

Thermo Scientific OXSAS

X-ray fluorescence analysis software

Thermo Scientific™ OXSAS software is the most modern software for X-ray fluorescence spectrometers. This innovative platform sets a new milestone in analytics thanks to its many convenient features. Ease of use is what you can expect from OXSAS, no matter what your requirements are. From simple tasks to complex jobs, all are defined easily and performed quickly.

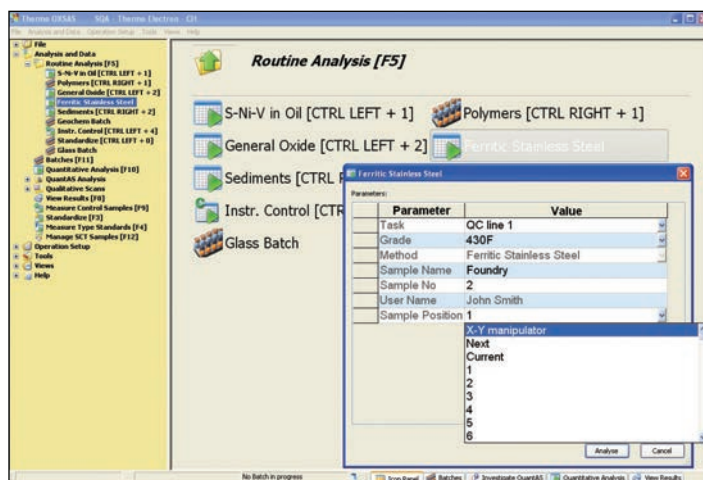


Figure 1. Routine analysis

With OXSAS, you can set up and carry out all your analysis jobs easily and quickly. And you can do a lot more. OXSAS is the most modern software for X-ray fluorescence spectrometers and shares functionality and design with its OES version. It implements state-of-the-art technology and software foundations. This makes it very powerful and easy to use. Your needs will expand in the future and you expect that your software will provide you with up-to-date solutions over the years. OXSAS is a new software platform that is designed to evolve to meet your needs throughout your instrument's lifetime.

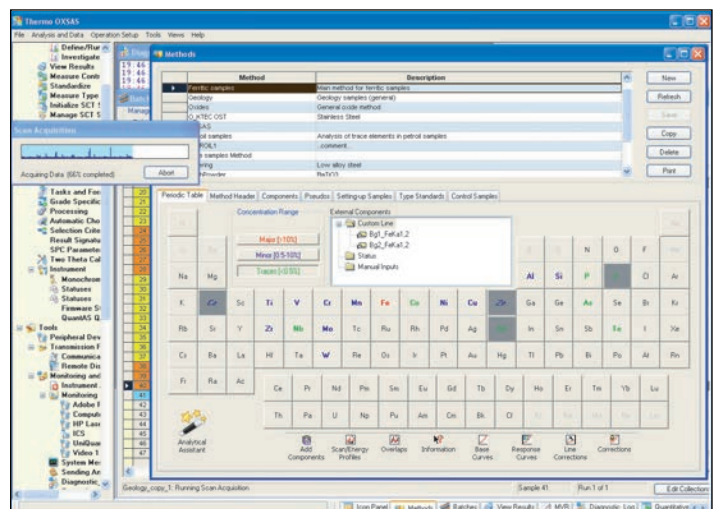


Figure 2. Modern, state-of-the-art User Interface for comfortable and powerful operation.

Key features and top benefits

- With OXSAS, you can perform rapid high quality analyses: routine analysis shortcuts lead you through the analysis operation
- Simple definition and comprehensive operation of sample batches. With support of priority samples. Makes unattended analyses handy
- Integrated Analytical Assistant guides the creation or extension of methods. With best analytical parameters for rapid and accurate analyses
- Fast calibration with multiple analyte curve display, instant base curve calculation, templates for edition and measurement of calibration standards
- Measurement uncertainty* and conformance probability on unknown sample analysis results
- Optional standardless analysis packages*: Thermo Scientific UniQuant™ software and the semi-quantitative QuantAS software offer additional analysis versatility
- Optional XRD goniometer channel for phase quantification. Allows combining XRF elemental analysis and XRD phase quantification in one result
- Flexible scans with graphical investigation tools
- Optional spot analysis and mapping with comprehensive graphical facilities on Thermo Scientific™ ARL™ PERFORM'X series instruments
- Multi-purpose analysis display with wide-ranging optional data. e.g. the analysis calculation steps help the validation of your methods
- Numerous customizable on-line processing functions, with manual or automatic application
- Comprehensive post-treatment of results, including export, e.g. in Microsoft Excel® format
- Full network and serial transmission capabilities
- Real on-line integrated SPC
- SCT samples management: gives the overview of the analytical capability of the instrument and of each method any time. The SCT samples status and history allow coordination of the control and standardization run with your analyses workload and plan
- Installation and Operation Qualification (IQ/OQ) for ARL PERFORM'X series instruments
- Effective monitoring and maintenance tools maximizes the system uptime

