UniQuant® 5

Let's compare...

Methods of Data Collection

Main features

Over the last decade most major x-ray spectrometer suppliers have developed software packages designed for the analysis of totally unknown samples for which no standards are available.

In most cases their approach is to use Fine-Step (FS) scanning of the complete spectrum to collect intensity data and Fundamental Parameters (FP) to calculate concentrations.

Although initially designated as Semi-Quantitative (SQ), these programs were capable of providing quantitative analysis of certain types of samples providing that the associated library of standards contained data of a suitable standard.

The unique approach developed by Omega Data Systems and subsequently incorporated in the latest version of UniQuant involves the use of Smart-Variable-Step (SVS) scanning of 114 fixed spectral positions evenly distributed over the entire spectrum.

As each position is tuned to the wavelength of a potentially present element the need to measure a very large number of spectrally interfering lines (necessary using FS scanning) is eliminated.

Strong interference's will quite often result in SQ programs automatically selecting an alternative line with the inherent risk of errors due to selection of an inappropriate library standard or additional spectral interference (line overlap) on the line selected!

In contrast UniQuant calculates and reports quantitatively the corrections made for the various line overlaps thus indicating which elements caused an interfering line and to what extent (in equivalent mg/kg).

But just how do these different approaches really effect overall analytical performance?

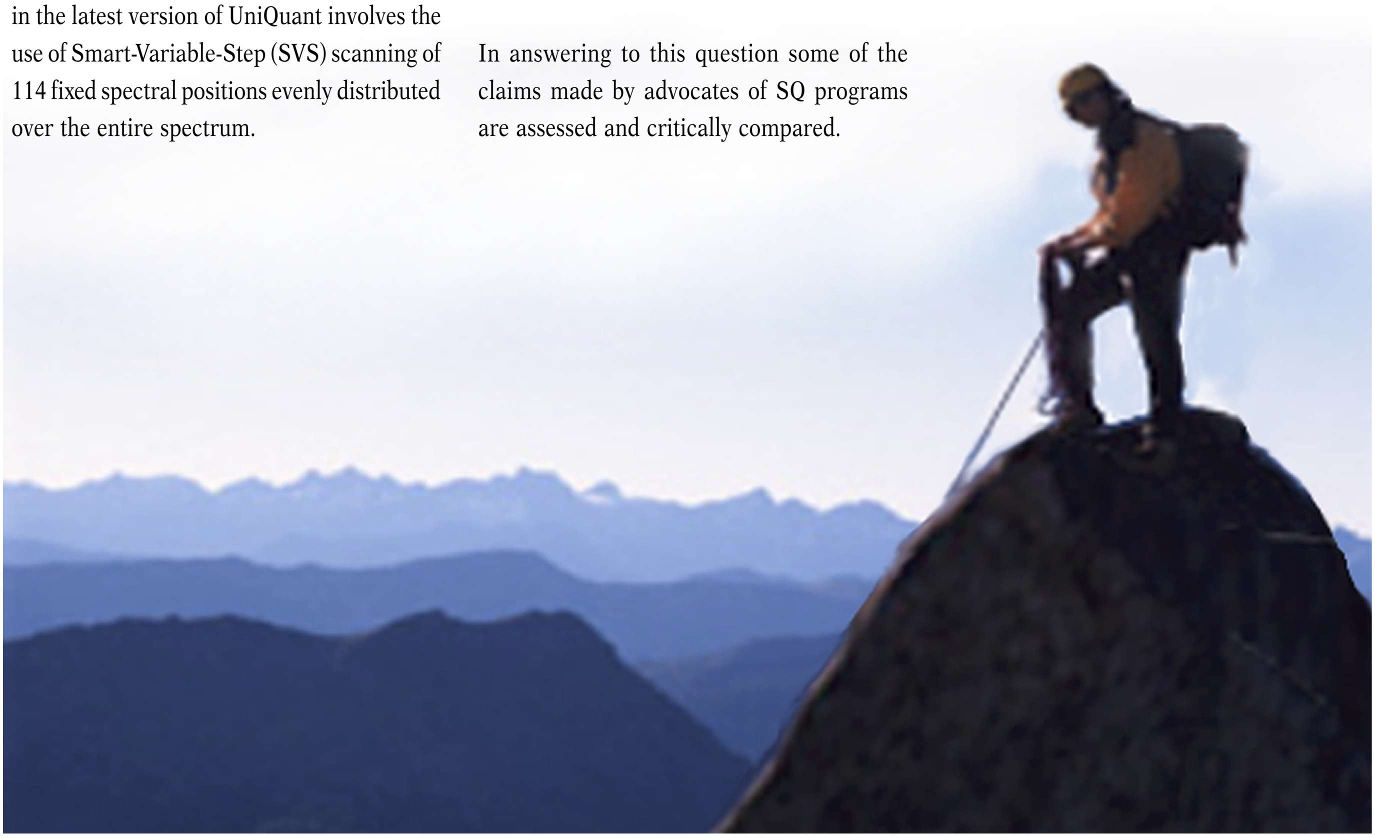
In answering to this question some of the claims made by advocates of SQ programs are assessed and critically compared.

