



**WRANE**

Water Research, Assessment  
and Networking Ecosystem

# What's in Water?

## Geochemical Evaluation

Presented by: Dr. Tracy Quan

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# How is water evaluated geochemically?



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# Outline

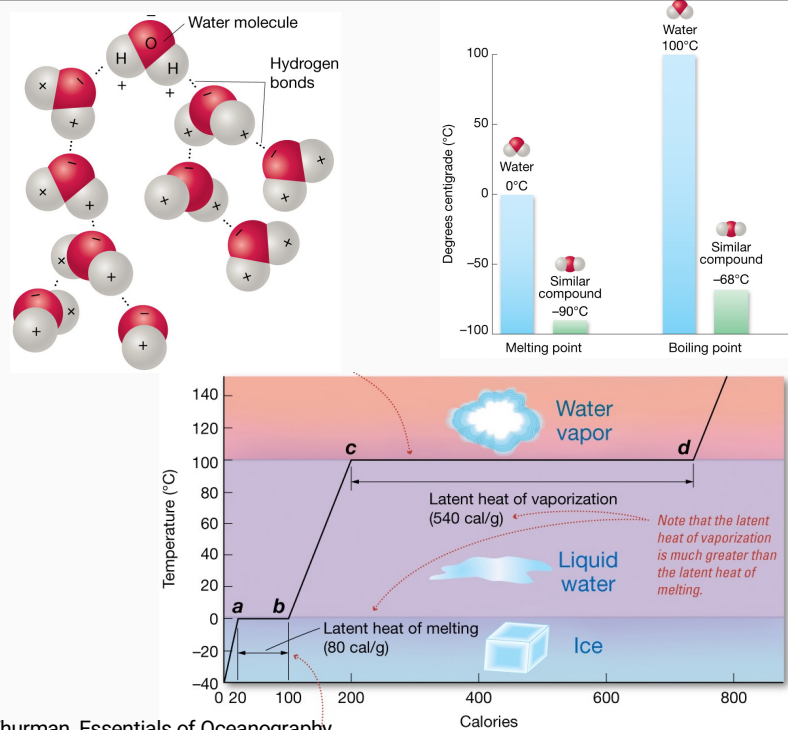
1. Why is water so (chemically) wonderful?
2. What are the conventional geochemical measurements to evaluate water?
  - pH
  - Alkalinity
  - Total dissolved solids (TDS)
  - Ions and salinity
  - Dissolved gases
  - Organic compounds



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## The Wonderful Water Molecule

- Polarity stabilizes dissolved ions
- Formation of Hydrogen bonds between water molecules give it stability and important properties
- High heat capacity stores energy, allows transport, drives climate

