofiliation. Please note that measuring times for the reprofiliation should be considerably shorter than you know it from your analytical measurements. Reason is that approx. 20 individual measurements are to be carried out for a reprofiliation and you certainly do not want to prepare the sample several times again. Moreover, the total time of the reprofiliation would become unnecessarily long. A typical measuring time in the case of the reprofiliation is 0.5 or 1 second.

Button Line Para.
Select at first an entry in the list field **'lines included into prof.'**. Then click this button in

order to open the dialog box Line Parameter SIM-Reprofiliation for the selected
line. There you can enter further specifications for reprofiliation process with the
selected line.
·Instead of using the button, you can also make a double-click in the list field on a
line entry in order to open the dialog.

See:

Menu Instrument
Program Development
Carry out a SIM-Reprofiliation
Profile Check
Dialog Box Source Parameters
Dialog Box Linie Parameters SIM-Reprofiliation

11.3.9 Dialog Box Linie Parameters SIM-Reprofiling

This dialog shows further specifications to lines which are measured and evaluated for
Reprofiling. The current line the dialog refers to, is indicated in the header line of the dialog.
This dialog is called from the dialog box SIM Parameter. The dialog box contains the
following dialog elements:

Combination field Measuring Cycle
In this field you select the measuring cycle with which the measuring of the line is to be
carried out. The lines for reprofiling are in general measured in the same measuring cycle.
However, it is possible to measure individual lines in another measuring cycle if a more
suitable intensity signal can be there achieved.

Check boxes Orientation Line
With this check box, you determine whether the selected line should be the orientation line.
The term orientation line ought to be understood as the line that determines the scaling of
the graphic representation of the course of profile. If several lines are selected for reprofiling
an optics, the line with the highest intensity achieves should be marked as orientation line.
The graphics program in the scan manager takes the current intensity value of this line as a
maximum for scaling. Consequently, all further lines of optics are displayed below the
orientation line and are not cut. If no orientation line is tagged, is the first line in the list field
of the dialog box SIM Parameters is used as orientation line.

Edit field Weighting
You determine with this edit field how strongly the signal of the current line should be
considered for reprofiling of an optics. This is important if more than one line is used for
reprofiling an optics. Enter numbers like 1, 2 or 3 for single, double or three times the
weighting. An entry 0 means, that the line is only indicated but not evaluated for the
quantitative analysis of the optimal profile position. If no value is entered for a line, then the
first line entry per optics is weighted by 1.

Button OK
Click this action key to close the dialog box. All changed entries are stored.

Button Cancel
Click this button to close the dialog box without saving the modified entries.

See:

Menu Instrument
Program Development
Carry out a SIM-Reprofiling

Profile Check
Dialog Box SIM-Parameters

11.3.10 Dialog Box SEQ-Parameter

`LAB`

The dialog views parameters of the SEQ Optic (Monochromator), which is optionally available. Especially the wave length range of the SEQ optic is stored here. From this dialog box the Dialog Box Wavelength Calibration may be called-up. Please not that this dialog box as well as the dialog box for wavelength calibration contain very sensitive data, which must not changed by the user but exclusively by authorized SPECTRO personnel. Wrong settings result in malfunction of your Spectrometer and bad analysis results! The dialog box contains the following dialog elements:

Group Box with Spectral

Edit Field from (nm) to (nm)
These edit fields view the limits of the spectral operation range of the sequential optic in [nm].

Combo Box Calibration
Here you may see whether the sequential optic is mechanically calibrated. If a calibration was carried out, it is displayed as calibration function *polynomial 2nd degree*. If the optic is not mechanically calibrated, the text *not calibrated* is displayed.

Edit Fields Number of Entrance Slits/ Number of Exit Slits
In these edit fields you see the number of lEntrance- and Exit Slits, the monochromator optic works with. The entry depends on the type of the installed monochromator.

Group Box Reprofiling Information
In this group box you find information necessary for Reprofiling of the monochromator.

Edit Field Entrance Slits
This field displays the number of the entrance slit used for the reprofiling.

Edit Field PM-Number
The entry in that field identifies the light sensor which measures the spectral line used for reprofiling.

Edit Field Peak Position
In this field you may see the position of the stepper motor given in mechanical steps, where the Peak is to be find, depending on the given combination of entrance slit and light sensor

Button OK
Click on this button to close the dialog box. All modified entries are stored.

Button Cancel
Click on this button to close the dialog box. Modified entries are not accepted.

Button Load
Click on this button to call-up the Dialog Box Wavelength Calibration, where the data for the mechanical calibration are stored.

See:

Menu Instrument
Program Development
Carry out a Reprofiling

11.3.11 Dialog Box Wavelength Calibration

The dialog box presents the wavelength calibration of the SEQ-Optic (Monochromator), which is optionally available for SPECTROLAB-S. The wavelength calibration is the connection between the steps of the stepper motor, which drives the adjusting mechanism of the SEQ-optic, and the wavelength to be measured. Unauthorized manipulation with the wavelength calibration may cause severe malfunctions - the Monochromator may no longer be used for analytical measurements!
Additionally this dialog brings the opportunity to take over the wavelength calibration of the SEQ-optic from an ASCII-file. This option is necessary for manufacturing the spectrometer.

Button OK
Click on this button to shut down the dialog box. All modified entries are stored.
Button Cancel
Click on this button to shut down the dialog box without reading-in the modified entries.

See:

  Menu Instrument
  Program Development

11.3.12 Menu Item Logbook

By means of this menu item you may open the logbook. The menu item is called-up from the Menu Instrument of the window on Program Development. The logbook is a journal file: error messages and selected warning notes are stored here, which possibly occur during the operation of the spectrometer. Consequently the entries into the logbook may be helpful for error diagnosis. The editor used to view the logbook, is the standard Windows editor. The logbook is written cyclically, i.e. the number of entries is limited. When the limit is reached, older entries are overwritten by new ones. Close the logbook view with the system menu of the editor.

See:

  Menu Instrument
  Program Development

11.3.13 Menu Item ICS Access

With this menu item you may open a program to check definite functions of the Instrument Control Server (ICS) directly. The menu item is called-up from the Menu Instrument in the window of Program Development. This menu item is for internal use only.

See:

  Menu Instrument
  Program Development

11.3.14 Menu item ICS Spy

By means of this menu item you may open a window, which displays communication and access authorization of the different program parts on the spectrometer control unit ICS. The menu item is called-up from the Menu Instrument in the window of Program Development. This menu item is for internal use only. Close the ICS-spion by means of the system menu of the window.

See:

> Menu Instrument
> Program Development

11.3.15 Menu item Initialize

By means of this menu item you may initialize the hardware of your spectrometer. The initialization of the spectrometer is also carried out during each restart of the spectrometer program. An initialization during the production process will be necessary if a new hardware component is installed or problems with the data transfer occur.

See:

> Menu Instrument
> Program Development

11.3.16 Menu item UV-Check

with this menu item you may start the measurement of the UV-check standard to test the absorption of short-wave light in the UV-Optik. This menu item is only important if your spectrometer is equipped with a UV-optic filled with nitrogen. The measure results are automatically compared with the set points which were found by a measurement during the installation of the spectrometer. The measurement was carried out with the Menu item UV-Transmission Test. The menu item is called-up from the Menu Instrument, submenu **Installation**, of the window on Program Development. Additionally the UV-check may also get started by means of an automatic prompt to carry out the UV-check. This prompt will be given in case a definite number of days passed on since the previous UV-check. The number of days between the UV-checks may be defined in a Parameter File. To carry out the UV-check, the Measure Window is automatically placed in the foreground. You are prompted to measure the UV-check standard. After single measurements and average calculation please press F9, **Next Sample**. Now the comparison between the intensities and the stored set values is carried out. The analytic program, which was called-up before the UV-transmission test, is reloaded again. If the difference between the set value and the current values is too big, a warning message will be displayed. Then please change the Oxiclear-Cartridge.

See:

> Change Oxiclear Cartridge
> Menu item UV-Transmission Test
> Menu Instrument
> Program Development

11.3.17 Dialog Box Dark Current Test

In this dialog box you enter the measure conditions and limit values for the Dark Current Test. These parameters are globally valid for all Analytical Programs. You can start the dark current test from the measure window in the menu 'instrument', Menu Item Dark Current Test.

The dialog box contains the following dialog elements:

Group Box Measure Conditions
  Edit Field Number of Measurements
  Here you enter the number of measurements to be carried out for a dark current test.

  Edit Field Measure Time
  Enter in this field the measurement time in seconds for the dark current test.

Group Box Limit Values Low Sample
  Edit Field Intensity Limit
  The intensities, which were present during the dark current measurement, are channeled specifically when compared with the intensities of the low sample(s) of the last **Standardization**. Enter in this field the % value which is accepted as dark current in relation to the low sample signal. Example: 10%.

  Edit Field Limit Value of Standard Deviation
  Enter here the % value which is accepted for the absolute (not relative) standard deviation of the dark current signal in relation to the low sample signal. Example: 0.5% means that the absolute standard deviation of the dark current for a specific channel must not exceed 5.0, when the low sample signal for this channel reach 1000 intensity units.

