Optical Emission Analysis Software

# Thermo Scientific OXSAS

Thermo Scientific<sup>™</sup> OXSAS is the most modern software for optical emission spectrometers. This innovative platform, also available for X-ray fluorescence spectrometers, 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.



Thermo Scientific<sup>™</sup> ARL iSpark<sup>™</sup>



Thermo Scientific<sup>™</sup> ARL easySpark<sup>™</sup>

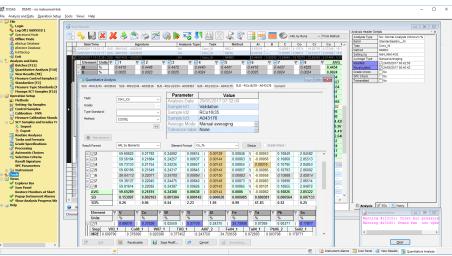


Figure 1. Modern, state-of-the-art user interface for comfortable and powerful operation

With OXSAS, you can set up and carry out all your analytical jobs easily and quickly. And you can do a lot more. OXSAS is the most modern software for Thermo Scientific optical emission spectrometers and shares functionality & design with its XRF 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 proven software platform that is designed to evolve to meet your needs throughout your instrument's lifetime.

### 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. Need to measure standards? OXSAS gathers and sets all data needed for you. Want to calculate sophisticated calibration curves? OXSAS allows you to have in one window numerical data & graphical display
- 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.

### 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. Allows preparing sample lists with their analysis parameters
- Fast calibration with multiple analyte curve display, instant base curve calculation, templates for edition and measurement of calibration standards
- Integrated Spark-DAT option
- Measurement uncertainty and conformance probability on unknown sample analysis results
- Multi-purpose analysis display with wideranging 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 Excel format
- Reports of method components and calibration curves
- 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
- Effective monitoring and maintenance tools maximizes the system uptime. Operation Qualification (OQ) for ARL iSpark Series.

### Developing expert analytical methods Picture clear method editor

The editor of methods allows easily defining the elements you need to analyze and the associated parameters for excitation, acquisition and concentration calculation. The internal standards definition and the line selection are also very simple. The necessary Setting-Up Samples, with the Type Standards and Control Samples can be also clearly defined together with the associated actions to be taken.

### 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.

Comprehensive mathematical formulae calculate pseudo values based on measured channels, status or manual inputs: the user selects the values to include in the formulae from the raw intensity up to the final concentration.

For some alloy analysis applications, the Type Standardization supplies ultimate accuracy for specific alloy types against a calibration.

The automatic method choice function selects the optimum analytical method, grade or type standard according to the analysis result without requiring any operator input. Particularly suited for the calibration curves selection per alloy family.

The recalculation of results helps you save time and operating costs. Without re-measuring samples, you can verify standardization, update a type standard, check unknown samples or include any value obtained by other techniques.

Measurements uncertainty\* can be displayed and transmitted along with the final sample analysis result. Associated to a grade check, this uncertainty can lead to conformity probability that elements match or not material specifications.

### Defining standards and calibrating your methods

OXSAS incorporates a comprehensive function allowing you to create and update calibrations at any time.

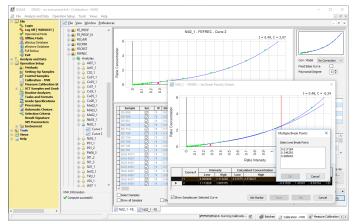
The correction model used for optical emission compensates for spectral interferences and for matrix interferences and uses the concentration of interfering elements for corrections. This enhances accuracy in comparison to intensity based models.

Calibration curves are calculated for absolute or ratio concentrations, depending on the definition of each component in the method's editor. Calibration curves are calculated using the multi-variable regression (MVR) algorithm. It uses the least squares regression to find the polynomial coefficients of the best fit curve. Additive or multiplicative corrections are simultaneously calculated together with the calibration curve, using linear or power model. The break point between successive curves of the same component can be graphically setup. Calibration curves can be calculated for physical components or formulae calculated pseudos. The line overlap for intensity corrections and background correction can also be performed.

The graphical User Interface is easy, flexible and clear: it displays the curves of multiple analytes combined with their numerical data, it allows comparing on screen the calibration among several different methods, it calculates and saves all base curves on a single click, etc.

Calibration standards are defined using an effective editor. You can import or export them using files in XML or CSV format, directly compatible with Microsoft® Excel for instance.