A new era in analytical software

- Integrated design. Thanks to a proper database structure and advanced software functions, OXSAS offers many sophisticated functions that you can apply in just one click. Want to review the spectra of a QuantAS analysis? Just search it and hit the show spectra button. Need to measure standards? OXSAS gathers and sets all data needed for you
- OXSAS breaks the limits for data capacity
- A new dimension in user-friendliness. Innovative software tools greatly help the comfort and speed of operation, such as:
 - Frequently used functions can be left open, a bar enables to quickly switch among them
 - Routine Analyses shortcuts greatly simplify operator's work
 - Recent analyses are shown in tabs
 - Instant edition of data sets using fill-down and increment-down tools
- OXSAS is a multi-processing application with amazing capability and potentials
- OXSAS comprehensive functionality enables the meeting of all your requirements

Develop expert analytical methods

Integrated analytical assistant

The editor of methods integrates an analytical assistant which helps defining the best analytical parameters. You simply define the elements you need to analyze from a periodic table, their chemical form, their concentration range and additional information related to the preparation of the sample. OXSAS Analytical Assistant proposes, in turn, the best corresponding parameters, suggests the analytical corrections and prepares the batch of scans and energy profiles to investigate the possible spectral interferences. Furthermore, the Analytical Assistant can be used to add elements to an existing method. Experienced users can take advantage of the speed of the Analytical Assistant. They can also use the Advanced Edition mode for customizing specific parameters.

Advanced analysis features

You can include in your method the acquisition of instrument status during quantitative analysis. Values measured or defined outside the instrument can also be included as manual input values in your methods.

Adjust and validate methods

OXSAS includes useful tools to help users fine-tuning their methods. The Analytical Assistant helps defining scan and energy profile measurement to check for possible overlap and background corrections. The calibration standards intensity update helps refining intensity corrections, e.g. overlap and background corrections without having to re-measure the samples. For quick identification of calibration problems, OXSAS can store and display all successive calculation steps from the raw intensities through to the final concentrations.

Perform analyses

Pre-defined parameters simplify your quantitative analyses

OXSAS assists your operators in achieving the analyses easily and quickly. Each OXSAS task includes a template of parameters including the sample identification, how to perform the analysis, how to display and process their result to meet the specific requirements for each sample category. Thanks to these mechanisms, running complex analysis jobs can be as easy as selecting the matching task and completing the predefined identity.

Parameters that can be controlled:

- Selection of the default analytical method. Alternatively, type standard calibration can be used. If a grade is selected, the analysis result is checked against this target upon completion of the analysis
- Sample identification with unlimited number of fields and up to 255 characters each. Data types are various: alphanumeric, numeric, lists, auto-incrementing with increment choice, date and time, fix text and operator name. Default value, mandatory input and maximum length can be defined
- Content and format of the display: e.g. wavelength, grade limits, uncertainty data, layout, color scheme, font details, element precision and units
- Manual or automatic processing of the result at the end of the analysis such as checking the result against grade limits and sending it

Individual quantitative analyses

The analysis screen can be adapted to each need. For highest versatility, users should keep all options open to select different tasks, methods, grades or type standards. In laboratories with uniform procedures, one can hide the unnecessary options for more clarity and speed of operation.

To save time, the user can start the analysis first, then fill the sample identification.

Routine analyses

For an even easier routine operation, shortcuts can start the analysis of samples individually or in batches on one click or one key press. The matching analysis template is preselected and you can predefine the value of parameters such as the method or the sample identification. You can also select which parameters your operators are allowed to edit.

Routine analyses can also call batches and are used to insert urgent samples in running batches as well.

Flexible batches for all your analysis jobs are quickly set up

OXSAS batches enable fast definition and analysis of sets of samples. Any rearrangement such as appending samples to a running batch, inserting priority samples, moving groups of samples to change their sequence, modifying sample data and measurement parameters is done easily and quickly. A batch can be interrupted and restarted at anytime.

Batches can be prepared in advance without limitation. A scheduler enables starting predefined batches at deferred times. Batch repetition is available too.

Speed functions allows incrementing or copying the value of an analytical parameter, an ID field or a sample position over the batch at one go. Positions can be chosen from a virtual view of the sample magazine, even by ranges.

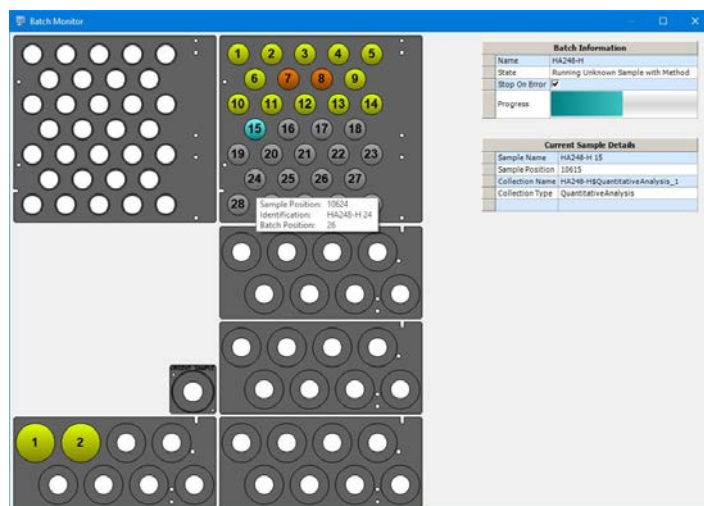


Figure 4. Batch monitoring with a graphical view of the magazine.