Group Box Reference Limit Value
  Edit Field Typical Intensity
  Reference Channels are not standardized, therefore there are no low sample intensities for these channels to assign the results of a dark current test to. This is why a certain percentage of the typical intensity of the reference channel is taken as limit value for the dark current test. Enter this numerical value here.

Button OK
Click this button to close the dialog box and to store the changed entries for the dark current test. The storage is globally valid for all analytical programs.

Button Cancel
Click this button to close the dialog box without storing the changed entries.

See:

  Menu Instrument (Program Development)
  Program Development
  Menu Item Dark Current Test
  Menu Instrument (Measure Window)
  Measure Window

11.3.18 Dialog Box Constant Light Test

You may set in this dialog box the measurement conditions and limit values for the constant light test. The parameters are globally valid for all Analytical Programs. You start the constant light test in the measure window of the menu Instrument, Menu Item Constant Light Test.

The dialog box contains the following dialog elements:

Group Box Measure Conditions

Edit Field Number of Measurements
Enter here the number of measurements, which will be carried out for the constant light test.

Edit Field Measure Time
Enter here the measurement time for the constant light test in seconds.

Group Box Reproduction
Edit Field Maximum Relative Standard Deviation
The relative standard deviation is calculated from the single measurement of the constant light test. Enter in this field the maximum permissible relative standard deviation. Example: 10%.

Edit Field Maximum Deviation from Average of the last 3 Constant Light Measurements
The results of the constant light measurement are stored. An average value is taken from of the last 3 constant light measurements. Then this value is compared with the current result. This criterion is only possible if a constant light test had been carried out at least 3 times before. Enter in this field the maximum permissible relative standard deviation in %. If you enter 0, a check in accordance to this criterion is disabled.

Button OK
Click this button to close the dialog box and to store the modified entries for the constant light test. The storage is done globally for all analytical programs.
Button Cancel
Click this button to close the dialog box. The modified entries are not stored.

See:

Menu Instrument (Program Development)
Program Development
Menu Item Constant Light Test
Menu Instrument (Measure Window)
Measure Window

11.4 Menu Extras (Program Development)

The menu **Extras** contains various menu items to view libraries and to call-up special functions. The following menu items are available:

➡ **Setup Output**
With this menu item you may open the Dialog Box Setup Output, to carry out the basic settings of the data output.

➡ **Format Sample-ID**
With this menu item you may open the Dialog Box Format Sample-ID, to define the look of the input dialog for sample data.

➡ **Standard Sample List**
With this menu item you may open the Dialog Box Standard Sample List, to change data of already defined Standard Samples or to define new standard samples.

➡ **Alloy Grade Library**
With this menu item you may open the Dialog Box Alloy Grade Library, to change data of already defined Alloy Grades or to define new alloy grades.

➡ **Line Library**
With this menu item you may open the Dialog Box Line Library, to view, complete, change the list of the possible spectral lines.

SPECTRO

→ **Interference Library**

With this menu item you may open the Dialog Box Interference Library, to view, complete, change the list of the possible Interferences.

→ **Master Standardization**

With this menu item you may open the Dialog Box Master Standardization, to start a Master Standardization.

→ **New Standardization Sample**

With this menu item you may open the Dialog Box New Standardization Sample to introduce a new standardization sample for the selected analytic program.

→ **User Management**

With this menu item you may open the Dialog Box User Management, to view, complete, change the list of the defined users.

→ **Program Import**

With this menu item you may open the Dialog Box Program Import to restore an exported Analytic Program.

→ **Program Export**

With this menu item you may open the Dialog Box Program Export to export an Analytic Program, to use it as data safeguarding and to re-import it later on - if necessary.

→ **Save Data**

With this menu item you may call-up an external program, for making a complete backup of all spectrometer data. The name of the backup program is stored in a Parameter File.

→ **Restore Data**

With this menu item you may call-up an external program to retrieve spectrometer data. The name of the backup program is stored in a Parameter File.

See:

Program Development

11.4.1 Dialog Box Output Setup

This dialog box is used for a basic setup on data output. This dialog-box is opened with the menu item **Output setup** in the Menu Extras of the window for Program Development. In this window you define whether the output is effected on several output units immediately after determination of data or when the complete analysis of a sample is finished. Additionally you see the type and the connecting interface of the printer installed and you can set a line based or a page based print mode. Furthermore you define a buffering of the results during a data transmission. The dialog box contains the following dialog elements:

Group Box Output Setup

In this window you define the moment to carry out **Print, Store, Transmit** of analysis results: an output **immediately** after analysis or the complete analysis (**block**). Note the following example: In the output parameters of a definite Analytical Program is defined that individual measurements, analysis results and average shall be printed. Provided that immediate output is defined, each single analysis result will be printed after each analysis. In case of deleting single measurements before averaging, the single measurements are documented on the paper. After averaging the average value is printed. In contrast to this the block output is printed after calling the next sample. In this example the print out only contains the not deleted individual measurements and the average and average with standard deviation respectively. Max 20 individual measurements are printed out in block mode. In case more than 20 measurements were performed, the last 20 are printed out. Storage and transmission of data is equivalent to print out. In any case an output of analysis results can be started manually independent from the settings in the output setup. Please use the Menu File in the Measure Window. Note the tips below on printer types.

Group Box Printer Setup

This window displays data on printer setup. The installation of a printer is effected in the Menu File (Program Development).

Display Field Device

The name of the active printer of your spectrometer is displayed in this field.

Display Field Port

This field displays the name of the interface the active printer is connected to.

Radio Button Line oriented printer

Click the radio button in case the printer installed is a line oriented printer. Line oriented printers use a continuous paper feed. Printers are able to print single lines without feeding the paper to the begin of the next page.

Radio Button Page oriented printer

Click the radio button in case the printer installed is a page oriented printer. Page oriented printers eject a complete page after each print task. Laser printers and most ink-jet printers are page oriented printers.

Note:

In case a page oriented printer is used, it is advantageous to set the block print output. If you would set immediate print, the printer uses a new sheet of paper for each single measurement.

Group Box Transmission Setup

In this field you define whether the analysis results shall be stored in a buffer for later manual data transmission or the transmission shall be effected online and automatically.

Radio Button Online

Click the radio button in case the recieving computer is always online and waits for data transmission. In case of a temporary interference with no possible data transmission, the analysis results are stored in a buffer file. During the next transmission of another analysis result the buffered file is transmitted too.

Radio Button Buffer
Click the radio button in case the recieving computer is **not** always online. The results to be transmitted are stored in a buffer file. The content of the buffer file is transmitted from the Measure Window with the Menu Item Transmit Buffered Data in the Menu File to the receive computer.

Radio Button Not installed
Click the radio button in case data transmission shall not be performed.

Button OK
Click this button to shut down the dialog box and to read-in the changed entries on output setup. The storage is effected globally and is not assigned to an Analytical Program.

Button Cancel
Click this button to shut down the dialog box without reading-in the changed entries.

See:

Dialog Box Output Parameter
Dialog Box Element Format
Menu Extras
Program Development

11.4.2 Dialog Box Samples ID-Format

This dialog box is used to define the shape of a sample description and the Dialog Box Sample ID-Format. The dialog box is opened with the menu item **Sample ID Format** in the Menu Extras of the window for Program Development.

Each Production Sample to be measured should be named in such a proper way that even after a longer period the analysis results can be clearly assigned to the sample. The dialog 'Sample ID-format' allows the definition of fields which are used as identification fields for the samples. It is possible to define up to 19 fields which may be filled with identification terms for each sample. Furthermore it is possible to calculate some field concentrations using the entries in other fields. The definition of the sample identification fields is valid for all Analytical Programs globally. The dialog box contains the following dialog elements:

Check Box Query
Click this field to query the sample identification terms automatically before the analysis starts.

Edit Field Pre-User Task
This edit field shows the names of the user task, which is called-up before opening the Dialog Box Sample Data in the measure window. This task may be used to complete a file with entries for the sample identification fields.
You select the user task through the button 'pre-user task'. But you may enter directly the name of the program to be selected into the edit field.

Edit Field Post-User Task
This edit field shows the names of the user task, which is called-up after closing the Dialog Box Sample Data in the measure window. This task may be used to provide other computers with this file including the entries in the sample identification fields for further processing.
You select this user task through the button 'post-user task'. But you may enter directly the name of the program to be selected into the edit field.

