

Spectroscopy Performance Note

Pseudo Elements: Use, Format, Example, Explanation & Discussion

Usage

An operator can utilize a pseudo element to assist in obtaining the correct analytical result between two analytical wavelengths, or as a calculator for a carbon equivalent. It should be noted that two analyte lines are required, one sensitive and one secondary, in case of sensitive line saturation or self-absorption. It is also possible to use the same wavelength for wide dynamic ranges by splitting the working curve into two separate curves—one covering the low and the other covering the high concentration ranges. Pseudo elements return the result of a comparative equation that the user defines in the GDS software.

Format

If the equation is set using a non-logical approach, an incorrect result will be displayed. When the equation is set correctly, however, it can simplify the testing process. When two lines are encountered for the first time, a new user may be confused as to which is more applicable. Once the equation has been entered and proven, the results for analytical lines can be hidden and only the pseudo element reported.

Example

Pseudo: Cr_calc

Formula: @IF([Cr_high]<V%,[Cr_low],[Cr_high])

[Cr_high] is less sensitive and is set for the high side of the working curve. Some degree of accuracy is needed toward the lower end of the curve so that normalization is not adversely affected. The use of the less than sign (<) as the comparator is strongly recommended.

"V%" is a switch point. It is a numerical Value representing percent of concentration that is logically compared to [Cr_high]. If [Cr_high] is found to be less than "V%", then the pseudo element "Cr_calc" will report the [Cr_low] result. "V%" needs to be validated in every method. It shall be set at a value where [Cr_high] maintains its accuracy and where [Cr_low] is now equally or more accurate.

Tips and Hints

- **Proper syntax is important! Pay attention to details!** When entering the formula, count the number of parenthesis (). The number of opening parenthesis should equal closing parenthesis. Be sure to use the exact name of the element in brackets []; e.g. [Cr425] not (Cr) or Cr.
- [Cr_low] is the more sensitive wavelength. [Cr_low] is the low concentration range of the working curve. It will give excellent analysis from the bottom up to "V%". More sensitive lines typically have lower standard deviations within their working range.
- When validating "V%", do not allow it to fall close to the user limit or range. Do not allow the pseudo to toggle back and forth at the switch point between the high and low curve sets.
- Use more decimal places to control the equation; e.g. enter "1.xxx", not just "1".



GDS500A

Discussion

1. Logistics for wavelength selection.
 - a. Choice of suitable analytical wavelengths may be limited necessitating separation of high and low concentrations at the same wavelength.
 - b. Curve fit between the low concentrations and high concentrations may benefit from using two analytical lines.
 - c. Separation of high and low concentrations allows them to be drifted independently.
 - d. Separation of high and low concentrations allows them to ratio to independent matrix wavelengths.
2. The "low" analyte should not be in control of deciding which result to report.
3. Working curves for sensitive wavelengths shall be linear. Avoid approaching saturation.
4. The ordering of elements is critical. Set the high curve on top of all other analytes of the same element. This is important for normalization to work.
5. When adjusting calibration curves start with the elements of highest concentration first and work down.
6. A method that contains three or more pseudo elements should be considered for cloning. It is perfectly acceptable to have multiple pseudo elements, however, for the sake of keeping the method clean, avoiding cockpit type errors and diagnosis of problems it is recommended that the method be split and dedicated to a specific alloy or family. This will reduce the need for multiple curves for "every" element.

Pseudo Element Table Examples

Pseudo Name	Formula	Range of "V"	Application Method
Cr_Calc	@IF([Cr357]<V%,[Cr425],[Cr357])	0.900 - 1.200	LAS, CI
Cr_Calc	@IF([Cr396]<V%,[Cr357],[Cr396])	10.000 - 15.000	STAINLESS
Ni_Calc	@IF([Ni225]<V%,[Ni341],[Ni225])	3.000 - 15.000	STAINLESS
Mo_Calc	@IF([Mo441]<V%,[Mo386],[Mo441])	10.000 - 16.000	NICKEL
Mn_Calc	@IF([Mn404.1]<V%,[Mn403.1],[Mn404.1])	3.500 - 8.000	LAS + Mn
Al_Calc	@IF([Al309]<V%,[Al396],[Al309])	1.000 - 5.000	COPPER
Si_Calc	@IF([Si288]<V%,[Si288.1],[Si288])	1.000 - 1.100	example using 1 wavelength w/2 curves
CE (carbon equivalent)	@ABS(((C165)+([Si288]+[P188])/3))	—	CAST IRON (all kinds, formula varies)



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