LIMS Requirements for Correct Use of Significant Figures and Rounding for Regulatory Compliance

Simple Mathematics and How It Impacts You

IMPORTANT NEWS

- Letter from Dr. Michael H. Shapiro
  Acting Assistant Administrator
  EPA Office of Water
  July 11, 2017

Part 1 of the Letter

- The Office of Water continues to recognize WSG 21 as an accurate approach when reporting drinking water compliance data.
- The regulatory limits established as Maximum Contaminant Levels (MCL) are expressed with the applicable number of significant digits permitted by the accuracy and precision of the specified analytical procedure.
- Drinking water health advisories, ambient water quality criteria and technology-based effluent limits are similarly expressed with the applicable number of significant digits.

Part 2 of the Letter

- In addition, for both SDWA and CWA compliance measurements, the EPA allows primacy agencies and permit writing authorities the flexibility to adopt the approach identified in "Standard Methods for the Examination of Water and Wastewater", 1050 B, 22n d Ed.

EPA Rounding Requirements-WSG 21

- All Maximum Contaminant Levels (MCL) contained in the National Interim Primary Drinking Water Regulations are expressed in the number of significant digits permitted by the precision and accuracy of the specified analytical procedure(s).
- **Data reported to the State or EPA should be in a form containing the same number of significant digits as the MCL.**

- In calculating data for compliance purposes, it is necessary to round-off by dropping the digits that are not significant. The last significant digit should be increased by one unit if the digit dropped is 5, 6, 7, 8 or 9. If the digit is 0, 1, 2, 3, or 4, do not alter the preceding number.
- Chemical and radiological data may be treated in like manner. Analytical results for mercury of 0.0016 would round off to 0.002 while 5.4 pCi/l of combined radium-226 and radium-228 would round down to 5 pCi/l.
  - *Joseph A. Cotruvo, Ph.D., Director Criteria and Standards Division, ODW (WH-550), April 6, 1981*

The Basics

- Do You Know the Details of This Excellent Mathematical Processes?

Which Regulation/Consensus Organization Defines Significant Digits and Rounding for Data Reporting??

Regulation/Consensus Organization	Yes/No
40 CFR part 141	NO
40 CFR part 136	NO
TNI (2007, 2016)	NO
WSG 21	YES
Standard Methods for the Examination of Water and Wastewater (22nd Ed.)	YES
ASTM E 29-13	YES

Rounding (Mult.,Div.,Sqrt., etc.)

- Standard Methods for the Examination of Water and Wastewater, 22nd edition, 1050
  - As a starting point, round off the results of any calculation in which several numbers are multiplied and divided to as few significant figures as are present in the factor with the fewest significant figures.
  - If the number 56 is an exact number (a count or a mathematical constant such as π), it has no error associated with it and is considered to have unlimited significant figures.
  - Standard deviations and standard errors often should be reported with extra digits (compared with single measurements) because they are calculated from variances and because they are square roots.

Decimal Point

- Significant Digits – Number of digits in a figure that express the **precision** of a measurement instead of its magnitude. The easiest method to determine significant digits is done **by first determining whether or not a number has a decimal point.**
  - START counting for sig. figs. On the FIRST non-zero digit.
  - STOP counting for sig. figs. On the LAST non-zero digit.
  - **Non-zero digits are ALWAYS significant**
  - Zeroes in between two non-zero digits are significant.
  - **All other zeroes are insignificant.**

SDWA MCLs

- https://www.epa.gov/ground-water-and-drinking-water/national-primary-drinking-water-regulations
- Chlorite 1.0 mg/L
  - Significant Figures 2
- Fluoride 4.0 mg/L
  - Significant Figures 2
- Nitrite 1 mg/L
  - Significant Figures 1 !!!!

POP QUIZ

What Should Be Reported ????

- MCL for Nitrate
  - 10 mg/L
- What is the Number of Significant Figures?
  - **2 ?**
  - **1 ?**
- If The Lab Determines a Result of 10.48, What Is The **Regulatory** Value For The Client?
  - 10.48 ?
  - 10.5 ?
  - 10. ?
  - 10 ?

Regulatory SDWIS Database False Violations

Laboratory Reporting Data to SDWIS

- Drinking Water Plant Laboratory Report
  - The Drinking Water Plants Nitrate is Determined by the Laboratory as 10.48 mg/L
  - That Result is Entered into SDWIS.
  - Laboratory or State Fails To Round Result to MCL
  - **Drinking Water Plant Receives a NOV**

NPDES Database Has The Same Problem

- Iowa DNR's Response:
  - A regulated facility must report the data received from their laboratory without manipulation. **If they are concerned with a compliance determination that does not account for accurate use of significant digits, then they could request that their contract lab provide data to the level of significant digits equivalent to those in the facility's permit limits.** Then the facility can report exactly what is received from the lab without concerns.

Let's See What We Know

- What Would a Regulator Do???

