Thermo Scientific ARL OPTIM'X Series
WDXRF Spectrometer

amazing performance
in WDXRF

Cement • Slags • Petroleum • Chemicals • Oxides •
Metals • Glasses • Ceramics • Alternate fuels • Food

Thermo
SCIENTIFIC

amazing performance in WDXRF

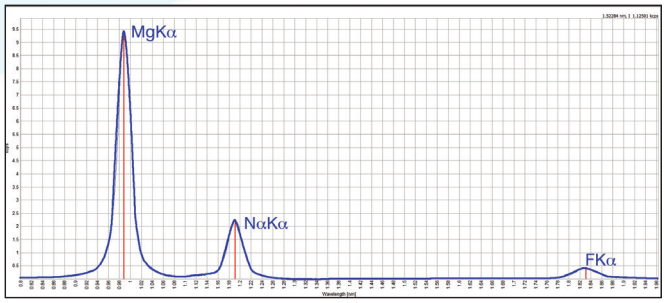
- 200 W analytical performance from 50 W power
- 500 W analytical performance from 200 W power

Wavelength dispersive X-ray fluorescence (WDXRF) is one of the most versatile analytical methods for elemental analysis of solids and liquids. Elements from boron to uranium can be analyzed in a wide variety of samples with high accuracy, precision and reliability. The technique and the analytical methods are mature enough to establish clear qualitative and quantitative characterization of diversified materials. Modern technological developments have helped to include WDXRF into standard test methods for analytical laboratories (ASTM and ISO norms for example) by virtue of its simplicity, flexibility, affordability and reliability. The cost per analysis is clearly advantageous over many traditional wet chemical and other spectroscopic methods.

A compact and independant WDXRF instrument

Continuing its tradition of innovation and leadership in WDXRF, our company presents a compact instrument, the Thermo Scientific™ ARL OPTIM'X spectrometer, with the choice of two power levels and the following salient analytical features:

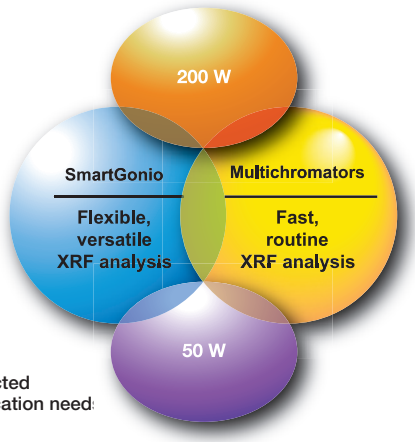
- Unique WDXRF platform with sequential and/or simultaneous capabilities
- Element coverage from carbon to uranium, depending on configuration
- Innovative UCCO technology (Ultra Closely Coupled Optics) for increased intensity, up to 210% higher than conventional geometry
- Unique compact SmartGonio device for sequential analysis
- Sequential-simultaneous configuration blending speed with analytical flexibility
- Multichromators for fast analysis
- High precision (short term and long term repeatability) thanks to temperature regulation of spectrometer and crystals
- Superior spectral resolution from low Z elements to heavy elements (~15 eV at CaKα)
- Optimum configuration for specific applications with simplified operation (compliant with ISO or ASTM standards)
- Stand-alone and autonomous operation without water cooling
- No gas supply required (depending on the configuration)
- Simple and direct sample introduction
- Automatic analysis of batches with sample changer
- Small footprint



Excellent resolution: Mg, Na and F peaks do not interfere on each other

Configuration for speed and flexibility

- Up to 8 elements simultaneously using 4 multichromators
- Sequential analysis with the SmartGonio
- Sequential-simultaneous analysis: SmartGonio and 2 elements simultaneously on one multichromator
- 50 W basic or 200 W optional power to achieve 2.5 times faster analysis



Configuration selected according to application need

ARL OPTIM'X

Large variety of samples

Many sample types can be analyzed on the ARL OPTIM'X spectrometer: conductive or non-conductive solids, liquids, loose powders, pressed pellets, fusion beads, pastes, granules and coatings. The instrument is always optimized for your specific application needs.

