## WERG method for calculating concentrations from ICP data

The ICP gives results of the element concentrations in the liquid aspirated into the plasma, in mg L-1. Where these concentrations are below the detection limits of the instrument and method, the data become “censored.” This means that the ICP cannot determine the real concentration of the sample, which is somewhere between the detection limit and zero. When this occurs, the data are not real numbers and therefore prevent further calculations, including dry weight concentrations or means.

To deal with this problem, WERG has developed a calculation procedure which takes into account the detection limit and results in a high estimate of the concentration. For example, if you used “zero” in place of all data below the detection limit (<DL), you could artificially skew your values lower than the true value, and thus obtain more statistically significant differences between experimental treatments. By replacing all <DL values with the calculated detection limit, you will prevent this and report conservative differences between treatments.

The instrument detection limits (DL) are calculated by three times the standard deviation of the mean of ten measurements of the calibration water blank, given in units of mg L-1. When analyzing solid samples that have been digested, the method detection limit (MDL) is the lowest value of confidence for the instrument given in units of mg kg-1. This is calculated by dividing the DL by the typical weight of the samples in the digestion solutions.

For QA/QC there are a number of strategies: running duplicate samples, using standard additions, and/or comparing the results with samples of a known concentration (certified reference materials, CRM). These are usually a material of the same type as the samples, whether soil, plant material, animal tissue. This material is treated as additional samples in the digestions and then the final concentrations are compared with values derived from multiple certified laboratories. The percent recovery is calculated to measure the deviation between analyses. These are not always comparable due to different digestion methods and instrument capabilities, but they give an estimate of recovery.

The following is a list of the procedure for calculating conservative concentration values in mg kg-1:

1. Determine the DL of the instrument.
2. Calculate the mean blank amount.
3. Subtract the blank from the sample concentrations mg L-1.
4. Multiply the concentration by the total extraction volume and the dilution factor, then divide by the sample weight = concentration in mg kg-1.
5. Determine the MDL by multiplying the DL by the typical sample extraction volume and the dilution factor, then dividing by the typical sample weight = concentration in mg kg-1.
6. Replace all sample concentrations which are below the MDL with the MDL value – this allows for further statistical analysis of the data.
7. Calculate the mean CRM concentration.
8. Compare the percent recovery of each element wavelength, keeping in mind differences in method etc.
9. Retain the wavelengths with the best recovery.
10. Compare the concentration results for each sample between different element wavelengths. If they are similar, consider using the mean or select one to report. Where they are very different, this may result from spectral or matrix interferences in the samples. In this case, you should review the spectra for causes of this difference. If no interferences are immediately apparent and correctable, reject the lines which are quite different from the others.
11. Where 50% or more of the samples are below the MDL, interpret this as all the samples being below the detection limits