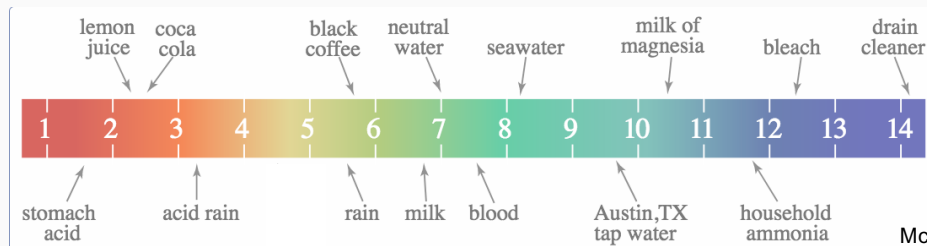


Trujillo and Thurman, Essentials of Oceanography

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# pH: a Master Variable

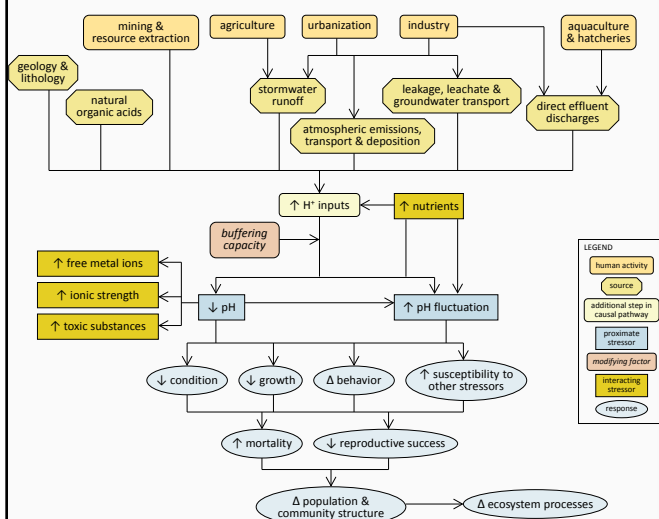
- $\text{pH} = -\log[\text{H}^+] = -\log[\text{H}_3\text{O}^+]$
- Most natural waters pH ~5.5-8.5
  - Acid mine drainage pH ~2.5-5.5
  - Alkaline waters pH >9



Mccord.cm.utexas.edu

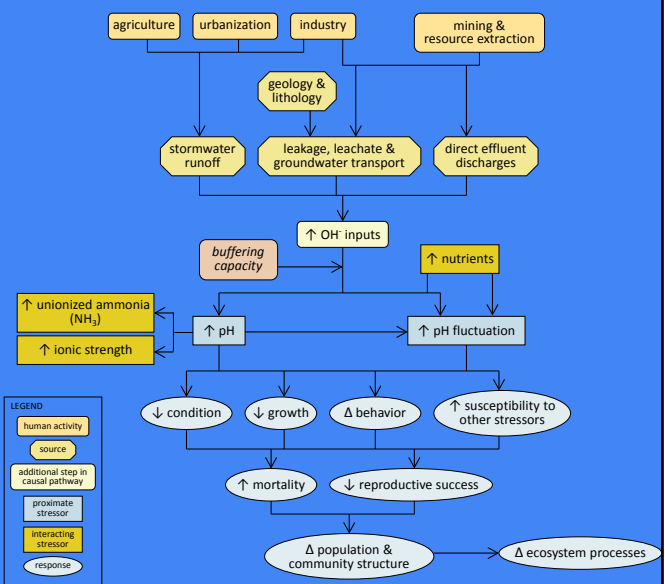
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## Low pH



EPA Conceptual Models

## High pH



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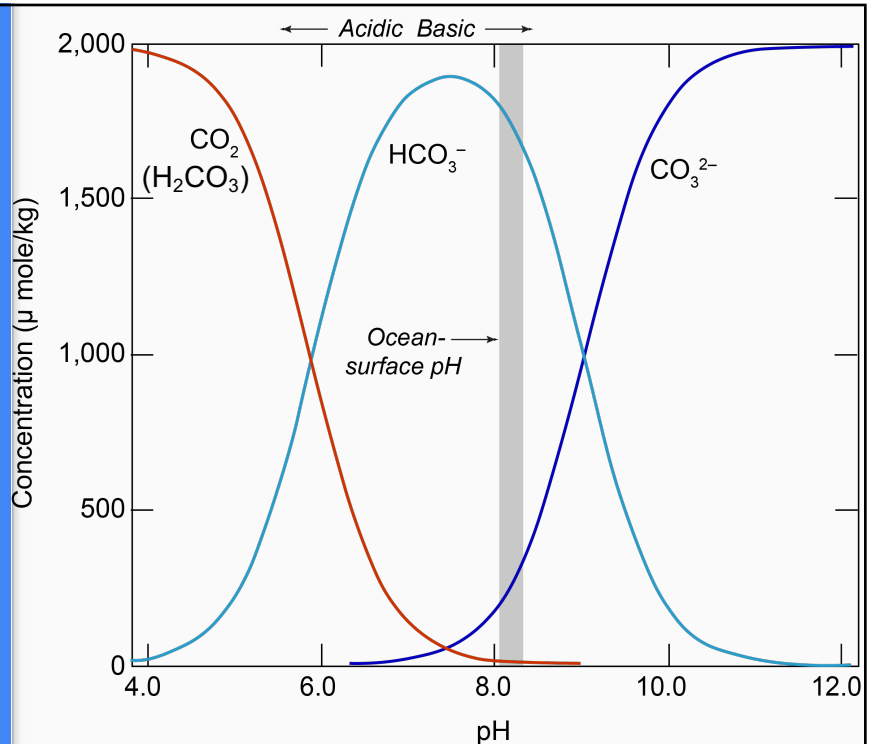
# Alkalinity