Setting batches of scan measurements is also very quick. The scan parameters or the processing parameters for QuantAS analyses can be adjusted directly from the batch screen.

All types of analyses and samples can be mixed in any order in a batch: quantitative, qualitative (scans), semi-quantitative (QuantAS) or standardless (UniQuant). The analysis of calibration standards, setting-up samples, type standards, control samples can also be grouped in batches.

The recurring measurement of samples such as control samples can be saved in lists for later reuse and instant insertion in any running or waiting batch. Lists can also be used as templates: they speed up the definition of the samples and the selection of their measurement parameters.

Several functions can define batches with minimum or no user input. Thanks to the built-in templates, most of the definitions are automatic. For instance:

- Calibration sample measurements
- Scans and energy profiles suggested by the Analytical Assistant for interference investigation
- Setting-up, control, or type standards that need to be measured: e.g. if their validity period has expired

Analyses defined by an external application*

Using the OXSAS option "Remote Sample Definition", sample analysis parameters and identification can be partially or entirely defined by an external application such as a LIMS. The external application can even launch the sample analysis reducing the operator's actions to sample manipulation only. It is also possible for the external application to define a complete list of samples that will be registered in a dedicated batch.

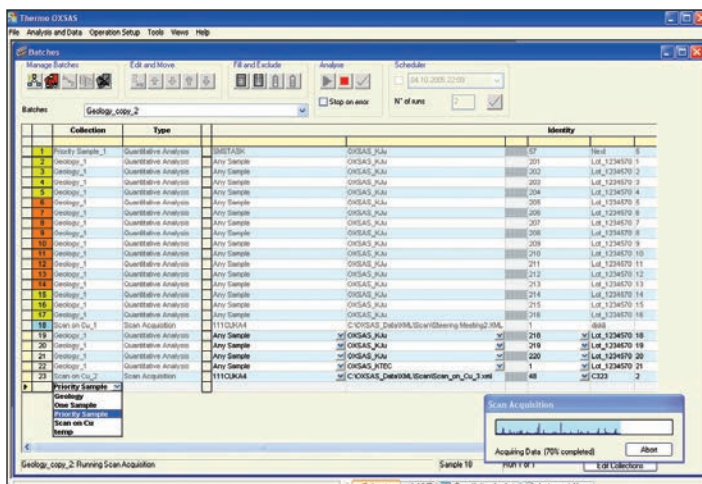


Figure 5. You can insert priority samples in batches during their execution. With powerful batch progression monitoring.

View, edit, validate and process analysis results

Upon completion of the analysis, the result is displayed according to the predefined format. The user can apply other formats for instance to check full details, such as calculation steps and non-reported elements.

Concentration values are displayed with up to 25 attributes (flags) with user definable colors and font styles, e.g. when values are out-of-calibration or above the checked grade range, and so on.

Identification and concentration of the analysis can be edited, if enabled. A result can also be recalculated, for instance using another calibration.

The result processing such as on-line transmission and grade checking, is performed directly after the analysis when set to automatic. This mode is ideal for routine analysis and batches. The processing can also be applied on user action and repeated as necessary. An operator validation can be made mandatory.

Recent analyses are shown in the analysis screen and are put in tabs next to the current one. Their access is very quick, e.g. for comparison. The next sample can even be started before processing the current analysis result.

Fast qualitative analysis

Two forms of digital scanning are available: step scanning for precise definition of peaks and continuous analysis. Multiple scans with different crystals and angular ranges can be defined and grouped per sample.

OXSAS can show all spectra of scan groups simultaneously. Automatic or manual peak identification and marking works throughout the complete group of scans. The user can also search for specific elements. The function displays as many different spectra as required: superimposed according to their range or in separate windows.

The color and thickness can be tailored for each curve. Information on each spectrum is displayed in a dedicated grid.

OXSAS allows showing the difference of multiple spectra. Background curves calculated with different polynomial can be displayed all together.

Other functions comprise zoom, scales, commenting and printing. Background positions and polynomial, 2 θ real values or even additional lines can be transferred from a scan spectrum into your methods to facilitate their setup.