General

In comparing the relative merits of FS and SVS scanning methods it should be noted that SQ programs and UniQuant differ fundamentally in the concepts used in generating net peak intensities. (i.e. gross peak intensity corrected for background continuum and spectrally interfering lines.

With SQ programs the use of FS scanning is an absolute requirement.
To be sure of adequate line overlap correction a potentially large number (> 1000) of spectrally interfering lines may need to be measured in addition to the 100 or so analyte lines.

With UniQuant this need has been eliminated resulting in much faster analysis.



For trace analysis

They say:
SQ programs with FS scanning produce better trace element performance than can be achieved by using a SVS approachî.

We say:
This is in complete contradiction to conventional methods for trace quantitative analysis using calibration standards and regression analysis based on measurements at fixed spectral positions.

In terms of trace element analysis of samples using SQ programs there are a number of factors which need to be considered in order to avoid potential problems.

Fine-step (FS) scanning carried out at relatively high speeds (to reduce total analysis time) requires that instrumental parameters are selected for highest possible intensity, at the expense of spectral resolution, resulting in more difficult line overlap corrections.

This problem can be partially solved for samples in which the trace elements to be expected are known by varying the scanning conditions in certain areas and or omitting specified spectral areas.

UniQuant employing SVS measures trace elements in very much the same way as in conventional analysis using a fixed time i.e. 10 seconds.
This should be compared to FS scanning where the dwelling time in the vicinity of the peak can be as low as 0.1 seconds.
The resulting lower limits of detection with UniQuant will be in general lower by a factor 10 or more in respect to those obtained using SQ programs which are not adjusted to sample specific conditions.

In calculating the background

They say:
FS aerow peak automatically measures background on either side of the peak as as a result, more accurate net peak intensities are obtained.

We say:
For simple cases, involving a peak without any spectral interference in its vicinity, the background under the peak can be easily calculated in this way.

However a typical “real life” situation involving background measurements on either side of an analyte line which is heavily interfered with, will present problems for SQ programs relying on finding suitable background measuring positions in the vicinity.

In such cases UniQuant accurately determines the background by measurements across the complete spectral range unlike limited range FS scanning which may result in an overestimation of background.

In confirming the presence of an element by using other lines of the same element

They say:
SQ programs offer the possibility of alternative line selection in cases where the principle line (usually Ka) of an element not expected to be present shows a net intensity.
In such cases additional scans over wider ranges can be made in order to verify the presence of other element lines (e.g. Kb, La)î.

We say:
UniQuant does not require additional measurements or checks due to its special unique algorithem, and in fact, for each peak intensity measured, a full report is given of its components e.g.

- Background continuum in equivalent mg/kg.
- Spectral impurity in equivalent mg/kg.
- Spectral line overlaps in equivalent mg/kg and from which elements.
- Counting error in equivalent mg/kg (only possible with UniQuant which measures for fixed times at the spectral line of interest.).

Conclusions

The combination of UniQuant 5 with the present generation of high power, high performance X-Ray spectrometers offers the potential for improved analytical performance for the analysis of completely unknown samples.

When compared to conventional SQ programs (based on Fine-Step-Scanning) Uniquant 5 provides a faster, more accurate and reliable means of both major and trace element determination in a wide variety of materials and sample types.

lines from unexpected elements. It should be clear that such specific approach may not work for less well known samples.

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