

LabSpeed: Reporting a different Species

Abstract:

Many times, it is important to report a result in a different form than the result that is generated by the instrument software. For example, it might be beneficial to report the concentration of elemental Calcium (Ca) as Calcium Carbonate (CaCO₃), or Magnesium (Mg) as Magnesium Oxide (MgO).

In this solution, a LabSpeed User Table is employed as a lookup table for species name and correction factor. The correction factor is applied in the Research Grid View to produce new data columns that contain the corrected output. Finally, the corrected output is displayed in a report.

LabSpeed Solution:

Step 1. Create a “Custom” User Table that contains an element symbol lookup column, a column for the corresponding Species Name and a column for the Factor.

User Table Column Properties

Column	Type	Usage
ElemSymb (lookup)	string	Element Lookup
SpeciesRpt	string	Label used for reporting
SpeciesFactor	double	Conversion Factor

Assign the User Table Reference Name (e.g. “Species”). Fill the table with the elements you wish to report as a different species. Leave out the ones that will report normally. The example below contains only two elements that will be reported as a different species.

User Table : Species		
ElemSymb	SpeciesRpt	SpeciesFactor
▶ Ca	Ca as CaCO ₃	2.4974
Mg	Mg as MgO	1.6583

The Factor was calculated as a ratio of the molecular / atomic weight.

Step 2. Reference the User Table in the Session Research Grid View by clicking on the “Value Columns” toolbar button in the Research Grid Designer. When finished, data rows that match the element symbols will be filled with the lookup values; those that don’t will be left blank.

Step 3. Add two Formula columns to the Elements table in the Research Grid Designer – one called “ElemRpt” to hold the reported element label (string) and one called “AverageRpt” to hold the corrected concentrations (double). These are formula columns

and so are filled using a formula. Formulas are typically entered using the click-and-drag Formula Builder, but may be entered manually as shown below:

Enter the following formula for the “ElemRpt” column:

```
if( isblank([SpeciesRpt] ), [ElemSymbol] , [SpeciesRpt] )
```

This formula checks to see if there is a SpeciesRpt entry for this element. If not, it assigns the normal element symbol; if so, then it assigns the SpeciesRpt element label.

Enter the following formula for the “AverageRpt” column:

```
if( isblank([SpeciesFactor] ), [Average] , [Average] * [SpeciesFactor])
```

This formula checks to see if there is a SpeciesFactor for this element. If not, it assigns the normal average concentration; if so, then it assigns a corrected average for this element.

The formula returns an unformatted value. Using the “sigfigs” function, the returned value may be formatted to 4 significant figures as shown below by extending the formula:

```
sigfigs(if( isblank([SpeciesFactor] ), [Average] , [Average] * [SpeciesFactor] ), 4)
```

The Research Grid will appear as below. SpeciesRpt and SpeciesFactor are filled for any element that matches the lookup row in the User Table. The added formula columns (header in green) contain updated values when a species factor exists, otherwise it contains the original value in the table.