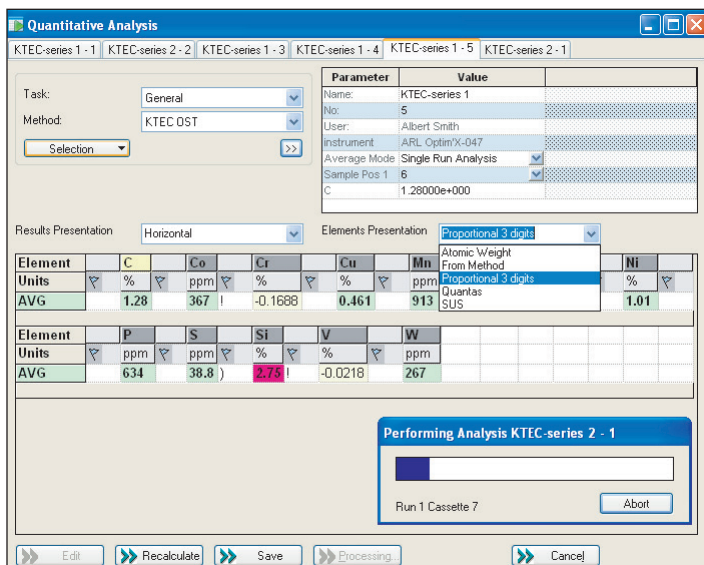


Figure 6. Recent analyses are displayed in tabs for easy access.

Integrated X-ray diffraction*

For ARL 9900 IntelliPower Series, a diffraction goniometer channel can be mounted inside the instrument. XRD quantified phases are automatically returned to OXSAS in order to produce a combined result with the XRF analysis.

Acquisition of the XRD diffraction channels is fully integrated in the XRF analysis. Consequentially, the sample must be registered only once in the system and all the powerful OXSAS analysis and result processing features are also available for combined XRF-XRD analyses: shortcuts, batches, grade check, result transmission and export, etc. This integrated solution is unique and is particularly valuable for process control monitoring.

Total elemental analysis

QuantAS*: Quantitative Analysis using Scans

Concentration levels in liquid or solid samples can be determined through the user-friendly optional QuantAS package. Five scans covering the spectrum of 70 elements from F to U are performed.

Smoothing, background subtraction, peak identification, overlap and matrix corrections, calculation of concentrations and normalization are done automatically for a fast and easy semi-quantitative analysis of unknown samples. Various options, like the calculation of an unanalyzed element or compound and Type standardization are available for ultimate accuracy.

QuantAS spectra can be viewed similarly to scan spectra and the user can interact with the peak identification procedure. Analysis results obtained by QuantAS can be processed just like any quantitative analysis.

Scan spectra and QuantAS spectra are stored in XML format enabling their exchange with other applications.

UniQuant* state-of-the-art standardless analysis software

The optional UniQuant* software provides standardless analysis for up to 79 elements when specific standards are not available and when samples can only be obtained in small quantities or as irregular shapes. Unknown liquid samples can also be analyzed very efficiently. Various options, like the calculation of an unanalyzed element or compound, the sample dilution (if unknown), multi-element monolayer or thin layers are available for ultimate accuracy. Moreover, the sample, flux and calculation information can be transferred to UniQuant allowing the automatic result calculation.

The QuantAS and UniQuant optional modules are fully calibrated in the factory, making them ready for immediate use on user's site.

Small spot analysis and mapping

The ARL PERFORM'X has optional hardware to photograph the sample and performs small spot analysis on any desired location. Using the same hardware, it is possible to scan a particular region of the sample in order to produce elemental mapping of this region (see Figure 7).

Spot analyses produce standard OXSAS results that are stored along with sample picture and spot location. These results can be transmitted to remote location using OXSAS result processing facility.

A graphical tool is used to show the results of mapping. This tool allows to display the mapping either in 2D or in 3D.

Map overlay options allow the user to combine mapping results with sample picture.

A report of mapping results can be printed or exported to an Excel® file.

(* OXSAS features, options or other Thermo Scientific products marked with an asterisk are described in separate product specification sheets. Please refer to them for more details.

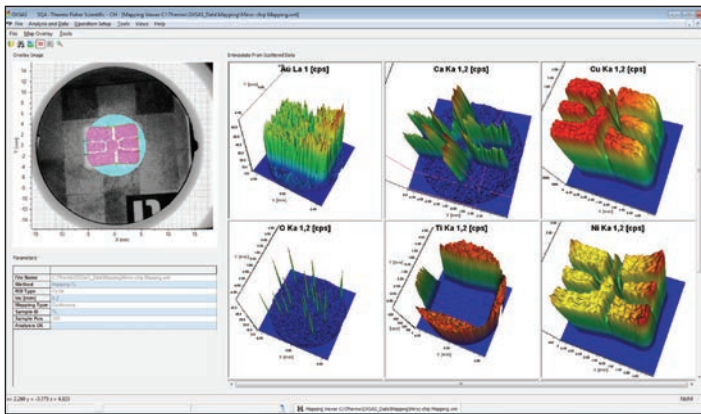


Figure 7. Small spot analysis on a specific area of the sample with results in 3D done by ARL PERFORM'X XRF spectrometer.

Instrument quality assurance

Control Samples: pro-active instrument control cannot be simpler

Control samples with their user specified limits (USL and LSL) can be defined to ensure quality of production samples analysis results.