Exclusive UCCO technology

UCCO – Ultra Closely Coupled Optics

- 200 W performance from 50 W power
- 500 W performance from 200 W power

Whole X-ray beam exciting the full sample diameter for highest efficiency: no photon loss during irradiation.

Sample holder

Miniaturized X-ray tube allowing close coupling with sample for optimized sensitivity.

Optimized for specific applications

- Petroleum industry – analysis of S (ISO 14596 or ASTM D2622), Pb (ASTM D5059) or other elements in gasoline, fuels and oils. The calibration curve for sulfur in oils and gasoline can be easily obtained for concentrations ranging from ppm levels up to 5% (see Fig. 1). At 50 W the excellent limit of detection of 1.4 ppm in 100 s (or 1 ppm in 200 s) is achieved. This good result is proven by the reproducibility test shown in Table 1. At 200 W power, the same precision is obtained in 50 s and the limit of detection decreases to 0.8 ppm in 100 s. The preconfigured ARL OPTIM'X Sulfur Analyzer is offered as a turn-key solution, details at **www.thermoscientific.com/optisulfur**
- Major and minor oxides in raw materials such as limestone, sand, feldspar, bauxite, magnesite and other mining applications as well as raw meal, clinker and cement. The ARL OPTIM'X analyzer shows excellent repeatability of analysis for such types of materials. For dedicated cement applications, the preconfigured ARL OPTIM'X Cement Analyzer is also available, please check details at **www.thermoscientific.com/opticement**
- For metallurgical slag analysis, the preconfigured ARL OPTIM'X Slag Analyzer delivers a turn-key solution, details at **www.thermoscientific.com/optislag.** As the calibration curve in Fig. 2 proves, the analysis of F can be carried out without problem either with the SmartGonio or with a fixed channel. The ARL OPTIM'X excellent precision is shown in Table 2 including data for fluorine.
- Major and minor oxides in products such as glasses, ceramics, refractories (more details in separate Application Notes)
- Polymers (see Table 3), paints, pigments, paper, ferro-alloys, silicon, metal sheets and other products where major and minor elements need to be monitored (check separate Application Notes for more details)
- Food industry for major and minor nutrients and other regulated elements in milk powders and cereals.Typical concentration ranges and the excellent limits of detection in milk powders at 50 W are listed in Table 4 below.
- For other wide-range and unknown material analysis, we offer the preconfigured ARL OPTIM'X Optiquantometer, details later in this brochure and at **www.thermoscientific.com/optilab**

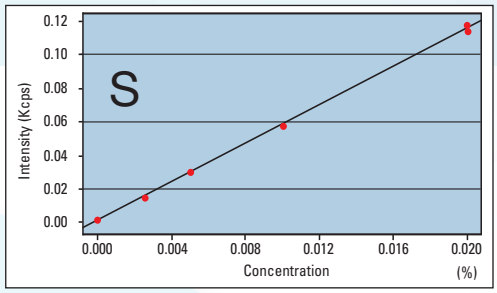


Fig 1. Calibration curve for S in oils and gasoline at 50 W (low concentration range)

Table 1. Excellent reproducibility for sulfur in oils at 50 W (120 s)

Sample	ppm
Cell 1	25.4
Cell 2	25.7
Cell 3	26.4
Cell 4	26.0
Cell 5	25.0
Cell 6	25.9
Cell 7	26.7
Average	25.9
Std. Dev.	0.58

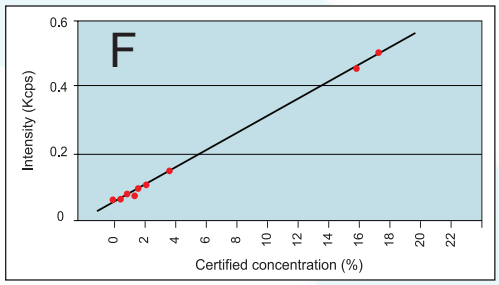


Fig 2. Calibration curve for F in slags. Standard error of estimate is 0.2% in a range from 0.1% to 17%

Table 2. Repeatability test on a pressed slag sample at 200W (6 consecutive runs). Total counting time 230 s for 13 elements - Fluorine is measured on a fixed channel.