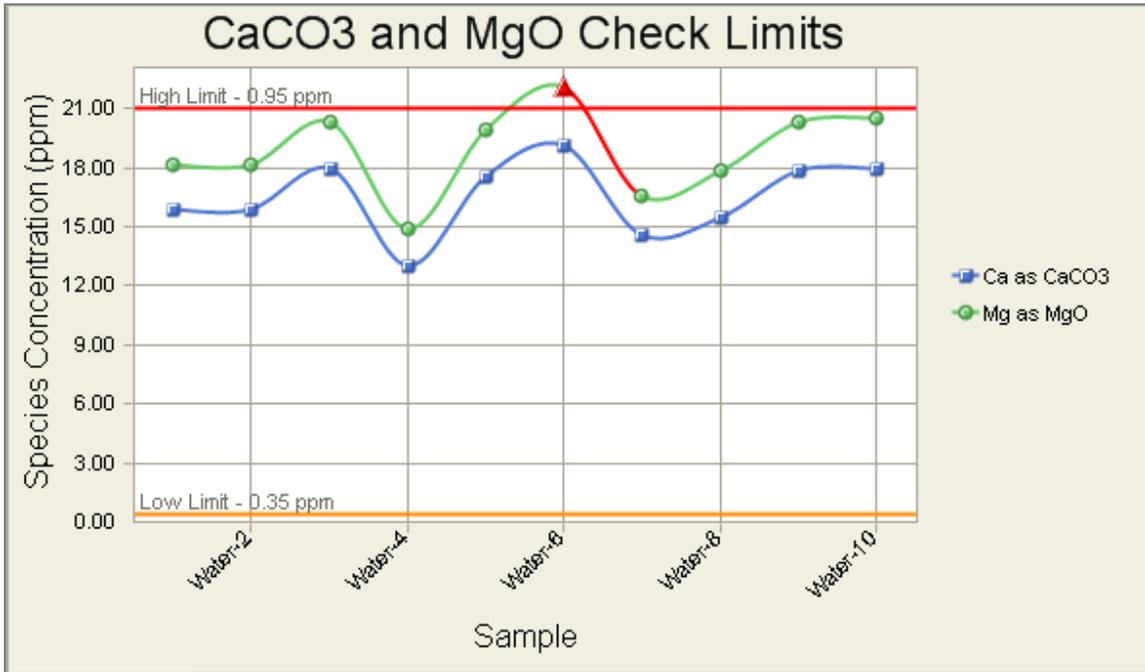
	Water-6	Unknown	5/2/2006 3:41:11 PM		WaterDemo	Section AJ72	1.1
	ElemSymbol	Units	Average	SpeciesRpt	SpeciesFactor	AverageRpt	ElemRpt
+	As	ppm	6.06310963067993			6.063	As
+	Ca	ppm	7.66249861427771	Ca as CaCO3	2.4974	19.14	Ca as CaCO3
+	Cu	ppm	4.39153604676863			4.392	Cu
+	Hg	ppm	1.91202792215952			1.912	Hg
+	K	ppm	24.7799237613445			24.78	K
+	Mg	ppm	13.3215982246017	Mg as MgO	1.6583	22.09	Mg as MgO
+	Na	ppm	36.4028133829749			36.40	Na
+	Pb	ppm	1.10228233399336			1.102	Pb
+	S	ppm	27.3608311075393			27.36	S
+	Zn	ppm	0.825025478937259			0.8250	Zn

The *AverageRpt* and *ElemRpt* data columns are available to all other Views in LabSpeed, including Tables, Charts and Reports as shown below.

Table

SampleName	As	Ca as CaCO3	Cu	Hg	K	Mg as MgO
Water-1	4.958	15.90	3.632	1.594	20.34	18.19
Water-2	4.992	15.92	3.632	1.593	20.46	18.18
Water-3	5.587	17.99	4.102	1.788	23.12	20.33
Water-4	4.105	13.04	3.004	1.299	16.86	14.89
Water-5	5.505	17.61	4.000	1.738	22.43	19.93
Water-6	6.063	19.14	4.392	1.912	24.78	22.09
Water-7	4.584	14.59	3.343	1.451	18.80	16.55
Water-8	4.911	15.53	3.577	1.547	20.01	17.87
Water-9	5.601	17.90	4.109	1.775	23.08	20.38
Water-10	5.609	17.95	4.092	1.780	22.95	20.54

Chart



Report

Water-6		5/2/2006 3:41:11 PM		Unknown	
Method	WaterDemo	Element Name	Average	Std Dev	%RSD
User		As	6.063	0.0504	0.8304
Corr Factor	1.1	Ca as CaCO3	7.662	0.0378	0.4935
Sample Wgt	1	Cu	4.392	0.0170	0.3860
Initial Vol	1	Hg	1.912	0.0206	1.0763
Final Vol	1	K	24.78	0.1968	0.7942
Folder	Section AJ72	Mg as MgO	13.32	0.0403	0.3023
Comment:		Na	36.40	0.2501	0.6871
		Pb	1.102	0.0086	0.7782
		S	27.36	0.2440	0.8917
		Zn	8.250	0.0033	0.3941