Methods of Evaluating Water Chemistry Data

Topics

- Data Quality
- Units and Conversion Factors
- Initial Data Review

Data Quality

Garbage In

Garbage Out

Data must be Accurate with Low Bias and High Precision

Accuracy

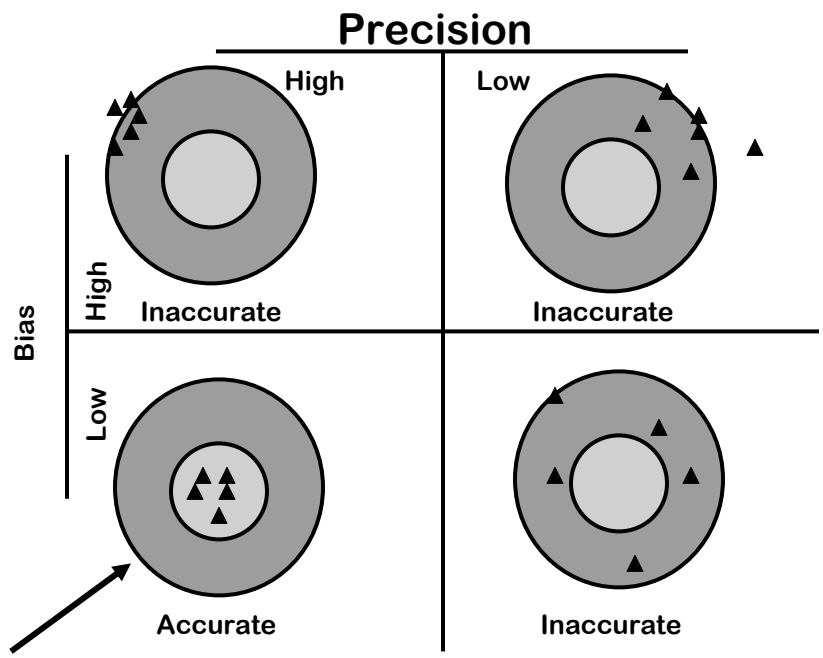
Combination of bias and precision that reflects closeness of a measured value to true value

Bias

Consistent errors of measured value from true value caused by errors in procedure

Precision

Measure of agreement among replicate analyses of a sample (standard deviation)



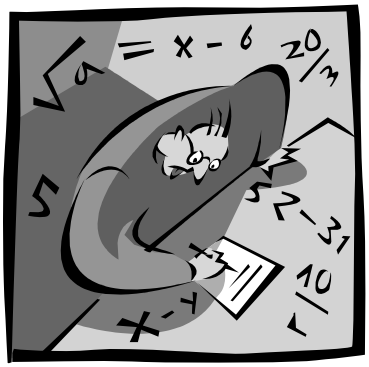
Units

PPM

Mg / l

μg / l

Meq / l



Weight-Per–Weight Units

Parts Per Million (PPM)

One part weight of dissolved mineral contained in one million parts by weight of water. This is the old U.S. system and not used today.

Weight-Per-Volume Units

Milligrams Per Liter (mg/l)

Mass concentration of dissolved solids per volume (liter) of liquid. SI system (metric) commonly used today. Generally for concentrations < 7000 mg/l 1mg/l = 1 ppm

Micrograms per liter (ug/l)

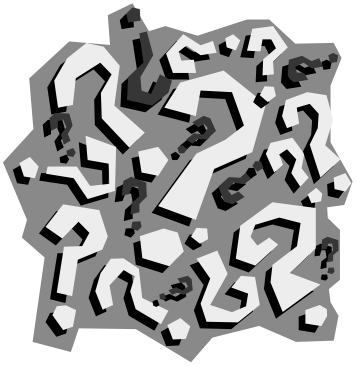
For trace elements many labs report values as ug/l. 1mg/l = 1000ug/l

Equivalent –Weight Units

Milliequivalents / liter (meq/l)

- Unit that recognizes that ions of different species have different weights and different electrical charges.
- In an analysis expressed in meq/l, unit concentrations of all ions are chemically equivalent.
- The total meq/l of cations should be equal to the total meq/l anions.

What Do These Units Mean?



Units of Measure Comparisons

Unit	1 Part / Million	1 Part / Billion	1 Part / Trillion
Length	1 inch /16 miles	1 inch / 16,000 miles	1 inch /16,000,000 miles
Time	1 minute /2 years	1 second / 32 years	1 second / 320 centuries
Volume	1 drop vermouth / 80 fifths gin	1 drop vermouth / 500 barrels gin	1 drop vermouth / 250,000 hogshead gin
Area	1 sq ft / 23 acres	1 sq ft / 36 sq miles	1 sq in / 250 sq miles
Quantity	1 bad apple / 2000 barrels	1 bad apple / 2,000,000 barrels	1 bad apple / 2,000,000,000 barrels

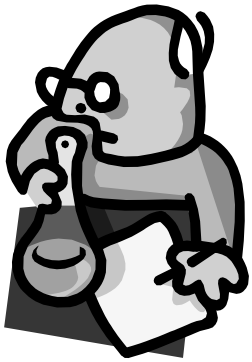
Initial Data Review

Checking for Correctness of Analyses

Cation/Anion Balance

Bad

Spot Data Checks



TDS

TDS Ratio

Good

Cation Anion Balance

$$\% \text{ difference} = 100 \times \left[\frac{\text{Sum Anions} - \text{Sum Cations}}{\text{Sum Anions} + \text{Sum Cations}} \right]$$

Units = meq/l

Criteria for acceptance = 5 – 10 %

Total Dissolved Solids (TDS)

- Sum of cations (mg/l) + Sum of anions (mg/l)
- Need a fairly complete chemical analysis (i.e., major cations and anions)
- TDS = [0.6 (alkalinity as $CaCO_3$) + Na^+ + K^+ + Ca^{+2} + Mg^{+2} + Cl^- + SO_4^{-2} + SiO_3^{-2} + NO_3^{-2} + F^-]

TDS Ratio

$$1.0 < \frac{\text{Measured TDS}}{\text{Calculated TDS}} > 1.2$$

TDS = sum of cations and anions in <u>mg/l</u>

Measured TDS should be higher than calculated TDS because a significant ion may not be included in the calculation.

Spot Data Checks

- Extreme values, either small or large, could indicate decimal error
- Compare to other samples from same site. Are there significant differences?
- Cation / Anion balance should be < about 5%
- Dissolved ion values < total ion values
- pH vs alkalinity – should not have low pH and high alkalinity

Spot Data Checks

- If carbonate is absent pH should be less than 8
- Ground-water sample should have low suspended solids
- Conductance > TDS
- Conductance multiplied by approx. 6 gives estimate of TDS

Spot Data Checks

- Common ionic ratios in ground water
  - NA>>K because the K is more readily removed from solution than Ca
  - Ca>=Mg because the most soluble minerals are sedimentary carbonates (calcite, dolomite and gypsum)
  - Ca>= SO_4 because the main source of sulfate is some variety of $CaSO_4$
  - In acid waters SO_4>Ca
  - Na>=Cl because the main source of Cl is NaCl and Na can have other sources

Class Exercise

Examine data table

Can you spot any problems?