Run #	CaO	SiO_2	Al_2O_3	Fe_2O_3	MnO	MgO	S	V_2O_5	TiO_2	K_2O	P_2O_5	Na_2O	F Mono
1	39.58	35.37	10.05	0.984	2.42	5.43	0.954	0.209	0.811	1.506	0.641	1.4	0.493
2	39.61	35.33	10.06	0.984	2.43	5.43	0.948	0.213	0.812	1.512	0.642	1.41	0.484
3	39.63	35.41	10.05	0.993	2.42	5.44	0.946	0.212	0.819	1.511	0.646	1.39	0.477
4	39.55	35.38	10.07	0.985	2.42	5.43	0.953	0.213	0.812	1.514	0.646	1.40	0.491
5	39.62	35.4	10.06	0.993	2.42	5.44	0.953	0.210	0.811	1.508	0.647	1.37	0.471
6	39.57	35.37	10.06	0.987	2.43	5.47	0.954	0.209	0.815	1.513	0.645	1.41	0.486
AVG	39.59	35.38	10.06	0.988	2.42	5.44	0.951	0.211	0.813	1.511	0.645	1.40	0.484
SD	0.031	0.028	0.008	0.004	0.005	0.015	0.003	0.002	0.003	0.003	0.002	0.015	0.008
Meas Time [s]	10	10	20	10	20	20	30	20	20	20	20	30	230

Table 3. Limits of detection for heavy elements in polymers at 200 W (100 s counting time). SEE: standard error of estimate with ranges from 0 to 500 ppm

		LOD in 100 s	SEE
Element	Line	[ppm]	[ppm]
Ba	Lα	2.6	17
Br	Kα	1.0	6.1
Cd	Kα	3.0	18
Cr	Kα	0.5	3.6
Cu	Kα	0.5	5.6
Hg	Lα	1.2	20
Ni	Kα	0.3	16
Pb	Lβ	0.9	24
Zn	Kα	0.3	6.2

Table 4. Limits of detection (LoD) at 50 W in milk powders prepared as pressed pellets (*cumulative counting time of SmartGonio for Na and Mg)

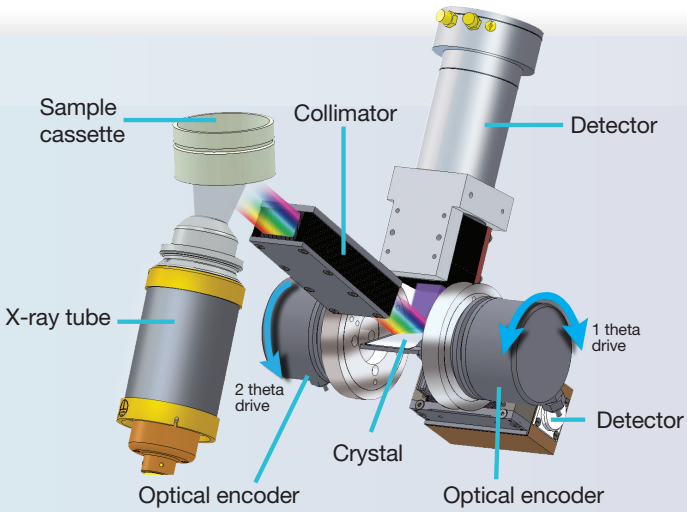
Element	Analytical device	Typical ranges	LoD (ppm in 60 s)
Na	Fixed channel	0 – 0.03%	20 ppm*
Mg	Fixed channel	0 – 0.12%	11 ppm*
P	SmartGonio	0 – 1.1%	4.4 ppm
K	SmartGonio	0 – 1%	2 ppm
Ca	SmartGonio	0 – 1.6%	10 ppm
Fe	SmartGonio	0 – 0.33%	2.1 ppm
Cu	SmartGonio	0 – 0.012%	0.6 ppm
Zn	SmartGonio	0 – 0.2%	2 ppm
Cl	SmartGonio	0 – 0.48%	10 ppm
Mn	SmartGonio	0 – 0.0023%	1.2 ppm
Se	SmartGonio	0 – 3.4 ppm	0.24 ppm