### Figure 2. All the data you need to produce accurate calibrations, clearly organized



Curve fit correlation displays analytical information such as: Standard Error of Estimate, Correlation Coefficient and Background Equivalent Concentration, and shows samples excluded from the calculations.

### Performing your analyses

#### Predefined parameters simplify your routine analyzes

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 category of your samples. Thanks to these mechanisms, running repeated jobs can be easily done by selecting the matching analysis template and introducing 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 during and upon completion of the analysis
- Management of the number of measurement runs and of the averaging method. The run averaging can be

selected to be controlled manually by the operator. Or it can be controlled automatically with no check, using reproducibility check against fluctuation tolerance limits or using statistical reproducibility check

- Sample identification with unlimited number of fields and up to 255 characters each. Data types are various: alphanumeric, numeric, lists, autoincrementing 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. element, uncertainty data, grade limits, 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.

### **Routine analyzes**

For an even easier routine operation, shortcuts can start the analysis of samples 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.

Alternatively, the routine analysis can be used to call a batch allowing the launch of repetitive jobs such as a standardization with a single click.

### Analyzes in easyOXSAS mode

easyOXSAS\* is an option offering the ultimate simplified user interface intended for production floor operators. No more menus to navigate, all necessary operations are simply launched from a button located in a left pane and system can be configured that the sample analysis operation requires no other action from operator then entering the sample identity and starting the measurement.

### Analyzes defined by an external application

Using the OXSAS option "Remote Sample Definition"\*, the 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 operators actions to the sample manipulation only. It is also possible for the external application action to define a complete list of samples that will be registered in a dedicated batch.

### **Flexible batches**

A batch is a list of samples and associated operations such as routine analysis, control samples or standardization update. Any change in measuring order and inserting or appending samples to a running batch, 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. The analysis of calibration standards, setting up samples, type standards and control samples can also be grouped in batches.

The recurring measurement of samples such as control samples can be saved in sample lists for later re-use and instant insertion in any running or waiting batch. Sample 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
- Setting-up, control, or type standards that need to be measured: e.g. if their validity period has expired.

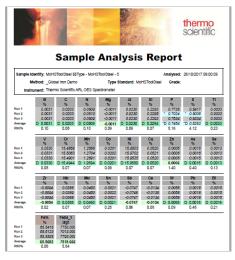
Speed functions allow incrementing or copying the value of an analytical parameter, an ID field or a sample position in one go.

## Viewing, editing, validating and processing analysis results

Upon completion of the analysis, the result is displayed according to the predefined format. If allowed, 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, etc.

### Figure 3. Result print-out with customizable logo and layout



The identity and the concentration of the analysis can be edited, if enabled. A result can also be recalculated, for instance using another calibration, or changing the selection of the runs to average.

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 analyses 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.

### **Instrument Quality Assurance**

# Integrated SPC (SPC-Full\* option): pro-active control cannot be simpler

SPC performs the routine check of the instrument using Statistical Process Control techniques. SPC features:

- The interval between control analyses can be set per sample. A scheduler reminds when the timer is over
- Immediate evaluation by SPC software and feedback for any element failing the tests
- 16 test rules supported: automatic detection of out-ofcontrol states using control limits, bias, trends, statistical distribution check, for example
- Check of the instrument or of specific methods using dedicated samples
- Different correction actions can be set up in case of control analysis failure
- Capability indexes (Cp, Cpk, Pp, Ppk).

### System standardization

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 standardization update is completed and the new factors are applied only when all required SUS have been measured.

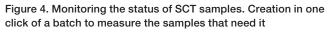
### Management of SCT samples

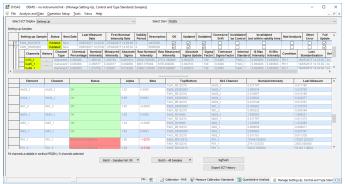
The SCT manager provides a central point for supervision, monitoring and maintenance of Setting-Up, Control and Type Standards samples:

• 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
- Create 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.





### **Operation Qualification and maintenance monitoring**

The ARL iSpark Series benefits from extra tools ensuring that instrument hardware is fit for sample analyses:

- Operation Qualification (OQ) monitors various instrument parameters to ensure the capability of the instrument to provide its best analytical performance
- The Instrument Maintenance facility monitors precisely the instrument usage (number of measurements, number of sparks) and asks operators for a maintenance of various instrument parts only when it becomes necessary. This ensures that instrument is always on top of its form.