X-Y-Coordinates Field

The two rows below the coordinates X = 1 to X = 1000 are used to display and design the sample identification fields. The entries fix the display of the fields on the screen. The number of rows (starting with 0) reserved for sample identification terms on the top of the Measure Window is adjusted in the Parameter File PS_GEN.ASC under 'Measure Window' in row 'MaxNumberIDRows'. A row of the Measure Window is fictitiously divided into 1000 horizontal positions; e.g. you want to display in the first row of the Measure Window 2 sample identification terms **Name:** and **Quality:**; the coordinates of sample identification terms should be selected as follows:

Name: X Start = 1, X End = 495, Y = 1
Alloy Grade: X Start = 505, X End = 1000, Y = 1

The display area in the field 'Name' stretches from the left screen margin up to short before the center, the display area in the field 'Alloy grade' from short behind the center up to the right screen margin. In case the entry in the field is longer than space is available, the entry is cut. The storage of the entry is always completely effected. The field coordinates of the example were consciously not selected from 1 to 500 and 501 to 1000 to prevent unification into one field.

Table Field Sample Identification Fields

Enter name, display position and type of the sample identification fields in this Table. The table contains the following columns:

Column Field Name

Enter the names of the sample identification terms in this field. You can enter max. 19 terms with a length of 15 characters each.

Check Box Edit

The check boxes indicate whether the content of a sample identification field in the Measure Window may be edited or not. This field is marked generally. In case a field is filled by a formula or a user task, it is sometimes desired to prevent any changes in this field. To secure the field, remove the mark from the respective check box.

Column Field Order

You define in this edit field the sequence of the sample identification fields in the Dialog Box Sample Data, used by the query process

Column Field X Start, X End, Y

This edit field defines the position of the field in the Measure Window. Y = 1 means: first row, Y = 2: second row, Y = 0: not displayed (see above: X-Y-coordinates field).

Column Field Field Type

The following field types are available in the combo box: Normal, Weight, Quality. It is not allowed to define more than one sample identification field of type 'Weight' or 'Quality'. These field types have a special use. Select the type 'Normal' for fields which shall not re-affect the spectrometer program.

Quality:
The entry in a field of quality type is evaluated for an Alloy Grade Test. Actually the type 'Alloy grade' can only be selected in the second sample identification field. The Measure Window displays a combo box for the alloy grade in the query dialog which is filled with all alloy grades of the current base.

Weight:
The entry in a field of weight type in the Measure Window is used for batch corrective calculations by the spectrometer program. The batch corrective calculation is an option for the spectrometer program. By means of this option it is possible to calculate type and amount of alloying elements necessary for a given batch, based on data like analysis results of actual batch and entry of the targeted alloy grade. This option can be used in metal manufacturing companies to calculate the kind and amount of alloying elements to achieve a defined target alloy grade of the batch.

Column Field Origin

The following field types are available in the combo boxes: Keyboard, Last, Operator defined formula, User defined sample Id's.

Keyboard
Select this entry to fill the sample identification field by means of the keyboard. This setting is most commonly used.

Last
Select this entry to pre-allocate the sample identification field with the entry of the last sample. In case of similar sample identifications for series of samples the required work can be reduced significantly. The pre-allocation may be modified or overwritten with the keyboard.

Operator defined formula
Select this entry to fill the sample identification field by means of a formula calculation based on entries in other sample identification fields. The formula may be freely adjusted. The definition is effected with a click on 'Edit formula'.

User defined sample-Id's
Select this entry to display the sample identification fields as a combo box. The combo box is filled with a list of all entries which are stored in the Parameter File PS_SID.ASC in the respective field.

External
Select this entry to fill the sample identification fields with information which are deposited in a file. The name of the file is EXT_SID.ASC. The file format is described in Data Formats. If you wish to get the sample identification fields automatically filled, the file EXT_SID.ASC must be in the subdirectory \INPUT of your Spectrometer software (different directories are also possible through an respective entry in the file EXT_SID.ASC; contact the Spectro service). The file with its desired entries may be provided e.g. by a superior host computer or in an network by another network computer. This file may be generated e.g. by an application which is called-up as a pre-user task See above 'edit field pre-user task'. If the file EXT_SID.ASC is not available though its origin is defined as external, the system waits for a defined period for this file, typically 60 seconds. You can adjust the waiting period in the Parameter File PS_SID.ASC. If the file was readout in the measure window to fill the Dialog Box Sample Data, it will be deleted automatically.

Column Field Formula

The edit fields display the formulas which are used to calculate the contents of the sample identification fields, provided that 'Formula' is selected in the field origin formula. The formulas are entered by means of a formula editor. The formula editor is positioned in the Dialog Box Edit Formula, which is called if you should try to enter data into this column field or you click the button 'Edit formula'.

Radio Buttons Positionate sample names / Enter operator defined formula

In case the box 'Enter operator defined formula' is selected, both is displayed, the sample name and all operator defined formulas which are connected with this name. In case the box 'Positionate sample names' is marked, general data on the sample names are displayed, e.g. the display position of the sample name on the screen output. Generally the radio button 'Positionate sample names' is pre-selected after opening the dialog box.

Button OK

Click this button to shut down the dialog box and to read-in the changed entries on the format of sample identification terms. The storage is effected globally and is not assigned to an Analytical Program.

Button Cancel

Click this button to shut down the dialog box without reading-in the changed entries.

Button Clear
Click this button to remove the entries in the highlighted area. Columns 'Field type' and 'Origin' are reset to field type 'Normal' and origin 'Manual'.

Button Edit Formula
Click this button to open the Dialog Box Edit Formula.

Button Pre-User Task
Click this button to select a program which will be executed before opening the Dialog Box Sample Data in the measure window. The selected pre-user task is displayed in the edit field pre-user task.

Button Post-User Task
Click this button to select a program which shall be executed after closing the Dialog Box Sample Data in the measure window. The selected pre-user task is displayed in the edit field pre-user task.

Button Default
Click this button to define the current settings as default values for generating new analytical programs.

See:

Menu Extras
Program Development
Dialog Box Sample Data
Data Formats
Parameter Files

11.4.3 Dialog Box Sample List

This dialog box is opened with the menu item **Sample list** in the Menu Extras in the window on Program Development or with several superordinated dialogs. The sample list displays a survey on all standard samples which are entered for the base of an Analytical Program (e.g. Fe-base or Al-base). Standard samples are e.g. calibration standards, standardization samples, type standardization samples, type calibration samples, control samples. As you can see from the examples, Standard Samples are used for a definite operation of the spectrometer. In contrast Production Samples are samples with unknown chemical compositions and shall be analyzed with the spectrometer.

The dialog contains the following dialog elements:

Edit Field Selected Standard
Use this edit field for a fast search for definite standards. Fill in the first characters of the standard searched for, and the list displays the entries starting with these characters.

List Box
Calling the list for the first time, all samples of the base are displayed which are entered up to now. By means of the button 'Filter' the selection may be influenced and limited to a special standard type (see below). The samples are listed in alphabetical order.

Button Close
Click the button to shut down the dialog box.

Button Edit

This button opens the Dialog Box Edit Standard Samples. Here you can change the type of standard, the concentration values and written comments on the standards. Type of standard means the intended use of a standard: e.g. calibration standard, type calibration sample, standardization sample, type standardization sample, control sample. A standard may cover several types of samples.

It is not possible to create new standards in this dialog box. Please use the button 'list'. This button is enabled when an entry in the list box 'proposed samples' was marked before. Multi-marking in the list box 'proposed samples' are not supported by this function. In case you marked several entries nevertheless, the Dialog Box Edit Standard Samples is displayed for the first highlighted sample.

Button New

The same dialog as 'Button Edit' is displayed. The difference is that no existing entry is transformed into a standard, but a new entry is generated.

Button Delete

The button gives the opportunity to remove an entry from the standard sample list. A query is displayed that you have to confirm the removal. As soon you confirmed the removal, the selected standard is deleted immediately. There is no way to undo the deletion, even if you should quit the dialog box 'Sample list' with the button 'Close'.

Button Filter

The button opens the Dialog Box Filter Settings for Standards Libary. This dialog box is used to select definite standards to be displayed in the list box. So the display may be limited to e.g. all standards of a special type.

Button Extern

Sometimes databases containing information on standard samples and concentrations exist in a company. These information can be read-in by the SPECTRLAB directly and are incorporated into the standard sample file. To proceed in this way, it is necessary to have the sample information, which shall be read-in, available in a special format as ASCII file. Ask the SPECTRO service for the file format. The read-in information on standard samples should be checked and edited respectively. With a click on the button 'External' the window 'File selection dialog' is displayed to load the above mentioned ASCII file. A conversion into the SPECTRO format is effected immediately. Please note that the ASCII file shall meet the format given by SPECTRO precisely. In case of non-observance not only the read-in procedure may fail, but also the complete file may be destroyed. We recommend you urgently to carry out Data Save before.

Button Copy

The button opens the same dialog as button 'Edit' and 'New'. In this dialog you can store a sample under another name and to modify some data, e.g. concentrations. Please note that the name for the new copy is not used by other files.

See:

Menu Extras
Program Development

11.4.4 Dialog Box Edit Standard Sample

This dialog box is used to edit standard sample data. Depending on the call by a button 'Edit', 'New', 'Copy', either terms on a definite entry of the standard sample is edited, or a new entry is generated or an entry is stored as a copy under another name may. The dialog box contains the following elements:

Edit Field Name
Enter a name for the standard, the size is limited to 30 characters. This field shall be filled unambiguously. Two standards with the same name for a base are not permitted.