- Alkalinity =  $-M_{H^+} + M_{HCO_3^-} + 2M_{CO_3^{2-}} + M_{OH^-} + M_{B(OH)_4^-} + M_{H_3SiO_4^-} + M_{HS^-} + M_{Organic\ anions} \dots$
- Represents the buffering capacity of a water body
  - Strong acids will convert anions to uncharged species
  - Strong bases will convert uncharged species to anions
- Keeps the pH relatively steady

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## Carbonate Alkalinity

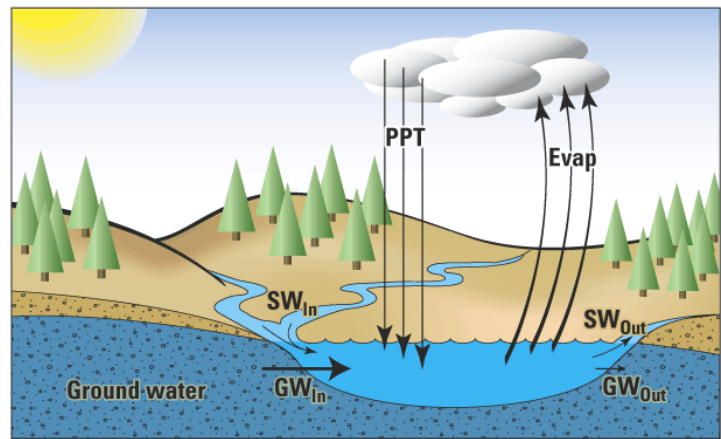
- $CO_2$  from the atmosphere dissolves in water, forming the carbonate buffer system
- At natural water pH, bicarbonate ion ( $HCO_3^-$ ) is the dominant form
  - Uptakes  $H^+$  to form carbonic acid ( $H_2CO_3$ )
  - Releases  $H^+$  to form carbonate ion ( $CO_3^{2-}$ )



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# TDS = Total Dissolved Solids

Any material dissolved in water, including ions, gases, organic compounds, metals, contaminants



NOT TO SCALE

## EXPLANATION

Evap	Evaporation
GW <sub>In</sub>	Ground-water inflow
GW <sub>Out</sub>	Ground-water outflow
PPT	Precipitation
SW <sub>In</sub>	Surface-water inflow
SW <sub>Out</sub>	Surface-water outflow

SERC

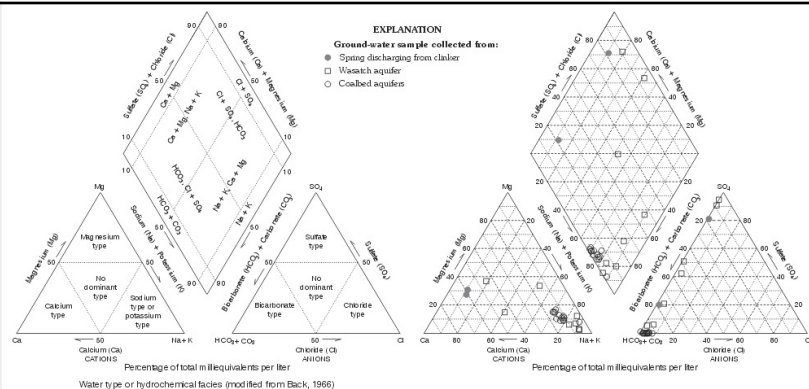


www.lakesuperiorstreams.org

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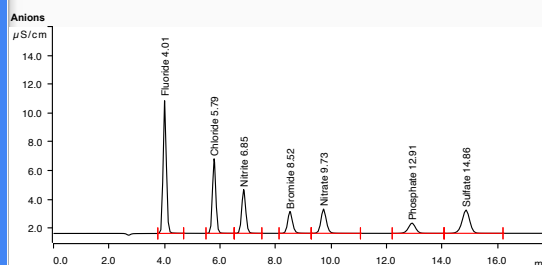
## Ions

