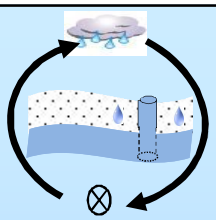


مرکز تحقیقات آبهای زیرزمینی (متآب)

Groundwater Research Center (GRC)

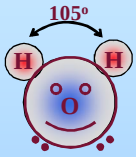
هیدروژئوشیمی و کیفیت منابع آب

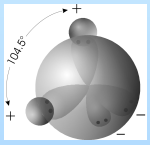
Groundwater Geochemistry

فصل اول

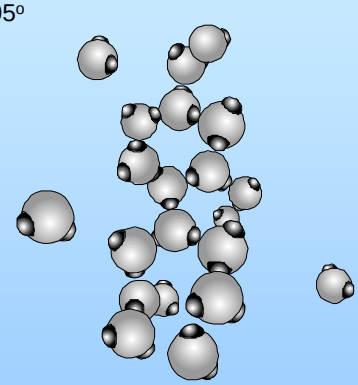
خصوصیات آب (Water Characteristics)

Water molecule is polar; angle between H-O-H is 105°





Density of water: Water is *Weird* (and wonderful) - one of the only substances whose solid state is less dense than the liquid phase; most dense at 4°C.



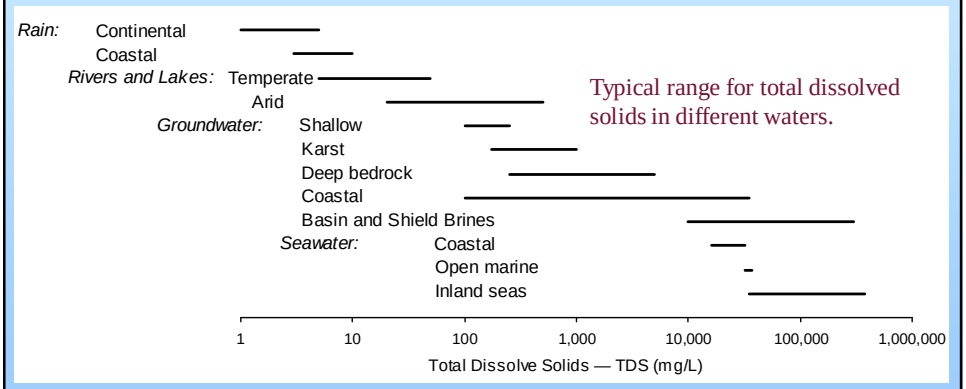
Hydrogen bonding and the tetrahedral structure of water

هدایت الکتریکی (Electrical Conductivity (EC))

- The ability of water to conduct electricity is call the Electrical Conductivity (EC) or Electrical Conductance.
- It is easily measured with a probe and is expressed in SI units as Siemens (= ohm^{-1}) per unit distance separating the prongs of the probe. The most commonly used units are microsiemens/cm = µS/cm= µmho/cm = $(10^6$ ohm cm$)^{-1}$ or milisiemens / cm.
- Measurements are highly dependent on temperature and are corrected to - and reported at 25°C
- Pure water does NOT conduct electricity; but water containing dissolved electrolytes does.
- EC is proportional to the concentration of electrolytes present in the water, and it is therefore related to TDS.
- EC can be used to estimate TDS

مواد جامد محلول (Total Dissolved Solids (TDS))

Total Dissolved Solids (TDS) is a commonly used indicator of the total amount of dissolved constituents in groundwater (= mass of solid residues obtained from drying a known volume of filtered groundwater) (usual units of mg / L, or ppm). TDS can be used as a way to classify waters (see following table).



Typical range for total dissolved solids in different waters.

شوری (Salinity)

Salinity is a similar term to TDS, which expresses the concentration of ions in solution. Like TDS, salinity can be expressed as mg/L, but is often expressed as parts per thousand (ppt). The following terms are used to qualitatively express salinity:

fresh	➔ 0 to 1000 mg/L	(0 to 1 ppt)
Brackish	➔ 1000 to 10,000 mg/L	(1 to 10 ppt)
saline	➔ 10,000 to 100,000 mg/L	(10 to 100 ppt)
Seawater	➔ 35,000 mg/L	(35 ppt)
brine	➔ greater than 100,000 mg/L	(>100 ppt)

رابطه بین TDS و EC

EC can be used to estimate TDS: TDS (mg/L) = A * EC (µS/cm)

For low salinity bicarbonate waters

TDS (ppm) ≈ 0.55 EC (uS/cm)

For high SO_4^{2-} waters

TDS (ppm) ≈ 0.75 EC (uS/cm)

For high Cl^- waters

TDS (ppm) ≈ 0.9 EC (uS/cm)