Calculate the MDL (40 CFR 136 Appendix B)

Which MDL Is Correct???

MDL = sdev × 3.143

Standard Concentration	**2.**	**mg/L**
Student T	**3.143**	
#	Raw Data	
1	2.752	mg/L
2	2.014	mg/L
3	2.159	mg/L
4	3.011	mg/L
5	2.451	mg/L
6	2.641	mg/L
7	2.048	mg/L
MDL (mg/L)		
Standard Deviation	0.38253665	**1.202313**
Standard Deviation	0.3825	**1.2022**
Standard Deviation	0.382	**1.200**
Standard Deviation	0.38	**1.19**

Incorrect Logic

Higher Than Acceptable MDL

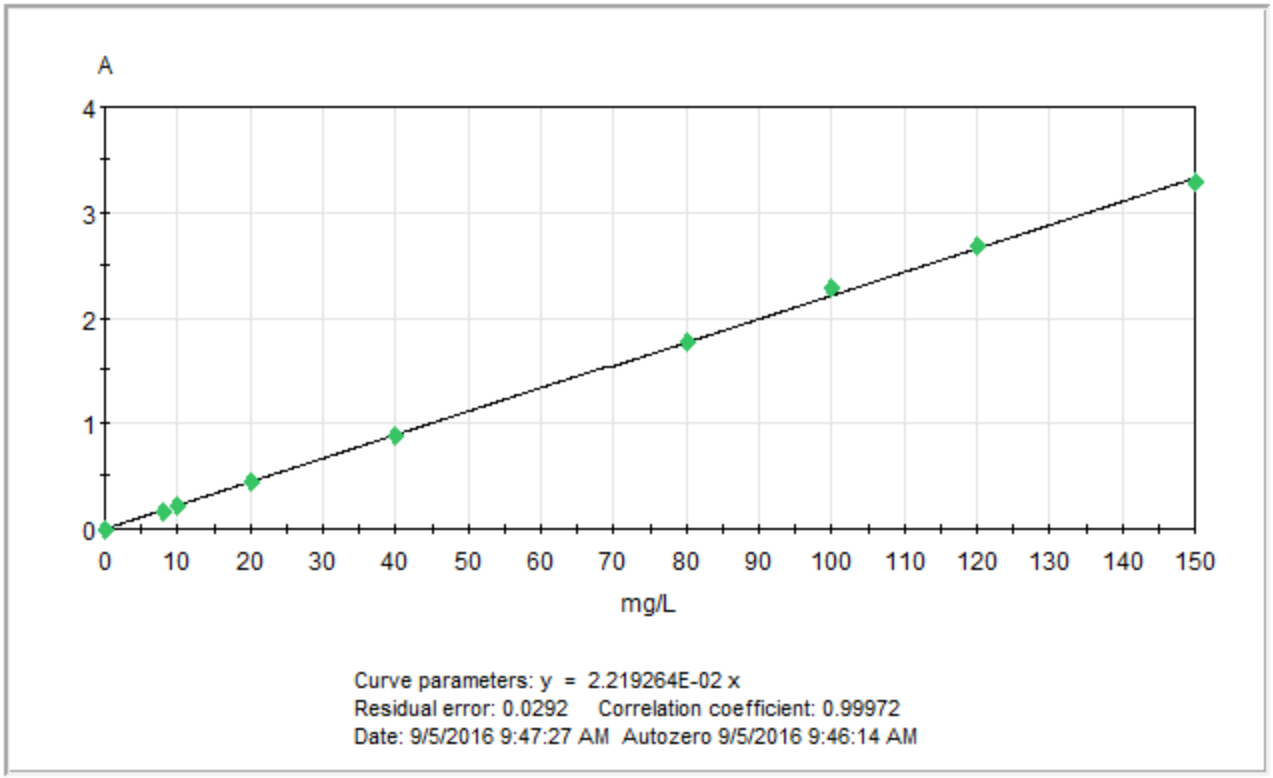
Standard Concentration	**2**	**mg/L**
Student T	**3.143**	
#	Raw Data	
1	3	mg/L
2	2	mg/L
3	2	mg/L
4	3	mg/L
5	2	mg/L
6	3	mg/L
7	2	mg/L
MDL		
Standard Deviation	0.53452248	**1.680004167**
Standard Deviation	0.5345	**1.6800**
Standard Deviation	0.535	**1.680**
Standard Deviation	0.53	**1.68**
Standard Deviation	0.5	1.6
Round to Unit		**2**

What Is Impacted by This Incorrect MDL Calculation?

- 40 CFR part 141 PROMULGATED METHODS!!
  - Some Require the **LRB < MDL!**
  - Some Require the **LRB < 2.2 x MDL!**
- A Higher Than Significant Digit Calculated MDL will allow **Failing LRBs to PASS!!!**

Other Significant Digit and Rounding Concerns

- Machine Software and Calculations That are Beyond Your Control



Given the Standards Concentration

What Can Be Used??

