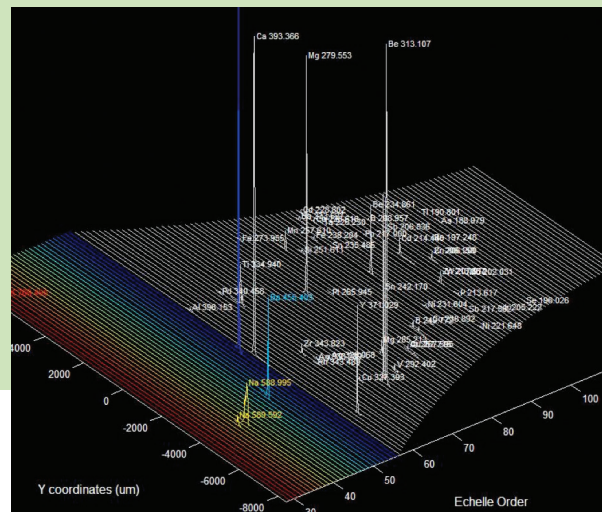


Universal Data Acquisition in Syngistix Software for Avio 550/560 Max ICP-OES

ICP-Optical Emission Spectroscopy



All the Data All the Time

Introduction

Historically, inductively coupled plasma (ICP) spectroscopy has been used for the analysis of multiple analytes with excellent speed, sensitivity and large linear dynamic range. Early ICP instruments used photomultiplier tubes for the analysis of single wavelengths, one at a time. Introduction of solid state detectors allowed for the simultaneous acquisition of all wavelengths and background information, resulting in data-rich analyses. However, even with these advances, most users still only utilize one wavelength per analyte, leaving the analyst with several questions:

- Did I use the best wavelength?
- What if I need information for another analyte?
- How can I achieve the appropriate detection or reporting limits?
- How can I handle all of the interferences in emission spectroscopy and still obtain the correct result?

Universal Data Acquisition (UDA), a proprietary feature within Syngistix™ for ICP software available on the Avio® 550/560 Max ICP-OES, addresses all of these questions by allowing for the simultaneous acquisition of all available wavelengths all of the time with a click of the mouse. UDA is much more than a semi-quantitative application. It will provide quantitative results without requiring a separate mode of analysis, uses virtually no extra storage space and can be added during your normal routine analysis. The resulting advantages of UDA are:

- Easy data validation
- Access to all analytes all the time – no reruns necessary
- Easy to establish reporting limits for any analyte
- Unmatched interference correction capabilities

Let's look at how UDA can help with several real-life case scenarios.

CASE 1 Is Your Data Validation Time Consuming?

One of the most important processes for an analyst is data validation. It is critical that the certainty of every reported result be known. With UDA, if any uncertainty exists with the results, it can be alleviated without ever rerunning the sample. In fact, multiple wavelengths can be reprocessed for each element to determine or confirm the correct result. Let's look at an example.

Let's say a performance test (PT) sample with an expected chromium (Cr) concentration of 0.020 ppm was measured but yielded a concentration of only 0.014 ppm – a 70% recovery, as shown in the Table 1. The test fails, which normally requires that the sample be rerun.

Table 1. Example of performance test without UDA.

Analyte	Mean Corrected Intensity (cps)	Concentration (ppm)	% Recovery
Cr 267.716	2203	0.014	70

With UDA, all that's required is to add other chromium lines to the method and hit the reprocess button. No reruns are necessary because UDA has already collected all information. After adding the other Cr lines and reprocessing, Table 2 shows that the Cr 205.560 line gives 100% recovery without re-running the calibration curve and sample. UDA not only saves precious time but can ensure accurate results.

Table 2. Example of performance test with UDA capability implemented.

Analyte	Mean Corrected Intensity (cps)	Concentration (ppm)	% Recovery
Cr 267.716	2203	0.014	70
Cr 205.560	1110	0.020	100
Cr 283.563	5015	0.022	110
Cr 284.325	2502	0.025	125
Cr 357.869	1561	0.024	120
Cr 206.158	1197	0.021	105

CASE 2 Tired of Re-running an Analysis for Additional Analytes?

Whether a lab is analyzing internal samples or those for an outside client, the potential for additional analyte requests exists. In some cases, the results reported initially may indicate a need for further analytical testing. At other times, changes to regulations may prompt a re-investigation of previous samples for new analytes. These requests may occur hours, days or even years later. UDA coupled with the UDA Standards Kit provide the capability to reprocess that data to include these new analytes without the need to rerun, as in the example below.

Have you ever run a sample for five analytes and been asked to reanalyze the sample for a sixth? With the combination of UDA

and the UDA Standards Kit, there is no need to recalibrate and rerun the sample. Just add the additional analyte(s) you need to the method and reprocess. The UDA standards contain virtually the entire periodic table, so you have already calibrated for all analytes even if you did not "run them" initially. If you started with a simple method, just add the additional analytes you would like into the method (as shown in Figure 1) and reprocess for quantitative results. UDA provides access to over 6,000 different analytical lines. The resulting echellogram allows all the selected analytes to be presented in a simple way.