AMAZING

Full automation with
Thermo Scientific ARL SMS-Omega
loading system connecting full
automatic preparation machines

Exclusive SmartGonio – Principle of operation

- Quantitative analysis of any element from F to U depending on configuration
- Angular positioning to ensure θ/2θ relationship between crystal and detector is achieved through Moiré fringe optical encoders:
  – excellent repeatability and angular precision
  – no friction, no wear and no maintenance
- Temperature regulation of crystals for best analytical stability
- Closest coupling with X-ray tube provides optimized sensitivity



Instrument control and data handling

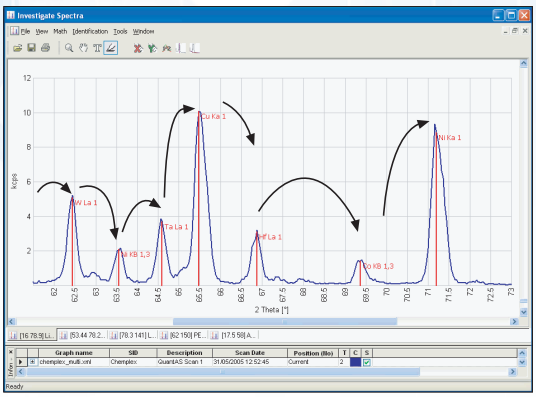
Operating the ARL OPTIM'X spectrometer and rapidly delivering highly accurate analytical reports are easily achieved through the state-of-the-art Thermo Scientific OXSAS™ software. Using Windows® 7 Professional operating system, OXSAS software is designed to evolve to meet customer's needs with up-to-date solutions throughout the lifetime of the instrument. All features and details can be found in the OXSAS software product specification sheet.

OptiQuant

The optional OptiQuant package is an optimized version of the renowned UniQuant™ program for the ARL OPTIM'X spectrometer. It provides "standard-less" analysis for up to 73 elements when specific standards are not available, or when samples can only be obtained in small quantities or as irregular shapes. All sorts of conductive or non-conductive solids can be analyzed. When helium environment option is fitted, analysis of loose powders, liquids and pastes can be easily accomplished. Additionally the OptiQuant program calculates the balance of unanalyzed elements present in the sample, e.g. organic and ultra light elements. Analysis by peak to peak hopping brings several advantages compared to scan based spectral processing:

- Better limits of detection
- Best counting time for each element
- Use of sample spinning for non homogeneous samples or to average out effects due to polishing grooves

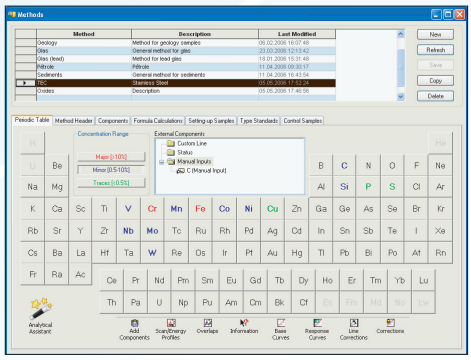
OptiQuant program is fully calibrated and pre-installed in the factory using the SmartGonio and thus ready for use immediately after installation at the customer site. Stable samples for setting-up and maintenance over time are included. The preconfigured version of the ARL OPTIM'X analyzer is called the ARL Optiquantometer. More details on **www.thermoscientifc.com/optilab**