Edit Field Description
Enter a description of the standard, the size is limited to 30 characters.

Edit Field Author
Enter your name or initials in this field to be able to identify the operator. The size is limited to 8 characters.

Edit Field Producer
Enter the producer or local supplier in this field. The size is limited to 30 characters.

Edit Field Comments
Enter in this field a comment on the standard, if desired. The size is limited to 64 characters.

Combo Box Alloy Group
Select the alloy group the standard shall belong to. In case the standard cannot be assigned to an alloy group or the standard belongs to several alloy groups, please select **none**.

Combo Box Base Element
This combo box is disabled. It is not possible to make a selection. But you can identify the base you are processing standard samples. In case you want to process standard samples of another base, you have to load a Analytical Program of this base in advance.

Check Boxes Standard Types
Calibration Standards, Standardization Samples, Control Samples, Diagnostic Sample, Type Stand. Samples, Master Stand. Samples, Type Calib. Samples, Sample for Reprofiling
Mark one or more standard types the edited standard belongs to. A multi-selection is possible.

Display Field Last Change
This field displays the date of the last change of the data of the standard sample. When you generate a new entry, the current data is displayed in this field.

Button OK
Click this button to shut down the dialog box and to read-in the entries.

Button Cancel
Click this button to shut down the dialog box. The selected filter and sort criteria are not applied to the standard sample list. The filter and order criteria valid before calling this dialog box are recalled.

Button Conc.
Click the button to open the Dialog Box Standard Sample Concentrations. This dialog box records element specifically the concentrations with units and concentration limits, if requested.

See:

Dialog Box Standard Samples List
Menu Extras
Program Development

11.4.5 Dialog Box Filter Settings

By means of this dialog box you define the display and sort filters for the list of standard samples. The dialog box is called from the Dialog Box Standard Sample List or from divers dialogs to select standards. Texts can be entered into the fields 'Author' and 'Producer' used as display criteria. An alloy group can be pre-selected with a combo box. There is an additional option to preset a concentration range for a definite element. In case you filled entries in several fields, the standard sample list displays the standards exclusively which fulfill all criteria simultaneously (AND-operation). A different behavior show the check boxes on the sample types: if you should click several boxes, all samples are displayed which belong at least to one of the selected sample types (OR-operation).
Additionally the sort order of the sample list can be changed. The dialog box contains the following dialog elements:

Group Box Filter Criteria
This group box contains the criteria to display standard samples in the standard sample list.

Edit Field Author
Enter the author into this field if you would like to use him as a display criterion. The standard sample list displays only standards with the preset entry in the field 'Author'.

Edit Field Producer
Enter the producer into this field if you would like to use him as a display criterion. The standard sample list displays only standards with the preset entry in the field 'Producer'.

Combo Box Base Element
This combo box is disabled. It is not possible to make a selection. But you can identify the base the loaded Analytical Program belongs. The standard sample list always displays just the samples of one definite base.

Combo Box Alloy Group
Select the alloy group the displayed standard samples shall belong to. In case you select none, the alloy group is not used as a filter criterion.

Check Box Concentration Range
Mark this field to make your selection with the concentration of a definite element in the standard sample. The element and the concentration range is defined in the next fields.

Combo Box Element
This field is used to select the element, on which the concentration entry shall be a filter criterion.

Edit Field Low
Enter in this field the low concentration value which shall be used as a criterion for sample selection. In case the entry is 0.000000, the low limit shall not be specified.

Edit Field High
Enter in this field the high concentration value which shall be used as a criterion for sample selection. In case the entry is 0.000000, the high limit shall not be specified.

Check Boxes Standard Types
Calibration Standards, Standardization Samples, Control Samples, Diagnostic Sample, Type Stand. Samples, Master Stand. Samples, Type Calib. Samples, Sample for Reprofiling
Mark one or more standard types for which all samples shall be displayed, provided that the criteria mentioned above are fulfilled. The individual standard types have an OR-operation. That means a sample is displayed, if at least one sample is a sample of the selected standard type. If you don't make a selection from these boxes, the criterion standard type will not be used.

Group Box Sort Criteria
This group box contains the criteria to sort the standard samples in the standard sample list.

Radio Button Sample Name
Click the radio button to display the standard samples sorted acc. to the names.

Radio Button Producer
Click theradio button to display the standard samples sorted acc. to the producer.

Radio Button Alloy Group
Click the radio button to display the standard samples sorted acc. to alloy groups.

Button OK

Click this button to shut down the dialog box. The selected filter and sort criteria are applied to the standard sample list.

Button Cancel

Click this button to shut down the dialog box. The selected filter and sort criteria are not applied to the standard sample list. The filter and sort criteria, which are valid before calling this dialog box, are recalled.

See:

Dialog Box Standard Sample List
Menu Extras
Program-Development

11.4.6 Dialog Box Standard Sample Concentration

In this dialog box you can edit concentration values for the elements of a standard sample. The data are recorded in a table. The dialog box is opened with the respective button 'Conc.' in the Dialog Box Edit Standard. The dialog box contains the following elements:

Table Field Selected Standard
In this Table you may enter elements and concentrations contained in the standards. Limit values may be entered additionally for standards of control sample type. The table contains the following columns:

Column Field Element
Enter here the symbols of the elements which are contained in this standard. In case the entry is not an element symbol of the classification of elements, a warning is displayed when the dialog box is quitted. But the entry is read-in.

Column Field Conc.
Enter the concentration of the respective elements in this field.

Column Field Unit
Select the unit for concentration inputs for the respective element. Units listed in the list box of the combo box are stored in a parameter file. Calculation factors for the units ppm, parts per million and ppb, parts per billion in relation to the base unit % are stored in the system. You can switch between these units, the values are displayed correctly.
If you update an older software version to the current software state, the unit calculation might possibly be not available directly. Please refer to the item 'Unit calculation' in the parameter files of the help function how to enable the unit calculation.

Column Field Lo.Lim. External, Lo.Lim. Internal, Hi.Lim. Internal, Hi.Lim. External
These fields are enabled in case the edited standard is a 'Control sample' type. Enter the limits between the control sample results are still accepted. In the Measure Window either internal or external limits are checked. These limit values are stored in a Parameter File.

Button OK

Click this button to shut down the dialog box. The changed entries are stored.

Button Cancel

Click this button to shut down the dialog box. The changed entries are not stored.

Combo Box Default Unit
Select the default value for the unit in this field. This unit is automatically set for the new element which is entered into a blank row of the table field. The units displayed in the list box of the combo box are stored in a parameter file.

Button Fill
Mark an area of several rows in the table field and press the button to copy data from the first row into the other highlighted rows. Entries in the column field elements are not copied.

Button Clear
Click the button to remove the highlighted area from the table field.

Button Print
Click this button to print the table.

See:

Dialog Box Edit Standard Samples
Dialog Box Standard Sample List
Menu Extras
Program Development

11.4.7 Dialog Box Line Library

The dialog box 'Line library' shows a list of about 1500 lines which can be supplemented or changed. The dialog box is opened with the menu item **Line Library** in the Menu Extras of the window for Program Development. The line library is the data source for the selection of lines to make measurements with the Monochromator. If you are working on a SPECTROLAB without a monochromator, the list is limited to information. Measuring other lines than the lines fixed installed is not possible. The dialog box contains the following dialog elements:

Row with Edit Fields
In this row you may edit the parameter of a selected line, or you may input data on a new, additional line.

List Box with Line Parameters
The list box displays the following data on each line:

Pri:
means priority. Rows marked with a (+) in this column are the mostly used lines of the respective element (line proposal). The marking makes the choice easier, because sometimes a very large number of lines is available.

El:
means element. The row displays the symbol of the chemical element of the lines.

WaveLen:
means wavelength. The row displays the wavelength of the line.

Sensitivity:
This column records the relative sensitivity of the lines. Sensitivity values are taken from literature. the higher the number, the more sensitive the line.

Order:
Class of order the line is measured. SPECTROLAB equipped with a Monochromator always performs measurements in first order.

Type:
There are two types if lines: the first type is radiated by atoms (marking I) and the second type is radiated by ions (marking II).

BEC:
Background equivalent concentration of lines (BEC), as far as described in literature.

DI:
Detection limit of lines (LOD), as far as described in literature.

Interference:
Known interfering elements may be entered here.

Radio Buttons Page Up / Page Down
Clicking the radio buttons you perform a paging through the list. When the displayed lines are positioned in the top or bottom end of the list, one of the two buttons is disabled.

Button OK
Click this button to shut down the dialog box. The changed entries are stored.

Button Cancel
Click this button to shut down the dialog box. The changed entries are not stored.

Button Edit
A click on this button copies the data of the selected row into the upper row containing the edit fields. Instead of a click on the button 'Edit' a double click on the selected line in the list box may have the same effect.

Button New
A click on this button removes the data from the upper edit row. Now the data of another row not jet in the list may be entered.