- The interval between control analyses can be set per sample. A scheduler reminds when the timer is over
- Immediate evaluation of control sample state with feedback of any element failing the tests.
- Check of the instrument or of specific methods using dedicated samples
- Different correction actions can be set up in case of control analysis failure

System standardization (drift correction) can be performed anytime, on operator decision, at scheduled intervals or as a response to a control request.

Urgent samples can be inserted between Setting-Up Samples (SUS). The new standardization is applied only when all required SUS have been measured.

SCT samples management

The SCT manager provides a central point for supervision, monitoring and maintenance of Setting-Up, Control and Type Standards samples:

- Display of the status of each SCT sample, whether they are good, have been invalidated or are out-of-date. Samples are sorted per type and / or per method
- Check additional information like the next measurement date and time

- Instant batch: schedules the SCT samples that require analysis for a selected method
- History: date and status of each SCT sample measurement. Detailed history for each channel with status, coefficients or errors

Installation and operation qualification (IQ & OQ for ARL PERFORM'X only)

The ARL PERFORM'X benefits from an extra software package that ensures proper instrument installation (IQ) and confirm that the instrument is fully operational (OQ).

The operation qualification is a full automatic process that can be launched after instrument maintenance or at any time when needed.

Process analysis results

Valuable functions allow you to process analysis results on-line. You enable them in the analysis tasks and specify if the user can interact with them. You define in which cases automatic operations will execute and their behaviors.

On-line processing can take place upon completion of the analysis. Moreover, the user can apply them later from the recent analysis view or from the result storage screen (View Results).

Result processing operations include:

- **Storage**, with full details
- **Printing**, to local or network printers defined in Windows® control panel
- **Transmission*** (option): results can be transmitted to computers, to serial printers and serial display terminals
- **Transfer to SPC:** transfer of the analysis results to SPC (Statistical Process Control program)

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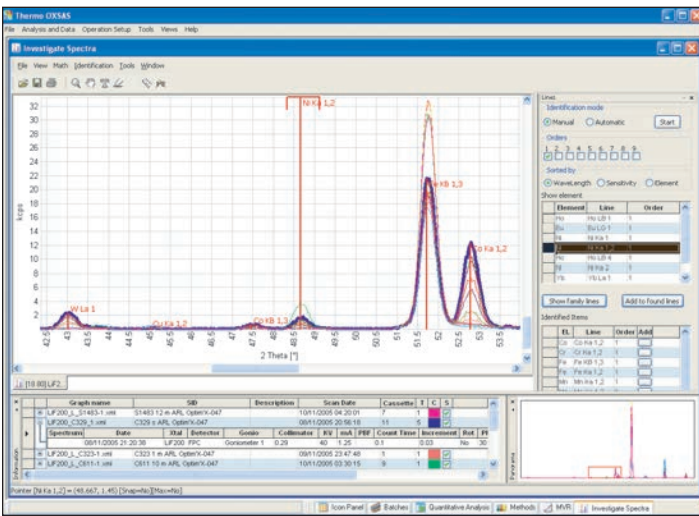


Figure 8. Display of spectra with their relevant data such as scan parameters, identified lines and elements.

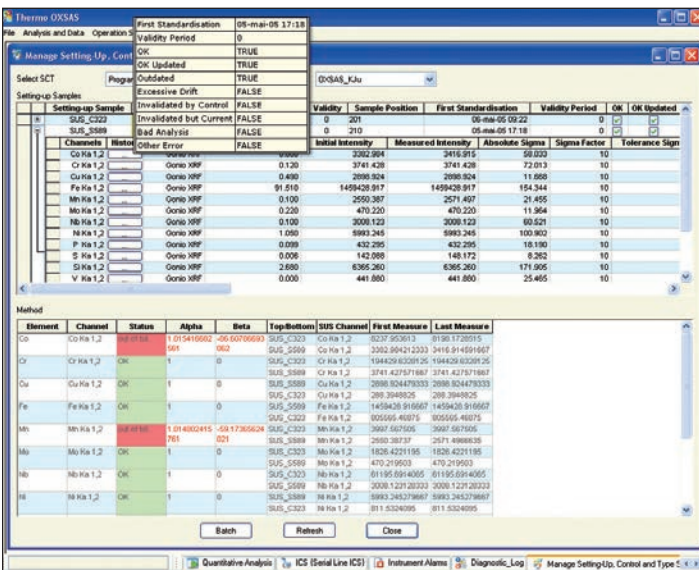


Figure 9. Monitoring the status of SCT samples. Creation in one click of a batch to measure the samples that need it.

Grade tests

Grade check: compares a result against pre-defined upper and lower limits of a target grade, alloy, product or material.

Grade limits can be displayed along with the result. Results can also be compared to two limit sets (inner and outer limits of grades).

The user selects the target grade when identifying the sample and it is checked automatically at the end of the analysis. Manual or automatic grade selection after the analysis is available too.