1. Slope
2. Correlation Coefficient (r^2)
3. What is the Result To Be Reported

Standards

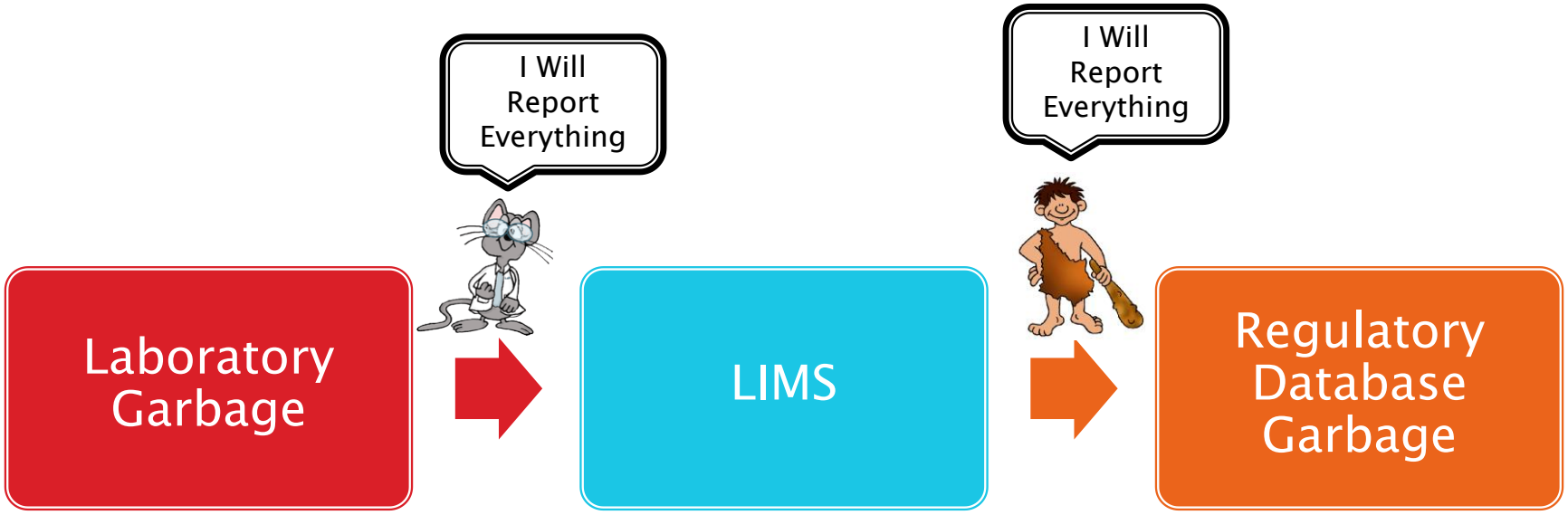
No.	Concentration [mg/L]	Ordinate [A]	Error [A]	Used
1	0.000	0.000	0.000	Yes
2	8.000	0.177	-0.001	Yes
3	10.000	0.227	0.005	Yes
4	20.000	0.445	0.001	Yes
5	40.000	0.890	0.003	Yes
6	80.000	1.782	0.006	Yes
7	100.000	2.280	0.061	Yes
8	120.000	2.674	0.011	Yes
9	150.000	3.275	-0.054	Yes

CHK2-...g-L_1 1	0.274	12.342
CHK2-...g-L_2 1	0.274	12.342
CHK2-...g-L_3 1	0.274	12.342
CHK2-...g-L_4 1	0.274	12.342
CHK2-...g-L_5 1	0.274	12.346
	Mean value	12.343
	Std.dev.	0.002
CHK3-...g/L_1 1	1.107	49.877
CHK3-...g/L_2 1	1.107	49.877
CHK3-...g/L_3 1	1.107	49.877
CHK3-...g/L_4 1	1.107	49.877
CHK3-...g/L_5 1	1.107	49.877
	Mean value	49.877
	Std.dev.	0.000

So What Needs To Be Done???

- LIMS Management
- Regulators
- Auditors
- Laboratories
- Consensus Bodies (TNI)

Remember Garbage Flow



What Should Be Done Now!

- WSG 21 and Letter from Dr, Shapiro clarifys the reporting of data **ALREADY REQUIRED** either in Promulgated Methods or in the CFRs.
  - **THIS IS NOT GUIDANCE or a NEW RULE!!!**
- You (All of You) Should:
  - Differentiate between machine rounding and manual rounding.
  - Allow internal rounding done by instrument software outside of the analyst's control be recognized as such.
  - Identify rounding and significant digits that are under the analyst's control either through manual or instrument transfer into the LIMS be required to meet the rounding and significant digits requirements identified by recognized standards.

Questions?

- Opinions, Comments,
  But Save the Rotten Eggs