Button Save
With a click on the button the content of the upper edit row is moved back into the list with its modified data. The button 'Save' is only enabled after a data set had been loaded into the upper row for editing.

Button Insert
With a click on the button the content of the upper edit row is moved into the list as new entry. The button is enabled after a new entry had been prepared with the button 'New'.

Button Delete
A click on this button deletes the selected row completely. Undoing is not possible!

Button Display
A click on this button calls up the Dialog Box Wavelength Display where the sorting order may be changed. Additionally a new start position within the list may be defined. By means of this it is not necessary any more to page downwards so often if data of an element far below in the list shall be edited.

See:

Menu Extras (Program Development)
Program Development
Menu Extras (Scan Manager)
Scan Manager

11.4.8 Dialog Box Interference Library

No description to this dialog box available.

11.4.9 Dialog Box Master-Standardization

No description to this dialog box available.

11.4.10 Dialog Box Wavelength Display

This dialog box is used to sort and select the list starting point for dialogs where a list of available spectral lines is displayed. The dialog box is called-up through the button *display*:

a) in the program development via the Menu Extras and the Dialog Box Line Library
b) in the program development via the Menu Instrument, *installed lines* and the Dialog Box Installed Lines, dialog box *line library*
c) in the scan manager via the Menu Extras and the Dialog Box Line Library
d) in the scan manager via the Menu Measure and the Dialog Box Select More Lines for Scanning

The dialog box contains the following dialog elements:

Group Box Sort Mode

Group Box Element + Wavelength / Element + Sensitivity / Wavelength
You define the sorting of the list of spectral lines by selecting one of these boxes. Depending on the position of calling-up the dialog, the last two check boxes may possibly not be available.

Check Box Best Lines
The limitation to display only the best lines (line proposal) is canceled by removing the mark from that box.

Check Box First Lines / Last Lines
Here you put the starting point in the list of spectral lines to the list start or list end. Depending on the position of the call-up of this dialog, the check boxes may possibly not be available.

Group Box Starting Point

Edit Field Element
You place the starting point in the list onto the first entry of the element which is entered in the field *element*, sorted according to the above mentioned special features. You can only make entries in this field, if the position of the call-up allows a variation of the element and the sorting criterion contains the element.

Edit Field Start Wavelength
You put the starting point in the list onto the wavelength, which is entered in the field *start wavelength*. The start wavelength may be valid for a single element or globally independent from any element. This depends on the sort criterion selected above.

Edit Field Sensitivity
You put the starting point in the list onto the minimum sensitivity, which is entered in the field *sensitivity*. The sensitivity may be valid for a single element or globally independent from any element. This depends on the sort criterion selected above.

Button OK
Click on this button to close the dialog box and to accept the current settings.

Button Cancel
Click on this button to close the dialog box with no resorting of the list of spectral lines.

See:

Dialog Box Installed Optics
Menu Instrument (Program Development)
Menu Extras (Program Development)
Program Development
Dialog Box Select More Lines for Scanning
Menu Instrument (Scan Manager)
Menu Extras (Scan Manager)
Scan Manager

11.4.11 Dialog Box New Standardization Sample

This dialog is used to replace standardization samples for the loaded Analytical Program. The dialog box is opened with the menu item **New Standz Sample** in the Menu Extras in the window on Program Development. The replacement of a standardization sample becomes necessary in that moment the standardization sample currently used is spent or lost. The replacement standardization sample may have the same or another name. The dialog box displays on the right half all available standardization samples of the respective Base, on the left side the samples currently used for standardization. At first make sure the new sample is existing in the standard sample library. If this is not the case enter the new standard with the button 'List'. The Dialog Box Standards Library is displayed. In this dialog box you can define new standards. In case you cannot find a previously defined standard, check whether the set filter suppresses the display of the standard you are looking for. The filter may be changed with the button 'Filter'. To replace a standardization sample, mark at first the sample to be replaced in the list box 'Selected samples'. Then highlight the new standard in the list box 'Proposed samples' and click the button <-Replace. The name of the new sample is displayed now behind the name of the old sample in brackets. After the measurement of the new standardization sample the old name is displayed in brackets. Please note the difference between calibration and standardization. This difference is explained in the glossary under Calibration and Standardization. the dialog box contains the following dialog elements:

List Box Selected samples
The box displays the standardization samples used. In case two names are inserted in one row, the name of the sample which is not used is put in brackets.

Button <-Replace
Click the button to replace the highlighted sample in the list box 'Selected samples' by the highlighted sample in the list box 'Proposed samples'. The name of the new sample is displayed in brackets behind the name of the sample currently used.

Button Parameter
A click on this button opens the Dialog Box Channel Parameter for Standardization Sample. You may here adjust parameter on standardization for the sample which was marked in the list box 'Selected sample'. This button is enabled after marking an entry in the list box 'Selected sample'. A multi-marking in the list box 'Selected sample' is not supported by this function. In case you marked several entries nevertheless, Dialog Box Channel Parameter for Type Standardization Sample is displayed only for the first marked sample.

Button Measure
A click on the button starts the measurement of all marked new standardization samples.
The intensity values determined are stored in the file of channel parameter as new
standardization setpoints of the new sample. The button 'Measure' is enabled after an entry
in the list 'Selected samples' was marked.

List Box Proposed Samples
The list box displays the available standards of the base to which the current edited
Analytical Program is assigned to. The standards may be taken into the list box 'Selected
samples'. Mark the sample which shall be used as replacement sample. Calling the dialog
the list box 'Proposed samples' displays all defined standards of the type standardization
sample. This list may be very extensive, consequently there is the possibility to display
standards with definite features. Please use the button 'Filter'.

Button OK
Click this button to shut down the dialog box. The selected samples are stored as
standardization samples for the Analytical Program.

Button Cancel
Click this button to shut down the dialog box without reading-in the changed entries.

Button Print
Click the button to print a list of all standardization samples used for the current Analytical
Program.

Button Edit
This button opens the Dialog Box Edit Standard Samples. Here you can change the type
of standard, the concentration values and written comments on the standards. Type of
standard means the intended use of a standard: e.g. calibration standard, type calibration
sample, standardization sample, type standardization sample, control sample. One standard
may cover several types of samples.
It is not possible to create new standards in this dialog box. Please use the button 'list'.
This button is enabled when an entry in the list box 'proposed samples' was marked before.
Multi-marking in the list box 'proposed samples' are not supported by this function. In case
you marked several entries nevertheless, the Dialog Box Edit Standard Samplesis
displayed for the first highlighted sample.

Button List
The button opens the Dialog Box Standards Library, which displays a list of all standard
samples, similar to list box 'Proposed samples'. Here you may edit standard data, similar to a
click on the button 'Edit'. In contrast to this in this dialog box you may define new standards.
The dialog called from this window may also be called with the menu item 'Sample list' in the
Menu Extras / Standards Library.

Button Filter
The button opens the Dialog Box Filter Settings for Standards Libary. This dialog box is
used to select definite standards to be displayed in the list box. The display may be limited to
e.g. all standards which are of a standardization sample type.

See:

> Carry out a Standardization
> Dialog Box Standardization Data
> Menu Extras
> Program Development

11.4.12 Dialog Box Automatic Program Selection

By means of the dialog box 'Automatic program selection' you may edit the switchover from the orientation programs with maximum 1 orientation program per Base to the specific analytical programs of the same base. In this dialog you define the program name. In the Dialog Automatic Program Selection, Concentration Ranges which is positioned one level below and which is called-up from this dialog, you may define the concentration ranges used as switchover cirterion for the respective elements. You may open this dialog box in the menu Menu Extras of the Program Development. For more details on the automatic program selection please refer to Automatic Program Selection in the glossary. The dialog box contains the following dialog elements:

Group Box define automatic program selection

Combo box Orientation Program
Here you may select the orientation program. If you didn't define and store a program as orientation program, the list of the combo box is empty. To check whether a particular program is defined as orientation program, you should open the **Dialog Box Global Parameter.**

Combo box Analytical Program
At first select an accompanying analytical program. All programs are displayed which have the same base like the orientation program.

Button Paste
Click on this button to insert the settings conc. the orientation program and analytical program done above into the table below. After the click on this switch the next analytical program is proposed for selection in the list.

Group Box select program for automatic program selection

Table of program switchovers
A double click onto a table line opens the **Dialog Box Automatic Program Selection, Concentration Ranges** similar to the button 'Edit'.

Column field Use
Unmark this check box if you want to deactivate the switchover between the programs of this line temporarily.

Column field Orientation Program
Here you see the selected orientation program

Column field Analytical Program
Here you see the assigned analytical program.

Column field Date and Time
Here you see the date and time of the effected assignment.

Button OK
Click on this button to close the dialog box and to accept the modified entries.

Button Cancel
Click on this button to close the dialog box with no acceptance of the modified entries.

Button Edit
Click on this button to define the element criterion for the switchover. the Dialog Box Automatic Program Selection, Concentration Ranges opens.

Button Delete
Click on this button to remove the highlighted row from the table.