Alternative grade check: in case the analysis did not match the target grade, OXSAS can successively try a list of alternative grades.

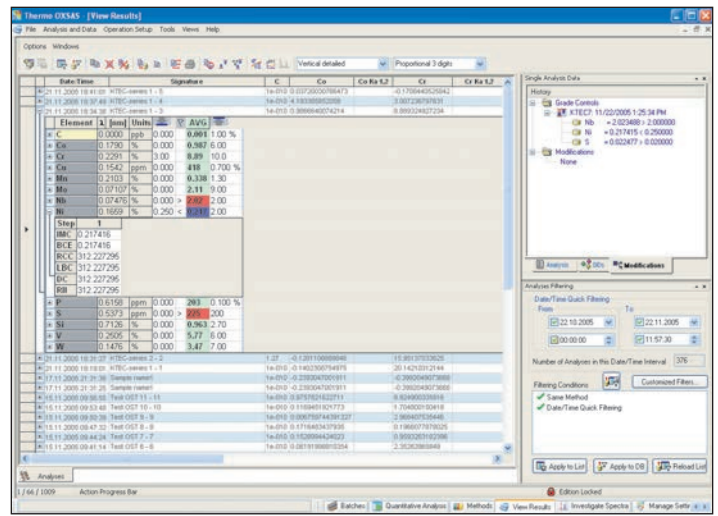


Figure 10. Grade check: display of the limits with the result and function history.

Charge correction* (option): Calculates the weight of materials to be added to a furnace charge to bring an out of specification material within limits. This charge correction procedure is cost optimized and will select materials that should be added to the charge to bring it within the specification limits.

SPC-Full, full Statistical Process Control package*

(option): a very useful software package to ensure quality of the instrument analyses and of your production samples. Allows on-line graphical display, evaluation and printing of the control charts and statistical data for control samples, Setting-Up samples, and unknown samples. SPC-Full provides the following additional features:

- Comprehensive charting capabilities and calculation of control limits
- Instrument standardization monitoring
- On-line transfer of unknown sample results, with automatic feedback to OXSAS. For monitoring production process, quality control jobs, etc.

SPC-Full allows Quality Assurance Managers to document permanently their Quality System, e.g. for audit purposes, study and revision procedures.

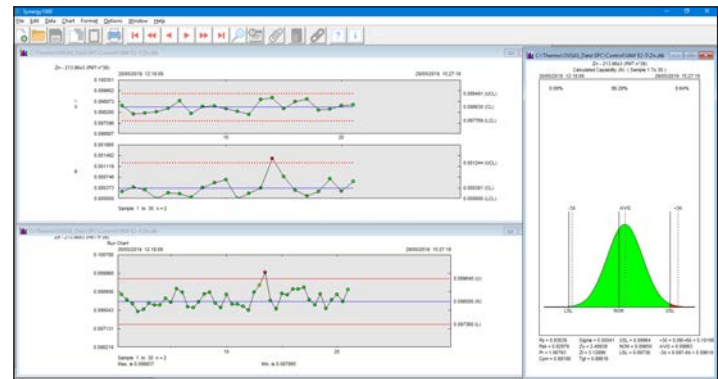


Figure 11. SPC-Full: Statistical Process Control with full charting capabilities.

Result storage with advanced query and post-treatment tools

Advanced result query filters

OXSAS saves automatically all analyses. You can search for specific analysis by simply giving an information and the system will propose all relevant analyses showing this information in one way or in another. Search can also be defined by date and/or by time, you can filter explicitly within the sample identity fields, the analysis parameters and other information fields.

You can even look for specific concentration ranges of selected elements, for analysis flags and further information. Wildcards are accepted. You can combine together as many filtering criteria as you need. Retrieving your results is that powerful.

Results post-treatment

All on-line functions can be applied and reapplied on stored results: result edition and recalculation, target and alternative grade check, transmission, printing and transfer to SPC. Moreover, the View Results permit exporting results in Excel or CSV formats, with possibility to select the element and arrange their format. When multiple results are exported in Excel format, their summary can be grouped in one sheet, or the details of each result can be displayed in separate sheets.

Thanks to these functions and to the filters, View Results allows exporting exactly the data you need. In addition, View Results calculates statistics of selected results.

More grade tests

View Results enables performing the following additional grade tests:

Grade search: searches the grade that the selected result is best matching and marks the result accordingly.

Grade sort: check the result against a group of selected grades and ranks them according to the variance.