Type of water	TDS (mg/L)	EC (µS/cm)
Fresh water	0 – 1 000	0 – 1 500
Brackish water	1 000 – 10 000	1 500 – 15 000
Saline water	10 000 – 100 000	15 000 – 150 000
Brine water	> 100 000	> 150 000
Potable water	< (2 000 – 3 000)	< (3 000 – 4 500)
Sea water	≈ 35 000	≈ 52 500
Rainwater		< 10's
River water		100's
Groundwater		10's – 10 000's
Distilled water		< 10's
Reverse Osmosis water		< 100's
1M NaCl	58 500	87 750
7-Up	440	660

(Units of Concentrations) واحدهای غلظت

Mass Fraction = mass of solute per mass of solution [$Mass_{solute}$ / $Mass_{total}$]

ppm (parts per million);
ppb (parts per billion);
ppt (parts per trillion)

$$ppm = \frac{\text{mg}}{\text{kg } H_2O}$$

Mass concentration = mass of solute per volume of solution [Mass / volume]

kg / m^3 or mg / L;
g / L also accepted

$$mg/L = \frac{\text{mg}}{\text{L solution}}$$

واحدهای غلظت - ادامه

m Molality = moles of solute per mass of solvent [mol / Mass]
mol / kg

$$m = \frac{\text{mol}}{\text{kg } H_2O} = \frac{\text{ppm}}{\text{gfw} .1000}$$

M Molarity = moles of solute per volume of solution [mol / volume]
mol / m^3;
mol / L

$$M = \frac{\text{mol}}{\text{L solution}} = \frac{\text{mg/L}}{\text{gfw} .1000}$$

واحدهای غلظت - ادامه

Equivalents per million (epm)

$$epm = \frac{ppm}{eq} = \frac{ppm}{gfw/z} = \frac{ppm}{gfw} \times z = m \times z \times 1000$$

miliequivalents per liter (meq/L)

$$meq/L = \frac{mg/L}{eq} = \frac{mg/L}{gfw/z} = \frac{mg/L}{gfw} \times z = M \times z \times 1000$$

نکته مهم (Important note)

With low salinity solutions (TDS less than about 10,000 mg/L), there is little difference between concentrations expressed as mg/L or ppm. Thus,

For TDS < ~10,000

ppm ≅ mg/L and $m \cong M$

مثال برای تبدیل واحدها

(Example for conversion of concentration units)

Calculate the concentration of Ca^{2+} in units of, m, epm, M, meq/L and mg/L given a measurement of 8500 ppm Ca^{2+} (gfw 40.1) (a) in a solution with a measured density of 1.20 kg/L at 25°C and TDS of 175,000 mg/L (0.175 kg/L) and (b) for a low salinity solution with 85 ppm Ca^{2+}, a measured density of 1.00 and TDS of 400 mg/L:

محاسبه خطای اندازه گیری (Charge balance error)

$$\text{Charge balance error (\%)} = \frac{\Sigma cat - \Sigma an}{\Sigma cat + \Sigma an} \times 100$$

Example: Determine the analysis error for these two geochemical analyses of spring waters, (values in mg/L):

	pH	Ca^{2+}	Mg^{2+}	Na^{+}	K^{+}	HCO_3^{-}	CO_3^{2-}	SO_4^{2-}	Cl^{-}
Spring A	7.55	72.5	32.2	132	10.6	177	0.27	126	213
Spring B	10.40	1.91	0.12	42.5	0.20	19.2	21.1	11.7	10.1
Converting data to meq/L									
(e.g. Ca^{2+} in Spring A = 72.5/40.1x2 = 3.62 meq/L)									
Spring A	7.55	3.62	2.65	5.74	0.27	2.90	0.01	2.62	6.00
Spring B	10.40	0.10	0.01	1.85	0.01	0.31	0.70	0.24	0.28

منشا عناصر در سفره های زیرزمینی
(FROM ELEMENTS TO AQUIFERS)