Button Print
Click on this button to print the table.

See:

Dialog Box Global Parameter
Menu Extras
Program Development

11.4.13 Dialog Box Auto. Program Selection, Concentration Ranges

By means of this dialog box you may edit the criteria for switching from orientation program to a specific analytical program. The concentration ranges recorded here are used as switching criteria. For further details please refer to the glossary under the head word Automatic Program Selection. The name of the orientation program and the current specific analytic program is viewed in the header line of the dialog. The dialog is called-up through the Dialog Box Automatic Program Selection. The dialog box contains the following dialog elements:

Table field element list
You may define in this Table the elements and their concentration ranges, provided that they shall be switching criteria. The table contains the following columns:

Column field Element
In this combo box you may select the elements. The list of the combo box supplies you with all elements for selection of the analytical program.

Column field Use
Unmark the check boxes of the elements which you temporarily want to disable as criterion for switching.

Column field Unit
elect in these combo boxes the units of the concentration data for the respective elements. Units displayed in the list part of the combo box, are stored in a parameter file. The units ppm, parts per million, and ppb, parts per billion, are linked with conversion factors for the base unit % in the system. You may switch between these units; the values are always displayed in the correct scale.

Column field Upper Limit / Lower Limit
Enter here the concentration limits, which are used as switching criteria.

Button OK
Click on the button to close the dialog box. The changed entries are stored.

Button Cancel
Click on the button to close the dialog box. The changed entries are not stored.

Button Cut
Click on the button to delete the entire active row.

Button Delete
Click on the button to delete the highlighted area in the table field.

Button Paste
Mark in the table field an area with several rows and click on this button to copy data from the first highlighted row into the other highlighted rows.

Button Print
Click on this button to print the table.

See:

Dialog Box Automatic Program Selection
Menu Extras
Program Development

11.4.14 Dialog Box User List and Passwords

5 user levels are implemented in the system, each with different access authorization for program parts and menus. The access levels are structured as follows:

A. Service (access for SPECTRO service for basic device settings)
B. Supervisor (access for responsible person for the stationary metal analyzer)
C: Level 1 (analyst)
D. Level 2 (shift leader)
E. Level 3 (employee)

The access of users of level 2 is limited to the Measure Window and sample management. Users of level 3 have access only to the Measure Window. The assignment of different access levels to the personnel operating the stationary metal analyzer prevents unauthorized change of sensitive program parameters and settings. Starting the spectrometer software, the operator has to enter his name and his password. In case no valid entry was performed, the spectrometer program aborts. A summary of the accessible menus for the different user levels may be taken from Software Structure.

A new incorporation of users and change of access levels can only be performed by the supervisor and the service. The password for the access to the service level is a combination of the password of the service (known exclusively by Spectro) and the password of the supervisor. Both passwords are entered one after the other linked by a hyphen (-).

The dialog box 'User list and password', displayed for the levels 'Service' and 'Supervisor', shows a list of all registered users and facilitates the correct assignment of the users to the levels. This dialog box is described below. Users of level 1 have no access to this dialog, the Dialog Box Edit User and Password opens automatically. Users of level 2 and 3 have no access to program development; there is neither an access to dialog box 'User list and password' nor to dialog box 'Edit user and password'.

The dialog box contains the following dialog elements:

Group Box Current User Data
The two fields in the first row display the current user and the access level. The edit field below displays the name of the company the spectrometer software is licensed for. Because this field is an edit field you may adapt the name in case of a company change.

Group Box Complete User List
The group box displays the list of all registered users together with the assigned user levels.

Edit Field User
The edit field displays the name of the user, whose adjustments on the access level shall be modified. The displayed name may be changed. Quitting the edit field the changed name is displayed in the list box 'User name and level'.

Combo Box Access Level
In this field you enter the access level of the respective user.

List Box User and Level
Here you see a complete list of all registered users and access levels.

Button OK
Click this button to shut down the dialog box and to read-in the changed settings on users and access levels.

Button Cancel
Click this button to shut down the dialog box without reading-in the changed entries on users and access levels.

Button New User
Click this button to define a new user. The Dialog Box Edit User and Password is opened.

Button Delete
Click the button to remove a user from the list.

Button Password
Click the button to change the password for the user selected. The Dialog Box Edit User and Password is opened.

See:

Menu Extras
Program Development
'Software Structure'

11.4.15 Dialog Box Edit User and Password

The dialog box 'Edit user and password' is used to enter new users and to change passwords. The dialog box is called up by users of access level 1 directly from the menu Extras (program development). Users of access level 'Service' and 'Supervisor' may open this dialog box through the preceding Dialog Box User Information.
The dialog box 'Edit user and password' contains the following dialog elements:

Group Box User Name and Level
The two **display fields** in the first row view the current user and the access level. Provided that calling up the dialog box is effected through the button 'New user' in the dialog box 'User list and passwords', the first field is an edit field to enter the user name, the second field is a combo box to select the access level.

Group Box User Identification
This group box is only visible for users of access level 1.

Edit Field Current Password:
Enter your current password. This is required to change your password.

Button Check:
After entering your password into the edit field 'Current password' click this button to check the entry. Provided you had entered the password correctly, you may access the edit fields in the group box 'Password'.

Group Box Password
Here you enter your new password.

Edit Field New Password
Type in your new password. The minimum length is 4 characters, the maximum 15.

Edit Field Retype Password
Then enter the new password in this edit field again. The repetition shall avoid typing mistakes during the entry which could lead to passwords of unknown shape, even for you.

Button OK
Click the button to shut down the dialog box and to read-in the changed password and user entry respectively.

Button Cancel
Click the button to shut down the dialog box without reading-in in the changed password and user entry respectively.

See:

Menu Extras (Measure Window)
Menu Extras (Program Development)
Measure Window

Program Development

11.4.16 Data Backup

A regular data backup should become a matter of routine for you. You may compare that data backup with the safety belt in your car. Hopefully you will never need it, but if the worst comes to the worst, it may be of inestimable value.

For example you will need the data backup if you had carried out extensive changes on settings and analytical programs of the Spectrometer software: now you may used the stored data to set back the system in its original state. Furthermore you will need the data backup for the case of a defect hard disk of the Spectrometer computer, which cannot be excluded. A new hard disk may be easily purchased. But what about the analytical programs, the standard samples files, the alloy grade library without data backup? Remember the time you had investigated for creating and optimizing these data!

Straight after finish of setup work you should accomplish a complete data backup of the entire Spectrometer directory from the hard disk and store it at a save place. So you get the possibility to retrieve the original installation condition at any time.

You may limit further data backups to files which were subject to changes. Save the subdirectories GENLIB, INSTDATA, METH, SETS, and STATUS.

When you store analysis results, the data are filed in the subdirectory RESULTS\NUMERIC. If you want to save the data, you should incorporate this subdirectory into the backup too.

If your SPECTROLAB-S is equipped with a Monochromator, you may store scans. You find them in the directory RESULTS\SCANS.

The backup is effected by a program which is part of the operating system Windows. In case of Windows 95 it is the program BACKUP.EXE, in case of Windows 3.11 it is the program MWBACKUP.EXE. The programs may be called-up directly from the Windows desktop. Even easier is the call-up via the Menu Extras of the program development. The menu items **Backup** and **Restore** call-up the respective programs. The precise program name and the path are stored in the Parameter File PS_GEN.ASC Depending on the configuration of your Spectrometer you may enter there the program name and path. Your partner at SPECTRO will support you with pleasure.

A selection of directories to be saved may be stored in catalogs of the data backup programs. If you call-up a program, you may add the catalog name and the backup will nearly run automatically.

Finally a nearly self-explaining remark: The data backup is not suitable for transferring analytical programs from one Spectrometer to another. Generally hardware and channel equipment are different, but the sensitivity of the photomultipliers are definitely not comparable.

The menu items **Export program** and **Import program** provide another possibility to save the analytical programs in the Menu Extras of the program development.

See:

Dialog Box Export Program
Dialog Box Import Program
Menu Extras
Program Development
Maintenance

Additional Maintenance

11.4.17 Dialog Box Program Import

This dialog box is used to re-import analytic programs which were exported before. The data source is a file named METXXXXX.EXP, which is generated during export of the programs (see Dialog box Program Export). XXXXX represents a five-digit figure which is identified by the analytic program. The import file may be on each drive (floppy drive, hard disk, and CD-ROM drive, provided the CD-ROM drive is equipped with the ability to write). Analytic programs may be exported to store them as data safeguarding.
Please note: The program export and later import will only give consistent data, if fundamental installation data, like installed lines and installed optics, are unchanged in the meantime! The dialog box contains the following dialog elements:

List box Programs to be imported
The list box displays the exported analytic programs which are stored under the selected drive and directory. The selected directory is displayed below the list box. It is the directory which was currently used for an export. In case the directory used for the last export is a floppy disk, the programs may only be displayed when the floppy disk is inserted. The following information is given about the programs:
Program name, Date of Export, Last Changes of the Program before the export and the current state of the same program on the hard disk. The current state of the program is displayed under the header **Existing Program, last Changes**. In case the method in the program data base of the device is deleted, the word **deleted** is displayed. Otherwise the date of the last change is shown. Please note: If you import a program, which is currently loaded in the program development or in the Measure Window, the program continues to be loaded. To get the imported program into the main memory, you have to load the imported program from the program data base of the device. You may use the Dialog box Load Program, which you can open by means of the menu item **Load program** of the menu **File**. To import programs from another spectrometer is impossible. The software recognizes the device, the program data come from. Programs which were generated by another spectrometer, cannot be loaded. Reason is that each analytic program is individually tailored on the device. Other spectrometers may have different assignment on selective channels and optic parameters. Even if two spectrometers are identically built-up, it is not possible to interchange analytic programs. The intensities, which are measured for a channel, may differ significantly between identical detector types.
Select one or more programs to be imported. Click on the respective program. If you would like to import more than one program, click on the next program immediately. To undo a selection, click on the respective entry again.