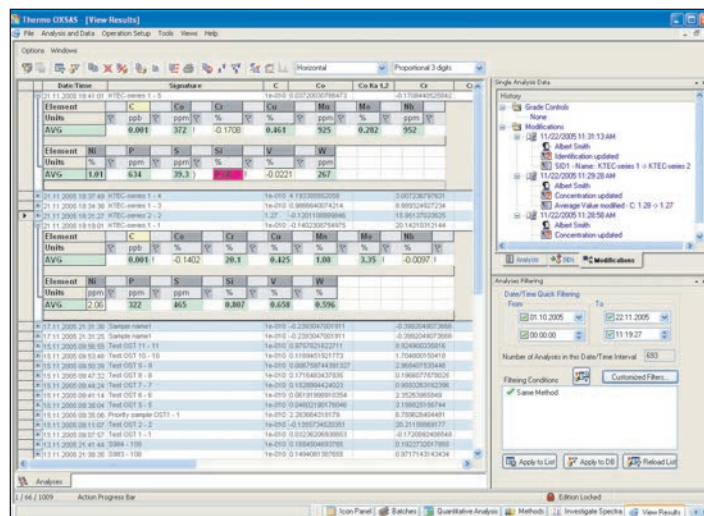


Figure 12. Query your stored results with advanced filters. View them with full details and modification history.

Modification history

Modifications performed on results are traced and can be viewed within a specific docking window. This includes the manual edition of sample identity and concentrations. For each history entry, OXSAS includes the name of the logged user, the date and time, the previous and the new values and the selected reason for change.

The history shows the reference to the original result for recalculated results. Grade check actions and results transmission with destinations are also logged and displayed in the history tree.

Quick operation

With time, view results stores a lot of results. Therefore, many functions can be applied on a multi-selection of results in one click to speed up the operation: print, export, statistics, grade check, even the recalculation and more.

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ARLcom data communication option*

OXSAS can be fitted with powerful and reliable transmission options that can transmit analysis results via network to applications running on other computers, to database servers, to LIMS, etc. It can also send them to your own computer enabling you to treat them with word processor, spreadsheet or database applications such as the Microsoft® Office programs.

Transmission over serial lines is available, whether you need to communicate to computers, to serial printers or to serial ASCII terminals. OXSAS can transmit results on-line to up to 16 destinations with for each one a different media and mechanism.

The result transmission solutions to computer applications or to files via LAN Local Area Network include:

- TCP/IP: computer task – to – computer task transmission
- File storage: transmission to files on local or network disks

The result transmission solutions to computers, printers or terminals over serial lines support the communication to:

- Computers using the Thermo Scientific Compac protocol
- Printers or visual display terminals using formatted telegrams

Software Destination Switch feature is integrated in ARLcom (available only with TCP/IP and Compac mechanisms). It automatically re-routes results to an alternative destination if the main one cannot be reached.

Utilities

- Easy learning of OXSAS thanks to contextual Help that describes the OXSAS functions with useful hints. Many tool tips give explanations directly in the software
- Security and data integrity with user accounts, password protection and configurable access to functions
- Translation or customization of software texts and messages into any language supported by Windows® Operating System
- Database maintenance: data backup and restore for settings and analyses

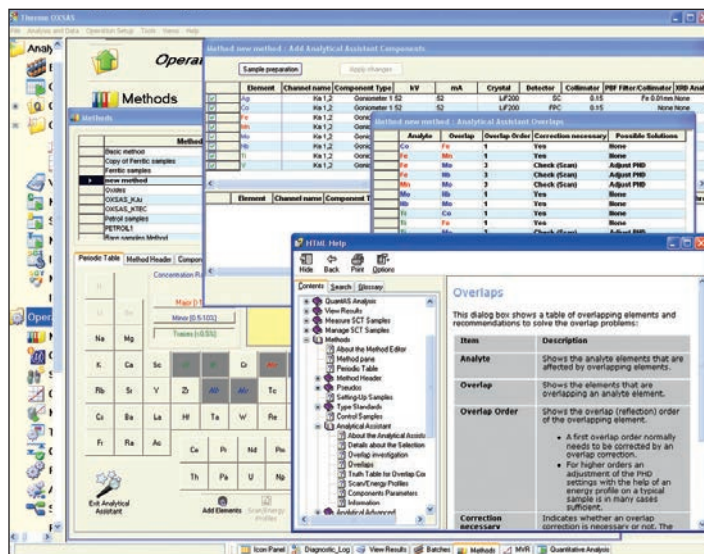


Figure 13. Contextual Help allows easy learning of OXSAS.

Monitoring, maintenance and service Peripherals monitoring

Monitoring the peripheral connections to OXSAS such as the instrument, the destination computers and the printers, makes their set up and troubleshooting very easy. Each peripheral has its own screen where all exchanged messages are shown.

System event logger

OXSAS logs system events and user actions allowing an efficient tracking of the operation and quick problem fixing.

You can set up your own display lists, files or destinations, where all events or only selected ones will be dispatched.

A fixed diagnostic log allows systematic investigation by our Technical Support. OXSAS comes also with defined logs dedicated to the instrument, calibration and SCT activities.

Full instrument automation option*

ARL SMS-2500/3500 series robotic systems and ARL SMS-XY/Omega systems offer a wide range of powerful automation solutions specifically designed for each Thermo Scientific ARL X-ray spectrometer. For even higher speed, increased productivity, less operational costs, improved quality and reliability of results.