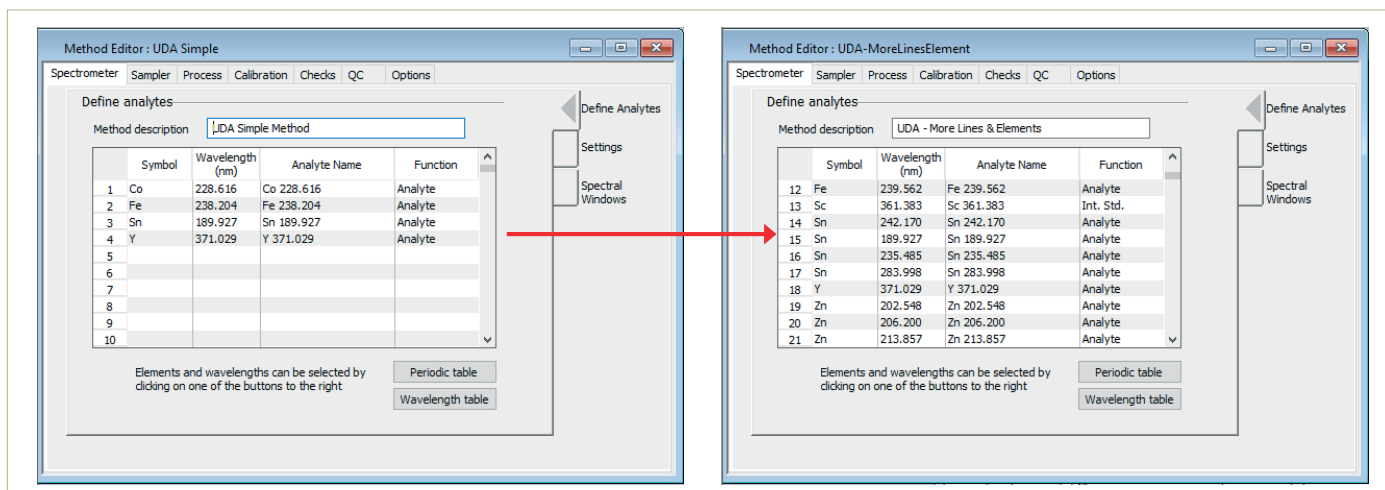


Figure 1. Example of adding elements to a method for UDA.

CASE 3 Determine Reporting Limits for All Wavelengths

Another common issue is determining whether or not the wavelength being used has the appropriate reporting limit for the analysis. Once again, most users run one wavelength and establish a reporting limit for only that wavelength. With UDA, the user can determine thousands of reporting limits at once and can simply choose the best one for the analysis, as in the following example.

Let's say that you included Mn at 257.610 nm in your method and then ran your IDLs, MDLs, or reporting limits on three non-consecutive days. That is a lot of time lost if you need to rerun it.

With UDA, you don't: just add the other Mn lines into your method, reprocess, and now you have validated limits for Mn 257.610, Mn 259.372, Mn 260.568, Mn 279.482, Mn 293.305, Mn 294.920 and Mn 403.075, as shown in Figure 2. If the UDA Standards Kit is used for the calibration, you can have reporting limits and MDLs for thousands of wavelengths.

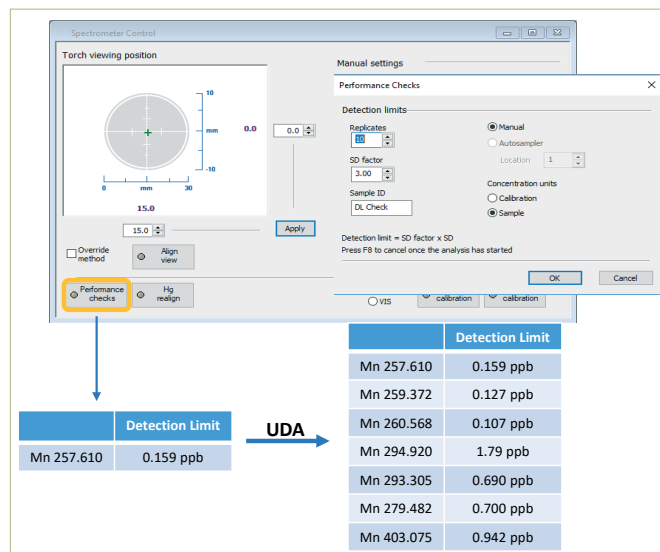


Figure 2. Example showing how adding analytes to a method can be added with UDA to determine detection limits without having to re-run anything.