List box Source Directory
This field displays the drive and the directory, the program will be imported from. The source directory is selected by means of the combinational field 'Change source directory'.

Combinational field Change Source Directory
Select the drive and the directory the analytical program is to be imported from. The selected directory is displayed in the above list box 'Source directory'. The list part of the combinational field displays the available drives of your computer (e.g. [-a-] and [-c-]) as well as the directories below. Clicking the entry [..], you move up one directory level.

Button OK
Click this button to carry out the import of the highlighted analytic programs. An additional question is displayed and you are asked to confirm the import once again. In case the imported program still exists in the program data base of the device, a respective message is displayed together with the option to overwrite the existing program.

Button Cancel
Click this button to shut down the dialog box without export a program.

See:

SPECTRO

Dialog box Program Export
Menu Extras
Program Development
Measure Window

11.4.18 Dialog Box Program Export

This dialog box is used to export analytic programs. The export may be effected to a floppy disk, a hard disk, and of course a CD-ROM, provided a CD-ROM drive is installed with the ability to write. Analytic programs may be exported to store them as data safeguarding. Consequently you are able to retrieve a defined level of the analytic programs at any time. This may be advantageous when you want to redo changes in an analytic program. Additionally you may restore your analytic programs in case of a faulty hard disk. To export an analytic program may take some minutes, especially if you want to export standard intensities too. The data occurrence for a single analytic program may be relatively high in case standard intensities shall be exported. This is why the error message 'Disk full' may be given during the exportation. In this case make the export to a directory of the hard disk. Using the BACKUP.EXE of Windows you may store this file on one or more floppy disks. The file, which is written during export and which contains the exported data, is named METXXXXX.EXP. XXXXX is a 5-digit figure identified by the analytic program. To import programs which were exported before, is carried out with the Dialog box Program import . Please note: The program export and later import will only give consistent data, if fundamental installation data, like installed lines and installed optics, are unchanged in the meantime!

Note:
A complete data record of your Spektrometer consists of more than just the analytic programs. This is why you should take care for a complete basic backup, which comprises e.g. the alloy grade library too.

The dialog box contains the following dialog elements:

List box Export program(s)
This list box displays all analytic programs which are stored in your Spektrometer. Select one or more programs you want to export. Click on the program to be exported. If you want to export more than one program, click the next program immediately. To undo a selection, click the program once again.
List box Target Directory
This field displays the drive and the directory, where the program will be exported. The target directory is selected by means of the combinational field 'Change target directory'.
Combinational field Change Target Directory
Select the drive and the directory the analytical program is to be exported. The selected directory is displayed in the above list box 'Target directory'. The list part of the combinational field displays the available drives of your computer (e.g. [-a-] and [-c-]) as well as the directories below. Clicking the entry [..], you move up one directory level.
Check box Export Standard Intensities
Mark this check box if you want to export standard intensities together with the other program data. Standard intensities are measured during the Calibration and are necessary to edit and to draw a graph of the calibration curves in the Regression Program. Provided that the program to be exported is a Global Standardization Program, the intensities of the standardization are exported too. When you export standard intensities, the export file may become very big.
Button OK
Click this button to carry out the export of the highlighted analytic programs. An additional question is displayed and you are asked to confirm the export once again. After the export of

each analytic program you are asked whether you want to delete the exported program from the program data base of the device. In case a program exists as an exported program on the target directory, a respective message is displayed together with the option to overwrite the existing program.

Button Cancel

Click this button to shut down the dialog box without export a program.

See:

Dialog box Program Import
Menu Extras
Program Development
Regression

12 Regression

The window on regression is called up from the window 'Program Development'. For each Logical Channel the equipment- and application specific calibration curves of your stationary metal analyzer are calculated and optimized. Calculating the calibration curves is performed by a Regression Calculation.

The screen of the regression displays a **data window** and a **graphic window** for one Channel simultaneously. Up to 20 channels may be loaded into the regression window at the same time. Consequently up to 20 data windows and 20 graphic windows are open simultaneously. Calculations are always performed on just one channel. If several channels in the regression window are open, the current channel is identified by the blue-highlighted heading of the graphic or data window.

Please find more details about the contents of graphic- and data windows below. But at first a description of the **menu**, the **tool bar** and the **status bar** are given.

In case the window for regression is active, the following menus are displayed:

→ Menu File
→ Menu Program
→ Menu Regression
→ Menu Window
→ Menu Help

Additionally the window for regression displays a **tool bar** for functions often used. The function is carried out by easy clicking on the respective icon. Obviously all functions of the tool bar may be called up by triggering the resp. menu item in the menu of the regression screen.

The following icons are available:

Click on this icon to display the Graphic Window and the Data Window of the current channel side by side on the screen. In case the graphic window is not active, it will be opened automatically. This icon corresponds to the menu item **Data & Curve** in the Menu Window.

Click on this icon to display the Data Window of the current channel in full-frame mode. This icon corresponds to the menu item **Data** in the Menu Window.

Click on this icon to display the Graphic Window of the current channel in full-frame mode. In case the graphic window is not active, it will be opened automatically. This icon corresponds to the menu item **Curve** in the Menu Window.

Click on this icon to display all opened windows in cascade mode. This icon corresponds to the menu item **Cascade** in the Menu Window.

Click on this icon to display all opened windows side by side simultaneously. This icon corresponds to the menu item **Tile** in the Menu Window.

Click on this icon to perform a new calculation of the Calibration Curve. This icon corresponds to the menu item **Calculate** in the Menu Regression.

Click on this icon to adjust filter settings for use of Calibration Samples. This icon corresponds to the menu item **Filter settings** in the Menu Regression.

Click on this icon to set calculation parameters. This icon corresponds to the menu item **Calculation model** in the Menu Regression.

Click on this icon to calculate a linear calibration function. This icon corresponds to the menu item **Linear model** in the Menu Regression.

Click on this icon to calculate a square calibration function. This icon corresponds to the menu item **Square model** in the Menu Regression.

Click on this icon to calculate a cubic calibration function. This icon corresponds to the menu item **Cubic model** in the Menu Regression.

Click on this icon to accept the calibration of the active channel. This icon corresponds to the menu item **Accept** in the Menu File.

The Status Bar is displayed down on the screen. It is divided into five fields. The first field displays the currently loaded analytic Program. The next field informs about the model of the Calibration Function. Possible alternatives for the selected calibration-polynomial functions are linear, square or cubic and automatic respectively, if the program selects the calibration function independently. The third field displays the weighting of the individual calibration samples. The next field in the status bar informs whether an Interference Correction (inter element correction) is carried out. The following texts are displayed depending on the case: Without IEC, with IEC, with IEC (locked). You may find details in the helptext Menu Regression. The fifth field displays the filter used on the selection of the calibration standard (Calibration Sample). There are two options: global filter and local filter.

### Operating the regression program

After calling up the regression program and selecting one or more channels with the **Dialog Box Load Channel**, the data window of the current channel is displayed. In case you had selected more than one channel, you may display the windows of the non-visible channels

with the **Menu Window** or the symbol buttons or .
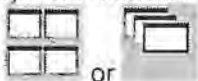
Apart from the data window, the window containing the graphic display of the calibration curve (graphic window) may be called-up for each channel. You open the window with the
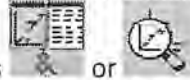
Menu Window or with the symbol buttons ⬚ or ⬚ on the tool bar.

Optimize your calibration curve by careful selection of the calculation (polynomial rank, weighting model) and a manual weighting of sample, if necessary. Please note that a higher polynomial rank does not automatically lead to a better fitting of the calibration curve to the calibration sample, even if standard error and correlation coefficient seem to prove it. Channels being linked with a Line Switch are to be checked carefully on the continuity of the calibration curves. Avoid definition gaps in the calibration range! The calibration ranges have to be preset by means of the Dialog Box Calibration Range.

Interferences of several elements amongst themselves are recognized in the Regression Calculation. To be able to do so, possible interfering couples have to be pre-determined either channel-specifically in the Dialog Box Interferences of the Menu Regression or globally in the Dialog Box Global Interferences of the Menu Program. The interferences are now calculated by the program. To determine the interferences especially Binary Samples are suitable. However the determination of interferences is not limited to binary samples. All selected calibration samples are used to calculate the interferences.

