

Qualitative XRF Data and Quantitative XRF Data

XRF is often thought of as a “black box” where a user can place a sample into the instrument and consequently the instrument will provide a quantitative elemental composition present in the sample. Although the instrument will indeed provide a “quantity” of the various elements present in samples – the accuracy and repeatability of these quantities should not be trusted or reported.

Qualitative XRF Data:

Qualitative XRF data is the essentially the raw data the instrument provides when analyzing a sample. This is the number of counts detected by the XRF detector from the element-specific fluorescent X-rays, displayed in graphical format. In the outputted spectrum, the x-axis displays the energies detected and the y-axis represents the counts detected at each energy.

This raw data is considered qualitative because it shows what elements are present (fluorescent X-rays are elements specific) but it does not provide information regarding how much of each element is present. Thus, just running an XRF spectrum knowing nothing about the sample is an excellent tool for elemental identification – essentially what elements are present in the sample. However, to get the amounts of the elements present, true elemental composition, requires further processing and normally many standards and/or calibrations.

Quantitative XRF Data:

Quantitative XRF is much more involved and, in the end, the user will obtain the quantities of elements present in a sample with accuracy that can be trusted. The best way to obtain quantitative XRF data is by making calibration curves, this requires the use of standards or samples of known concentration. Essentially a set of samples of known concentrations, containing the elements of interest, are run by the XRF to relate peak heights/intensities to known concentrations. Once this is achieved, the unknown sample is run against the curve so that its “height” can be calibrated for concentration.

For the best accuracy achievable with XRF data, there are 4 main criteria that should be met:

1. Calibrants/known samples used for calibration should be an appropriate material for the unknown materials being analyzed (ie don't use a solid metal reference for a powdered material sample)
2. Samples should be homogeneous
3. You must have samples/standards of known concentration available in order to create calibration plots.
4. Sample must be “infinitely thick” – meaning it is thick enough to attenuate the X-rays from the XRF. (Guidelines – for metal samples – make sure they cover the entire window of the instrument, for soils/loose powders ensure the material as at least an inch thick worth of samples after compacting)

If you cannot meet the above requirements, you can process the raw data so that you can compare results between similar samples. For instance, by curve fitting the peaks of interest (elements of interest) you can obtain a relative amount of a specific element present in the sample (the area under the curve for the specific element). Doing this for samples that you wish to compare can be done such that you can compare the relative amounts of elements within different samples.