#### Processing your 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:

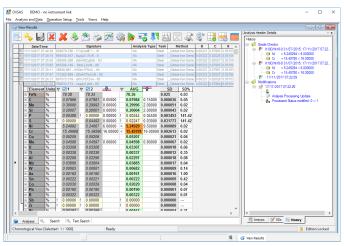
Automatic storage, with full details.

**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.

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

### Figure 5. Grade check: display of the limits with the result and function history



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).

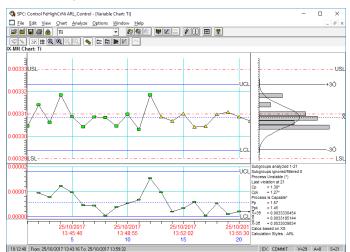
The user selects the target grade when identifying the sample and it is checked automatically at the end of the analysis. Manual or automatic grade selection after the analysis is available too.

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

**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): allows on-line graphical display, evaluation and printing of the control charts and statistical data for control samples, setting-up samples, and unknown samples.



### Figure 6. SPC-Full: Statistical Process Control with full graphics and capability indices

Figure 7. Clear reporting of analytical operation

Method Standardisation Report FELAST							thermo scientific	
Instrument: ARL iSpark						ARL ISpark 8860 - Demontration database		
Setting up Samples of M	lethod : Current State Review							
Fe01_RE12/210		Last Analysis OK, drift updated.						
Fe02_RN11990 Last Analysis CK, drit updated Fe03_R011915 Last Analysis CK, drit updated Fe03_R011915 Last Analysis CK, drit updated Fe04_R01477 Last Analysis CK, drit updated Fe04_R014915 Last Analysis CK, drit updated Fe04_R014915 Last Analysis CK, drit updated Fe04_R01495 Last Ana								
Fe07 S423255/01								
Channel Name	Alpha			Alpha Beta Statua				
A07.1	0.96	0.96 0.000		OK				
Setting-up Samples	SUS Channel Status	Nomina	Lost	Current	Abs. Diff.	Diff. %	Current D	
Low Fe01 RE12/210	Outdated	0.01233	0.01260	0.01234	0.00001	0.08	18/05/2017 14:33	
High: Fe02_RN19/80	Outdated	0.94582	0.97360	0.96180	0.01598	1.69	18/05/2017 14:33	
Channel Name	Alpha	Alpha		Alpha/Beta Status				
As01_1	1.06	-0.0006		OK				
Setting-up Samples	SUS Channel Status	Nomina	Last	Current	Abs. Diff.	Diff. %	Current D	
Losc Fe01_RE12/210	Outdated	0.03747	0.03631	0.03624	0.00124	3.30	18/05/2017 14:33	
High: Fe02_RN19/80	Outdated	0.36783	0.36625	0.35110	0.01673	4.65	18/05/2017 14:33	
Channel Name	Alpha		Absolute Beta	Alpha/Deta Sta	tus			
As01_2	1.04		-0.0001	OK				
Setting-up Samples	SUS Channel Status	Nomina	Last	Current	Abs. Diff.	Diff. %	Current D	
Low: Fe01_RE12/210	Outdated	0.00889	0.00865	0.00859	0.00029	3.29	18/05/2017 14:33	
High: Pe02_RN19/80	Outdated	0.16488	0.15911	0.15805	0.00683	4.14	18/05/2017 14:33	
Channel Name	Alpha		Absolute Beta	Alpha/Beta Status				
801_1	1.06	1.06		OK.				
Setting-up Samples	SUS Channel Status	Nomina	Lost	Current	Abs. Diff.	Diff. %	Current D	
Low: Fe01_RE12/210	Outdated	0.01509	0.01455	0.01434	0.00076	4.94	18/05/2017 14:33	
High: Fe02_RN19/80	Outdated	0.08358	0.08158	0.07947	0.00408	4.89	18/05/2017 14:33	
Page: 1	SoftWare Nam	SoftWare Name: OXSAS Version No: 2.5.2.3417					27/10/201	

SPC-Full provides the following additional features:

- Comprehensive charting capabilities and calculation of control limits
- Automatic control chart display after each analysis
- 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.

### Result storage with advanced query and posttreatment tools

#### Advanced result query filters

OXSAS saves automatically all analyses. You can search for specific analyses by simply giving an information and the system will propose all relevant analyses showing this information one way or another. Search can also be defined by date and/or by time.