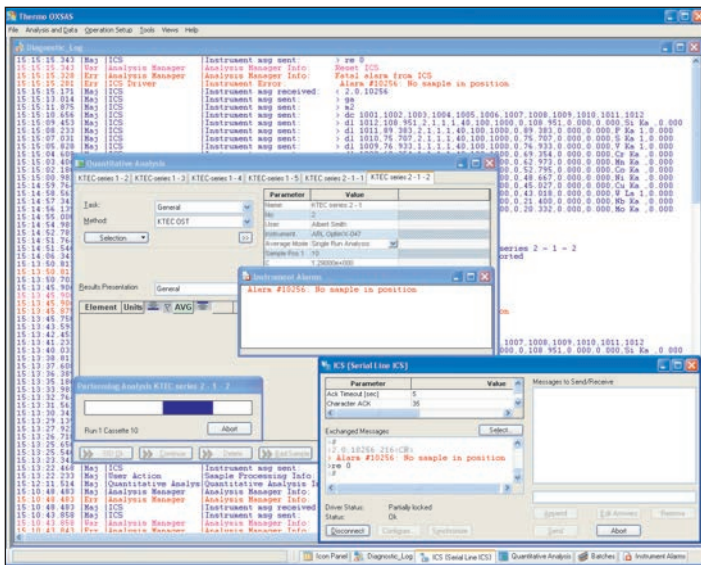


Figure 14. Easy setup and troubleshooting: e.g. with the peripheral communication monitoring and the event logger.

OXSAS innovative features

- Modern User Interface providing comfort and fast operation
- Speed functions for edition in grids
- Triple navigation style: menus, tree and icons meet everyone's preference
- Simple routine analysis start based on one button operation
- Templates for fast sample batch set-up. Deferred start using a scheduler
- Quick method setup with fully integrated Analytical Assistant that recommends the best measurement and correction parameters
- Unique solution where phase quantification can be merged with the XRF elemental analysis to form one single quantitative result
- Calibration: novel intuitive and comprehensive user interface with multiple analytes curves display
- Refined fundamental XRF parameters alphas calculation for best accuracy
- Recent analyses view
- Result query using advanced filtering
- Setting-up, Control and Type Standard status monitoring (SCT). One click creation of a batch with all samples requiring analysis
- Easy use and learning thanks to contextual help and tool tip
- Integrated Microsoft® SQL Server relational database

Remote instrument control

The OXSAS OEM Mode allows the connection of an external computer through a LAN to control and monitor the operation of the instrument and its sample loader, if fitted. This includes the definition and the execution of the analyses and the processing of their result.

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OXSAS standard features

- Triple software navigation
- Integrated Microsoft® SQL Server Express relational database which stores your set up data and analyses
- Quantitative analysis using tasks with analysis parameter template
- Flexible batch for all types of samples and analyses, with support of priority samples and scheduler
- Shortcuts for starting your routine analyses, measurements of SCT samples and batches. With shortcut keys (keyboard accelerators)
- Integrated Analytical Assistant to set up methods with measurement and corrections parameters
- Manual inputs and status. Pseudo values computed on intensities, concentrations or any calculation steps
- Variable counting time on peak and background positions
- Mathematical treatments of element intensities permitting advanced background and matrix corrections
- Calibration curve determination using multi-variable regression with a range of correction models and integrated theoretical alphas calculation
- Measurement uncertainty and conformance probability*
- Powerful flexible sample identification
- Automatic Method Choice
- Step scanning and digital continuous scanning. Scan spectra investigation, including peak identification and background subtraction formulae
- Manual and automatic result processing
- Flexible result display and printing

- Element display with units. Precision: dynamic (proportional), fixed number of decimals or of significant digits. ASTM rounding supported
- Result validation and edition
- Grade check against single or double limit sets, grade search and sort
- Concentration result recalculation
- Result storage and post-treatment with powerful database query filters. Statistics. Export to other applications
- Instrument check with Control samples
- Standardization, with history
- Type standardization, with history
- Management of SCT samples
- Instrument alarm monitoring
- System event logging
- Peripheral device monitoring
- Integrated contextual help
- Text customization and translation
- Accounts with password protection
- Database maintenance tools
- Instrument Installation and Operation Qualification (IQ & OQ) with ARL PERFORM'X

OXSAS options

- QuantAS*: semi-quantitative analysis package
- UniQuant*: standardless analytical software, full package
- ARLcom* Package including: LAN network result transmission and serial result transmission to computers and to ASCII terminals
- Charge correction*: Allows weight of materials calculation to be added to a furnace charge to bring an out of specification material within limits
- SPC-Full*: Statistical Process Control, full graphical package extension
- Spot analysis and mapping with ARL PERFORM'X
- Remote Sample Definition*: Allows samples registration by an external application through TCP/IP communication
- Extension allowing the instrument automation with the ARL SMS-2500/3500 series and XY/Omega/PFX systems
- OEM Mode allows the connection of an external computer through a LAN to drive OXSAS for monitoring and control of the instrument operation

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Find out more at thermofisher.com/oxsas