CASE 4 Interference Correction by Interelement Correction (IEC) or Multicomponent Spectral Fitting (MSF)

In a typical analysis, the user must contend with perhaps tens of thousands of emission lines that may interfere with the chosen analyte line. Many regulated analyses require interference correction. It is important to confirm that the correct line is being used for the matrix being run. How can the optimal correction model be created? And, if the model being used is not correct, must the entire method development process be repeated? UDA is an easy answer to these questions without requiring re-analysis or new method development. UDA saves an immense amount of setup time and will improve laboratory productivity. Let's see how.

Interference Correction

All the interference solutions that are needed for the calculations have been run with UDA activated, thereby acquiring all the data for all the wavelengths. Simply use the IEC or MSF tool, choose your alternative correction wavelength or profile, and reprocess with the new model, as shown in Figure 3. There is no need to start over with method development.

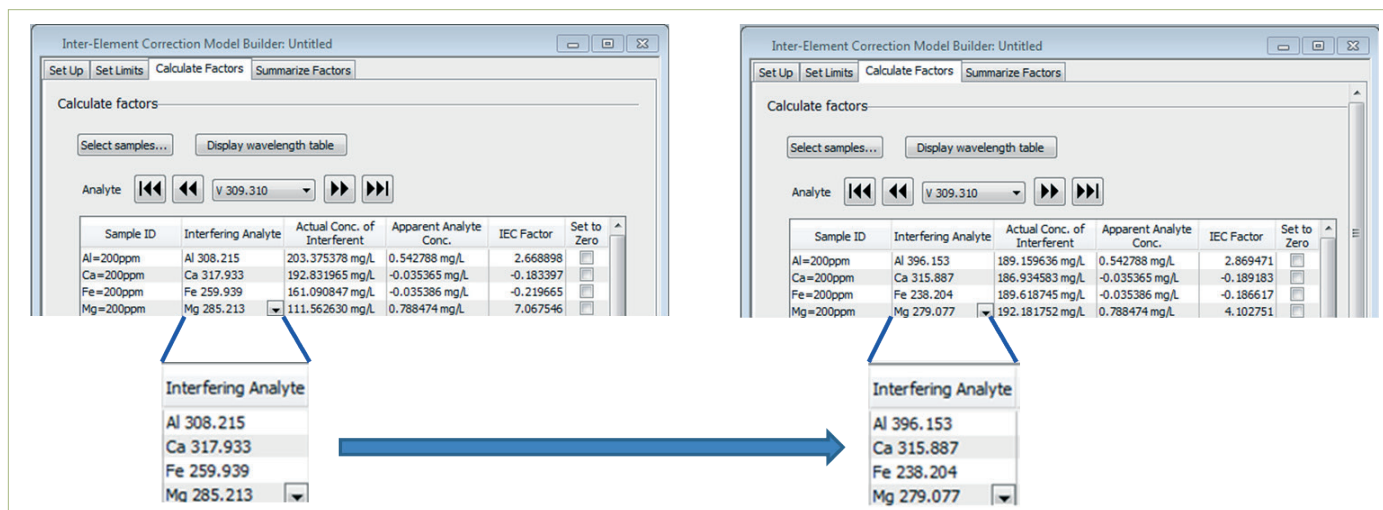
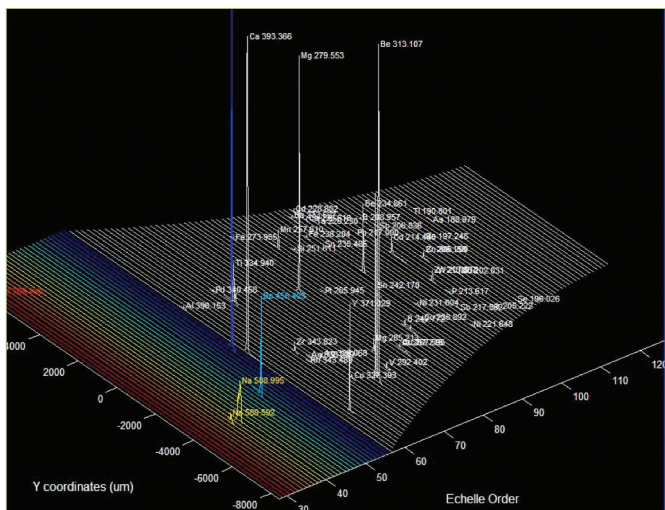


Figure 3. Example of updating IECs by adding new wavelengths with UDA.

Summary

Universal Data Acquisition, only available on the Avio 550/560 Max ICP-OES, is a unique tool that acquires data for all available wavelengths. This ability allows results to be attained for analytes not in the original method: simply add the desired elements and wavelengths to the method and reprocess the data to attain accurate results for new analytes. The outcome: simplified data validation, access to all analytes without having to rerun samples, easily established reporting limits, and improved interference correction capabilities. UDA enhances a lab's capabilities and increases confidence in results.



Echellogram showing a number of peaks with analytes added via UDA.



UDA Standards Kit (Part No. N9306225).

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