You can even look for specific concentration ranges of selected elements. Wildcards are accepted. You can combine together as many filtering criteria as you need.

### **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.

### **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 result 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.

### **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.

Result transmission to computer applications or to files via LAN Local Area Network. Includes:

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

Result transmission to computers, printers or terminals over serial lines. Supports 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.

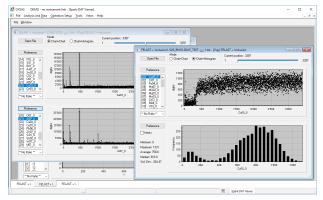
### **On-line Spark-DAT option\***

With Spark-DAT, the digital acquisition and treatment of individual spark signal means a dramatic growth of analysis information material. Fully integrated in OXSAS, it operates on-line supplying values in an instant, where classical techniques can take hours!

With on-line Spark-DAT, new analysis opportunities are possible: determination of soluble/insoluble parts of the elements, on-line metal cleanness determination and inclusions control. Inclusions control includes the chemical determination, the number of inclusions and their sizes.

OXSAS allows to mix in one method both conventional elemental analysis and Spark-DAT analysis. It is designed for evolution, new algorithms can be added at any moment. Algorithms are available as standard or as options. You may even provide your owns!

#### Figure 8. Spark-DAT viewer



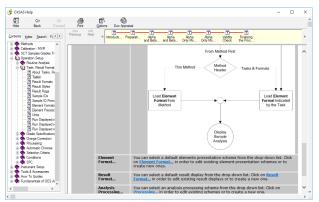
### Full instrument automation option\*

With the Thermo Scientific<sup>™</sup> ARL<sup>™</sup> SMS-2500/3500 series robotic systems. For even higher speed, increased productivity, less operational costs, improved quality and reliability of results.

### Utilities

- Easy learning of OXSAS thanks to on-line 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

### Figure 9. On-line contextual Help allows easy learning of OXSAS



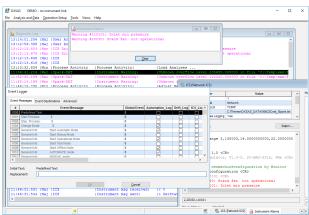
Database maintenance: data backup and restore for settings and analyses

### Monitoring, maintenance and service Monitoring of the peripherals

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 come. 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.



### Figure 10. 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 everyones preference
- Simple routine analysis launch based on one button operation

- Templates for fast sample batch set-up
- Quick method setup with all necessary parameters well organized
- Calibration: novel intuitive and comprehensive user interface with multiple analytes curves display
- 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 online contextual Help and tool tips
- Integrated Microsoft® SQL Server relational database.

### **OXSAS** standard features

- Triple software navigation
- Integrated Microsoft® SQL Server relational database which stores your set up data and analyses
- Quantitative analysis using tasks with analysis parameter template
- Shortcuts for starting your routine analyses and measurements of SCT samples. With shortcut keys (keyboard accelerators)
- Flexible batch for all types of samples and analyses, with support of priority samples and scheduler
- Manual inputs and status. Pseudo values computed on intensities, concentrations or any calculation step
- Calibration curve determination using multi-variable regression with graphical and numerical data in one window display
- Measurement uncertainty and conformance probability\*
- Powerful flexible sample identification
- Automatic Method Choice
- 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 (target and alternative) 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 files in Excel or CSV format
- Standardization, with history
- Type standardization, with history
- Management of SCT samples
- Argon Management (ARL iSpark only)
- Operational Qualification (OQ, ARL iSpark only)
- Maintenance management (ARL iSpark only)
- Instrument alarm monitoring
- System event logging
- Peripheral device monitoring
- On-line contextual help
- Text customization and translation
- Accounts with password protection for secured operation
- Database maintenance tools.

### **OXSAS** options

- ARLcom\* Package including: LAN network result transmission and serial result transmission to computers and to ASCII terminals
- SPC-Full\*: Statistical Process Control, full graphical package extension
- On-line Spark-DAT\* (ARL iSpark only)
- Extension allowing the instrument automation with the ARL SMS-2500/3500 robotic systems
- Charge correction\*: Allows weight of materials calculation to be added to a furnace charge to bring an out of specification material within limits
- Remote Sample Definition\*: Allows samples registration by an external application through TCP/IP communication
- easyOXSAS\*: Simplified user interface for operators.

(\*) 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.

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