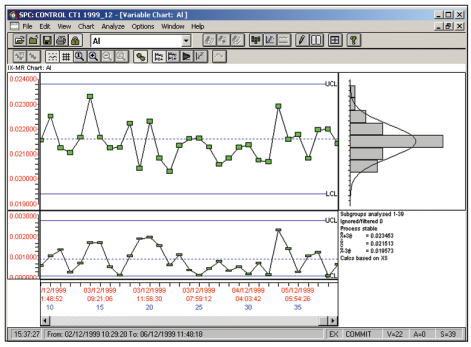
OptiQuant uses 'peak hopping' to acquire intensities for more than 121 line positions

UniQuant and OptiQuant are world's most renowned standard-less packages

SOFTWARE



The Analytical Assistant helps definition of analytical programs, calibration and instrument use



Statistical Process Control – Typical screen

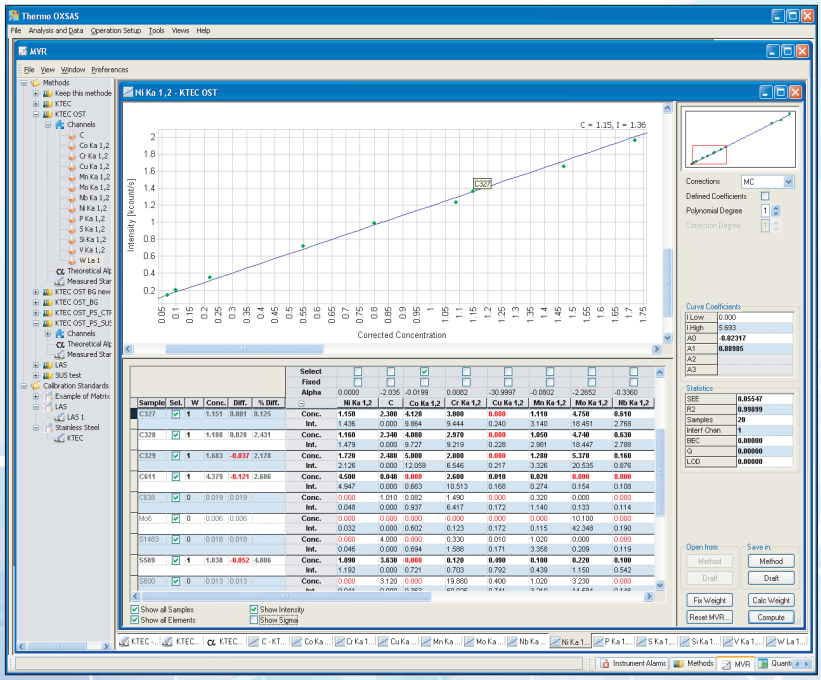
Fast qualitative analysis

Step scanning provides precise definition of peaks with a resolution of 0.001°. For rapid qualitative analysis, continuous digital scanning allows fast acquisition of spectra at speeds up to 327 °/min. Identification of the peaks representing the detected elements is automatic.

Accuracy made easy

The on-line Analytical Assistant helps quick and correct definition of analytical programs and calibrations. The multi-variable regression (MVR) program is used to build the various calibration curves. The influence of interfering elements in multi-component matrices is minimized thanks to correction models leading to better accuracy of analysis. These models are:

- Line overlap correction
- Additive correction on intensities
- Additive correction on concentrations
- Multiplicative correction on intensities
- Multiplicative correction on concentrations
- Multiplicative and additive corrections on concentrations
- COmprehensive LAchance (COLA) with 3 term alphas is used with NBSGSC fundamental parameters program, which simulates analytical calibrations for homogeneous materials. Inter-element correction factors (theoretical alphas, now with matrix and LOI/GOI elimination) are calculated and used as known coefficients in the MVR. This minimizes the number of standards necessary to produce calibrations and improves the accuracy of analysis



MVR calibration curve: real concentration vs. intensities

Turnkey calibrations

Ex-works calibrations can be delivered for various materials such as:

- Petroleum industry products using the PetroilQuant program and/or ASTM & ISO methods
- Iron, hot metal and slags
- Copper, bronze and brass
- Aluminum and alloys
- Ferro-alloys
- Cement and clinker
- Various oxides through the General Oxide calibration
- Traces in soils and sediments
- Polymers and coatings
- Minerals such as lime, limestone, dolomite and sands
- Glasses
- Milk powders and cereals

Analytical specifications are available on request for all the above calibrations as well as for custom made calibrations.