- Charged atoms/molecules
  - Most common cations are  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Na}^+$ ,  $\text{K}^+$
  - Most common anions are  $\text{HCO}_3^-$ ,  $\text{Cl}^-$ ,  $\text{SO}_4^{2-}$
- Originate from dissolution of rocks/minerals, contamination
- Serve as nutrients, form shells, also evaporite minerals
- Can be used to trace water source, biogeochemical processes, rock-water interaction



Bartos and Ogle, 2002 (USGS)

Figure 13. Trilinear diagram showing water types for ground-water samples collected from springs, Wasatch aquifer, and coalbed aquifers, eastern Powder River Basin, 1998. Nondetections set to 0.0 milligrams per liter.

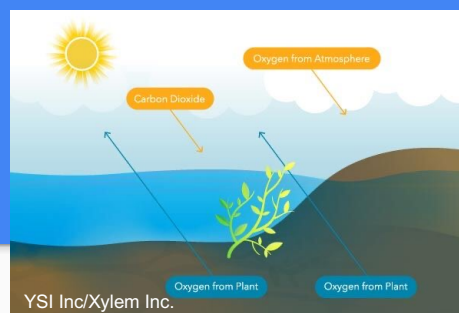


Anion standard run on ion chromatograph

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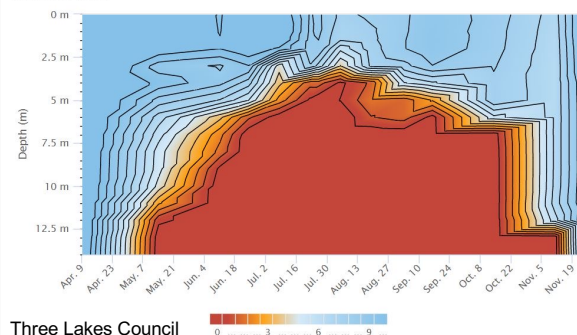
# Dissolved Gases

- Gas molecules dissolved in water including  $O_2$ ,  $CO_2$ , methane,  $H_2S$ 
  - Exchange with the atmosphere through diffusion, aeration
  - Internal sources such as photosynthesis, decomposition of organics
  - Release from sediments
- Important to health of water body
  - Dissolved  $O_2$  a master variable
  - Stratification and anoxia



Dissolved Oxygen Levels for 2018

Lake Waccabuc  
Westchester County



Three Lakes Council

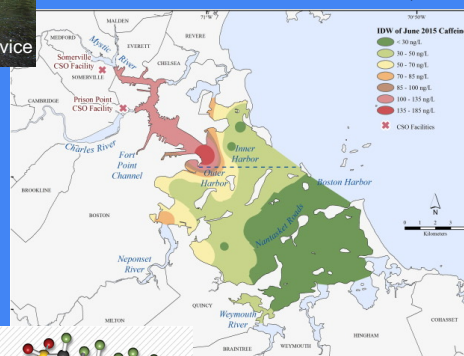
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# Organic Compounds

- Carbon-based compounds
- Natural organic compounds
  - Tannins, humics, dissolved organic matter
- Anthropogenic organic compounds
  - Industrial pollutants, wastewater, agrichemicals, oil spills; microplastics



Cantwell et al., 2016



**PFAS**  
PERFLUOROALKYL AND  
POLYFLUOROALKYL  
SUBSTANCES



FIRE  
RETARDANT  
FOAMS



ELECTRONICS



FAST FOOD  
CONTAINERS



MICROWAVE  
POPCORN  
BAGS



NONSTICK  
COOKWARE



PERSONAL  
CARE  
PRODUCTS



STAIN-  
RESISTANT  
CARPET

Cook and Steinfeld-Darling,  
Water Online

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# Geochemical measurements can characterize a water system

Evaluate environmental  
conditions, biogeochemical  
processes, and anthropogenic  
influences



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## Acknowledgements

Contact us:

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[Cas.okstate.edu/wrane/index.html](http://Cas.okstate.edu/wrane/index.html)



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## Additional Information:

- [Water Quality Information by Topic](#): USGS  
Water Science School



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