Lecture #2

Intro: Expressions of Concentrations and Natural Abundance

(Stumm & Morgan, Chapt.1 & 3.4)
(Pg. 4-11; 97-105)
(Pankow, Chapt. 2.8)

(Benjamin, 1.2-1.5)
Molarity

- One mole of any substance contains $6.02 \times 10^{23}$ (Avogadro’s number) elementary chemical units (e.g., molecules).
- It is very convenient to measure concentrations in moles, since reactions conform to the law of definite proportions where integer ratios of reactants are consumed (e.g., 1:1, 1:2, etc.) on both a molecular and molar basis.
- It is calculated by:

\[
Molarity = \frac{mass}{L} \times \frac{1}{GFW}
\]

- Often use M, mM, µM (molar, millimolar, micromolar)
  - To represent: moles/L, $10^{-3}$ moles/L, $10^{-6}$ moles/L
Normality

- Like molarity, but takes into account the stoichiometric ratios of reactants and products
- Measured in equivalents per liter

\[ \text{Normality} = \frac{\text{mass}}{L \cdot \frac{GEW}{Z}} \]

- And Z is an integer related to the number of exchangeable hydrogen ions, or electrons the chemical has, or its overall charge

\[ GEW = \frac{GFW}{Z} \]
“Complete” water analysis

<table>
<thead>
<tr>
<th>Species</th>
<th>mg/L</th>
<th>meq/L</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bicarbonate</td>
<td>153</td>
<td>2.5</td>
</tr>
<tr>
<td>Chloride</td>
<td>53</td>
<td>1.5</td>
</tr>
<tr>
<td>Sulfate</td>
<td>19.2</td>
<td>0.4</td>
</tr>
<tr>
<td>Calcium</td>
<td>44</td>
<td>2.2</td>
</tr>
<tr>
<td>Magnesium</td>
<td>10.9</td>
<td>0.9</td>
</tr>
<tr>
<td>Sodium</td>
<td>25.3</td>
<td>1.1</td>
</tr>
<tr>
<td>Potassium</td>
<td>7.8</td>
<td>0.2</td>
</tr>
</tbody>
</table>
Anion-Cation Balance

- **Cations**
  - Ca\(^{+2}\)
  - Mg\(^{+2}\)
  - Na\(^{+}\)
- **Anions**
  - HCO\(_3\)^{-}
  - Cl\(^{-}\)

**Conc. (mequiv./L)**

- Total Hardness
- Carbonate Hardness
- Non-carbonate Hardness

- SO\(_4\)^{-2}
- K\(^{+}\)
Common Constituents

- N, P, and S containing compounds are often expressed in terms of their elemental concentration.

 Examples
  - 66 mg of $\text{(NH}_4\text{)}_2\text{SO}_4$ added to 1 L of water
  - 85 mg of $\text{NaNO}_3$ added to 1 L of water
Example: element/group conc.

Consider a solution of Ammonium Sulfate prepared by dissolving 66 g of the anhydrous compound in water and diluting to 1 liter. What is the concentration of this solution in:

a) g/L?
b) moles/L?
c) equivalents/L?
d) g/L as sulfate?
e) g/L as N?
Example (cont.)

- a) 66 g/L
- b) The gram formula weight of ammonium sulfate is 132 g/mole. So, using equation 2.7, one gets:
  - Molarity = \((66 \text{ g/L})/(132 \text{ g/mole})\) = 0.5 moles/L or 0.5 M.
- c) Without any specific information regarding the use of this solution, one might simply presume that either the sulfate group or the ammonium group will be the reacting species. In either case, Z should be equal to two (product of the oxidation state times the number of groups). So:
  - Normality = 0.5 moles/L * 2 equivalents/mole
  - = 1 equivalent/L or 1.0 N or N/1.
d) The GFW for sulfate is:
   - \( \text{GFW} = 32 + 4 \times 16 = 96. \)
   - The molarity of sulfate is:
     - \( \text{Molarity} = 0.5 \text{ moles-} (\text{NH}_4)_2\text{SO}_4/\text{L} \times 1 \text{ mole-} \text{SO}_4/\text{mole-(NH}_4)_2\text{SO}_4 \)
     - \( = 0.5 \text{ moles-} \text{SO}_4/\text{L} \)
   - Then, one gets
     - \( \text{mass/L} = \text{Molarity} \times \text{GFW} \)
     - \( = 0.5 \text{ moles-} \text{SO}_4/\text{L} \times 96 \text{ g-SO}_4/\text{mole-SO}_4 \)
     - \( = 48 \text{ g-SO}_4/\text{L} \)
e) The GFW for nitrogen is simply 14:

- The molarity of nitrogen is:
  
  \[
  \text{Molarity} = 0.5 \text{ moles-}(\text{NH}_4)_2\text{SO}_4/\text{L} \times \frac{2 \text{ moles-N}}{\text{mole-}(\text{NH}_4)_2\text{SO}_4} \\
  = 1 \text{ mole-N/L}
  \]

- Again, one gets:

\[
\text{mass/L} = \text{Molarity} \times \text{GFW} = 1 \text{ mole-N/L} \times 14 \text{ g-N/mole-N} \\
= 14 \text{ g-N/L \ or \ 14 g NH}_3\text{-N/L}
\]
Calcium carbonate units

- Used for major ion concentrations in drinking waters
  - Alkalinity
  - Hardness

- Since CaCO\textsubscript{3} is divalent (Z=2) and its GFW is 100 g, its GEW is 50 g
  - 50 g/equivalent or 50 mg/meq
  - 50,000 mg/equivalent
Elemental Abundance

- O
- Si
- Al
- Fe
- Ca
- Na
- Mg
- K
- Ti
- H
- P
- Mn
- F
Concentration of inorganics in fresh water

From: Stumm & Morgan, 1996; Benjamin, 2002; fig 1.1

Figure 15.1. Cumulative curves showing the frequency distribution of various constituents in terrestrial water. Data are mostly from the United States from various sources. (Adapted from Davies and DeWiest, 1966.)
Rock-WQ Connection

- Water Solutes reflect rock mineralogy; e.g.
  - Limestone
    - CaCO₃, mostly
  - Dolomite
    - CaMg(CO₃)₂, mostly
  - Gypsum
    - CaSO₄

“Stiff diagram”
From Hounslow, 1995
Water Quality Data; Analysis and Interpretation
• To next lecture