Specifications of the Thermo Scientific ARL OPTIM'X XRF spectrometer	
Element range	Fluorine (Z=9) to uranium (Z=92) with 2 detectors fitted. Fluorine to Iron (Z=26) with FPC detector fitted (Carbon (Z=6) can be fitted as fixed channel)
Spectrometer environment	Vacuum for solids, helium for liquids and loose powders
Spectrometer design	Analysis devices contained in a temperature controlled vacuum chamber made of grey cast iron
Spectrometer arrangement	X-ray tube inclined at 66° under sample for optimum incidence
Spectrometer capacity	Simultaneous configuration: Four Multichromators (covering eight elements) Sim-seq configuration: SmartGonio + one Multichromator (covering two elements)
UCCO technology	Ultra Closely Coupled Optics offering largest solid angle for most efficient irradiation of the total sample surface: 50 W power providing excitation similar to 200 W or 200 W power providing excitation similar to 500 W
X-ray excitation	Air cooled Rh anode end window tube with thin Be window (0.075 mm). Other anodes available on request. 50 W version: Solid-state high frequency generator of maximum voltage 50 kV and maximum current 2 mA (combinations to be chosen to be at 50 W) 200 W version: maximum voltage 50 kV and maximum current 10 mA (combinations to be chosen to be at 200 W). Max. line voltage variation 230 V -15% to +10%. Stability ± 0.0002% per 1% variation
SmartGonio	Fully automatic, gearless, microprocessor controlled compact goniometer using optical encoders Total angle range: 0 ° -150 ° 2 θ (Flow proportional counter: 17 ° -150 °, Scintillation counter: 0 °- 90 °). Continuous digital scans: from 0.25 °/min to 327 °/min.
Multichromator	Fixed channel using dual curved crystal optics allowing analysis of two elements simultaneously. Sealed detectors available for all elements from sodium (Z=11). Flow proportional or scintillation detectors also available depending on element. Dual pulse height integration to discriminate and correct for 2nd order peaks. Note: some elements can only be fitted as single channel monochromator
Counting electronics	Multi-channel analyzer to discriminate peaks of higher energies. Digital Automatic Gain Control (AGC) for pulse shrinking correction. Automatic dead time correction ensures linearity of response up to 2 Mcps on flow proportional counter and 1.5 Mcps on scintillation counter
Sample loading	Basic: 1 position for cassette or liquid cell. Optional: 13 position autosampler
Automation	ARL SMS-Omega full automation with transport link from/to fully automatic sample preparation machines for pressed pellets or fused beads or solids
Sample holders	Sample cassettes with maximum size of sample: height 26 mm, diameter 52 mm. Liquid cell: height 22 mm, external diameter 40 mm Exposed opening: 29 mm diameter (basic). Rotation of sample holder in analysis position: 6 to 60 rpm
Dimensions and weight	H 126 cm, W 88 cm, D 82 cm with basic sample loading. System weight: approximately 260 kg
Laboratory information	Optional phone service support through modem connection
Power requirements	1.5 kVA single phase at 50 W; 1.7 kVA single phase at 200 W

Safety standards	
Electrical and protection	EN IEC 61010-1 (Safety requirements for electrical equipment for measurement, control and laboratory use. Part 1: General requirements)
Radiation	Full protection system: Swiss directive ORaP RS 814.501 and German directive RöV BGB1.IS.114
Electro-magnetic immunity	EN CEI 61326-1 (Electrical equipment for measurement, control and laboratory use – EMC requirements – Part 1: General requirements)
European directives	2006/95/EC (LVD) Low Voltage Directive 2002/95/EC (RoHS) Restriction of Hazardous Substances Directive 2002/96/EC (WEEE) Waste Electrical and Electronic Equipment Directive

Thermo Fisher Scientific (Ecublens) SARL, Switzerland is ISO certified.

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