The **Data Window** displays in the upper part numerical and narrative details about the calibration curve. See also Data Window for more information.

The **Graphic Window** displays the calibration curve of the current channel. See also Graphic Window for more detailed information.

Link between graphic window and data window

Clicking single symbols in the graphic window selects the respective standard in the data window. Reversely a selection of a standard in the data window causes a marking the respective symbol in the calibration curve. Select a simultaneous display of graphic and data

window by means of the symbol button ⬚ on the tool bar.

See:

Regression Calculation
Data Window
Graphic Window
Program Development

12.1 Regression Calculation

Description of the calculations used in the regression module for Spark Analyzer

To calculate the calibration curve the method of least squares is applied.

Method of Least Squares
A polynomial curve is fitted to the measured samples based on their measured intensity and the entered concentration. The method to fit a curve to these points is "method of least squares" which means that the sum off all squared distances between the curve and the points is minimized.

A third degree polynomial could be expressed us:

$$y_i = b_0 + x_i * b_1 + x_i^2 * b_2 + x_i^3 * b_3$$

where i represents the running sample number, y the concentration, x the intensity and b the equation factors.
The function to be minimized could be expressed as:

$$\sum_{i=1}^{n}(y_i - (b_0 + x_i * b_1 + x_i^2 * b_2 + x_i^3 * b_3))^2$$

or in a matrix form:

y = X*b+f

where f is the distances between point and curve.
The solution to this could be expressed as:

$$b = (X'*X)^{-1} * X' * y$$

Weighted regression
Giving certain samples in the regression more importance is called weighting. In the calculation this is done by adding a weight vector to the expression above. The solution will be changed into:

$$b = (X'W^{-1}X)^{-1} X'W^{-1}Y$$

Now any weighting method is easy to apply, manual entry, 1/◆Int², 1/Conc, 1/Int, etc.

Inter Element Corrections (IEC)
To correct for influences from one element to the other, called inter element corrections, certain corrections are applied.

The correct for spectral overlap:

$$Int_i = Int^0_i + f_{ij} * C_j$$

Where Int^0_i is the measured intensity, Int_i the corrected intensity, f_{ij} the correction factor and C_j the concentration of the disturbing element. The correction is often called additive or translational because of that the effect is not dependent on the concentration of the disturbed element. In almost any case the correction factor will be negative when the correction formula is defined as above.

Interferences caused by plasma effects can often better be corrected by:

$$Int_i = Int^0_i * (1 + f_{ij} * C_j)$$

Now the effect is also depending on the concentration of the disturbed element. This correction is often called multiplicative or rotational and occurs with both positive and negative correction factors.

If these correction model is added to the calibration curve above the original equation:

$$C_i = a_{i0} + a_{i1} * Int_i + a_{i2} * Int_i^2 + a_{i3} * Int_i^3$$

into:

$$C_i = a_{i0} + a_{i1} * (Int^0_i + f_{ij} * C_j) + a_{i2} * (Int^0_i + f_{ij} * C_j)^3 + a_{i3} * (Int^0_i + f_{ij} * C_j)^3$$

This will cause a non linear equation system as i.e.

$$a_{i1} * (Int^0_i + f_{ij} * C_j)$$

is equivalent to:

$$a_{i1} * Int^0_i + a_{i1} * f_{ij} * C_j$$

And now two unknown variables a_{i1} and f_{ij} are not added but multiplied.

To solve the non linear system it is divided into two steps, first the calibration curve is calculated and after that the correction factors. This procedure is repeated automatically until the fit is not improved anymore.

Correlation Coefficient and Standard Error

To be able to quantify how well a curve fits the calibration samples, two measures of fit can be used, the correlation coefficient and the standard error of estimate.

The correlation coefficient is defined as:

$$r = \sqrt{\frac{\sum(C_{ber} - C_{mittel})^2}{\sum(C_{zert} - C_{mittel})^2}}$$

where C_{ber} is the calculated concentration, C_{zert} the certified and C_{mittel} the average concentration of the set of samples. The correlation coefficient is without dimension and therefore not affected by concentration interval etc. It is normally very close to 1.

The standard error of estimate (SEE) is calculated as:

$$SEE = \sqrt{\frac{\sum_{i-1}^{n}(C_{i,zert} - C_{i,ber})^2}{n - m - 1}}$$

where $C_{i,zert}$ is the certified and $C_{i,ber}$ the calculated concentration. N is the number of samples and m the number of variables used in the regression, n-m-1 is the so called *degree of freedom*.

Error Messages during Regression Calculation

In case not enough samples were measured to be able to carry out the calculation for the preset calculation model, an error message **"not enough standards"** is displayed. To calculate a n-degree polynomial n+1 data points are necessary. Consequently a square polynomial requires at least 3 data points (measured samples). Each interference to be recognized requires another data point.

In case the calculation of the calibration function cannot be carried out due to other reasons, the error message **"Singular Matrix"** is displayed.

See:

Measurement Evaluation
Regression
Data Window
System Description

12.2 Menu File (Regression)

This menu is used to load channels for the regression, to accept and todiscard operation results, to call-up printer operations, to stop the regression program. The following menu items are available:

→ **Load Channel**

Select this menu item to open the Dialog Box Load Channel (Regression). By means of this dialog box you may load individual channels for the regression. You may call-up this menu item with the shortcut <F4> too.
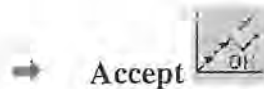
→ **Accept**
Select this menu item or click on the icon displayed to store the regression data of the active channel. Note: here is no possibility to undo the storage! After closing the regression window and the program development, the system prompts you to store the changed program. Then the regression data become component of the analytic Program.
Tip: work on the regression data always in a copy of the analytic program. So you get the possibility to use the original analytic program again, if the modifications proof to be disadvantageous.
You may call-up this menu item with the shortcut <F9> too.

Note once again: The regression data are the key data of the spectrometer. Faulty determination of the calibration curves influence the accuracy of the analysis results immediately!

→ **Discard**
Select this menu item to discard the regression data of the active channel without storing them. The data window and the graphic window - if opened - of the channel are closed.

→ **Print Data**
Select this menu item to print the regression data of the active channel. You may call-up this menu item with the shortcut <Ctrl>+<P> too.

→ **Print Curve**
Select this menu item to print the graphic display of the Regression Curve of the active channel. You may call-up this menu item with the shortcut <Ctrl>+<G> too.

→ **Print All**
Select this menu item to print the regression data and regression curves of all Channels of the Analytic Program. It is not necessary to load the channels into the regression program. The regression program loads the channels for the print operation one after another automatically. You may call-up this menu item with the shortcut <Ctrl>+<A> too.

→ **Exit**
Select this menu item to shut down the regression program. Changed calibration curves are not automatically accepted by the program development. Consequently you should not forget to store the modified calibration curves you want. By means of the menu item **Accept** (s.a.) you may store individual calibration curves.

See:

Regression
Program Development

12.2.1 Dialog Box Load Channel (Regression)

This dialog box is used to load single channels to be edited in the regression program. It opens automatically as soon as the regression program is called-up. Additionally the dialog box may be opened in the window Regression with the Menu File to edit further channels. The dialog box contains the following dialog elements:

Table Field Logical Channels for Regression

In this Table you select the channels to be edited. The selection is done by a click with the mouse cursor on the respective table row. To undo the selection click another time on the row. You may load 20 channels max. to be edited in the regression program. When you call-up this dialog into the regression program to load further channels for edition, you only need to mark the new channels. Channels marked before remain opened. They are not loaded again to preserve the determined regression data. To edit the data in the columns is not possible. The table contains the following columns:

Channel

In this column you see the names of the analytic channels, entered in the Dialog Box Channel Parameter.

Wavelength

In this column you see the wavelengths of the spectral lines which are connected with the analytic channels.

Low Limit, High Limit

In this column you see the lower and upper calibration range to be edited in the Dialog Box Calibration Ranges in the Menu Program.

Accepted

These check boxes indicate whether a channel had been already stored together with its calibration function (accepted). The storage may be effected with the menu item **Accept** in the Menu File.

Button OK

Click on this button to shut down the dialog box and to load the selected channels into the regression program. At first the Data Window is opened for the selected channels.

Button Cancel

Click on this button to shut down the dialog box. No further channels are loaded into the regression program to be edited.

See:

> Menu File
> Menu Program
> Menu Regression
> Regression
> Program Development

12.3 Menu Program (Regression)

This menu contains menu items to view and to modify data of the analytic Program, as far as they are of significance in the regression window. The called-up dialog boxes are identical with the dialog boxes you call-up in the Program Development for that purpose.

➡ **Element Parameters**

Select this menu item to open the Dialog Box Element Parameters and to edit the parameters for the elements. You may call-up this menu item with the shortcut <Ctrl>+<2> too.