Periodic Table of the elements

IA												IIIB	IVB	VB	VIB	VIIB	VIIIB
1.00 1 H 1	IIA						←	VIIIA	→	IB	IIB	10.8 5 B 6	12.0 6 C −4 −2 0 4	14.0 7 N −3 0 3 5	16.0 8 O −2 0	19.0 9 F −1	4.00 2 He 0
6.94 3 Li 1	9.01 4 Be 2																20.210 Ne 0
23.011 Na 1	24.312 Mg 2	IIIA	IVA	VA	VIA	VIIA						27.013 Al 3	28.114 Si 4	30.115 P −3 5	32.116 S −2 0 4 6	35.517 Cl −1	40.018 Ar 0
39.119 K 1	40.120 Ca 2	45.021 Sc 3	47.922 Ti 4	50.923 V 5	52.024 Cr 3	54.925 Mn 4 3 2	55.826 Fe 2 3	58.927 Co 2 3	58.728 Ni 2	63.529 Cu 1 2	65.430 Zn 2	69.731 Ga 3	72.632 Ge 4	74.933 As −3 3 5	79.034 Se −2 0 4 6	79.935 Br −1	83.836 Kr 0
85.537 Rb 1	87.638 Sr 2	88.939 Y 3	91.240 Zr 4	92.941 Nb 3 5	95.942 Mo 4 6	98 43 Tc 7	101 44 Ru 3 4	103 45 Rh 2 3 4	106 46 Pd 2 4	108 47 Ag 1	112 48 Cd 2	115 49 In 3	119 50 Sn 4 2	122 51 Sb 3 5	128 52 Te −2 0 4 6	127 53 I −1	131 54 Xe 0
133 55 Cs 1	137 56 Ba 2	139 57 La 3	178 72 Hf 4	181 73 Ta 5	184 74 W 4 6	186 75 Re 7	190 76 Os 3 4	192 77 Ir 2 4 6	195 78 Pt 2 4	197 79 Au 1 3	200 80 Hg 2	204 81 Ti 1 3	207 82 Pb 2	209 83 Bi 3 5	209 84 2 4	210 85 At −1	222 86 Rn 0
223 87 Fr 1	226 88 Ra 2	227 89 Ac 3															

140 58 Ce 3	141 59 Pr 3	141 59 Nd 3	145 61 Pm 3	150 62 Sm 3	152 63 Eu 3	157 64 Gd 3	159 65 Tb 3	163 66 Dy 3	165 67 Ho 3	167 68 Er 3	169 69 Tm 3	173 70 Yb 3	175 71 Lu 3
232 90 Th 4	231 91 Pa 5	238 92 U 4 6	237 93 Np 4 5	244 94 Pu 4	243 95 Am 3	247 96 Cm 3	247 97 Bk 3 4	251 98 Cf 3	252 99 Es	257 100 Fm	258 101 Md	259 102 No	260 103 Lr

توضیع عناصر در پوسته زمین
(Distribution of elements in the Earth's crust)

Principal elements of the Earth's crust, by weight

Element	Atomic Number	Crustal Abundance %	Element	Atomic Number	Crustal Abundance ppm
O	8	46.6	P	15	1050
Si	14	27.7	Mn	25	950
Al	13	8.13	F	9	625
Fe	26	5.00	Ba	56	425
Ca	20	3.63	Sr	38	375
Na	11	2.83	S	16	260
K	19	2.59	C	6	200
Mg	12	2.09	Zr	40	165
Ti	22	0.43	V	23	135
H	1	0.14	Cl	17	130

عناصر تشکیل دهنده سنگ ها (The rock forming minerals)

- ***Silicates***
  - Fe — Mg (mafic) minerals
  - Feldspars
- ***Clay minerals***
  - Serpentine — $Mg_3Si_2O_5(OH)_4$
  - Chlorite — $(Mg,Fe,Al)_6(Si,Al)_2O_{10}(OH)_8$
  - Smectite — $Na(Al,Mg)_2Si_4O_{10}(OH)_2$
  - Kaolinite — $Al_2Si_2O_5(OH)_4$
  - Illite — $KAl_2(Si_5Al)O_{10}(OH)_2$
- ***Carbonates***
  - Calcite — $CaCO_3$
  - Dolomite — $CaMg(CO_3)_2$
  - Siderite — $FeCO_3$
  - Magnesite — $MgCO_3$
- ***Evaporites***
  - Sulfates:Gypsum — $CaSO_4 \times 2H_2O$
    - Anhydrite — $CaSO_4$
    - Mirabilite — $Na_2SO_4 \times 10H_2O$
    - Epsomite — $MgSO_4 \times 7H_2O$
    - Jarosite — $KFe_3(SO_4)_2(OH)_6$
  - Chlorides:Halite — NaCl
    - Sylvite — KCl
  - Carbonates:Trona — $NaHCO_3 \times Na_2CO_3 \times 2H_2O$

عناصر تشکیل دهنده سنگ ها -ادامه

- ***Phosphates***
  - Fluorapatite — $Ca_5(PO_4)_3F$
  - Chlorapatite — $Ca_5(PO_4)_3Cl$
  - Hydroxylapatite — $Ca_5(PO_4)_3OH$
  - Carbonate-apatite — $Ca_{10}(PO_4)_6(CO_3)H_2O$
- ***Sulfides***
  - Pyrite — FeS_2
  - Mackinawite — FeS
  - Chalcopyrite — $CuFeS_2$
  - Sphalerite — (Zn,Fe)S
  - Galena — PbS
  - Pentlandite — $(Fe,Ni)_9S_8$
  - Cinnabar — HgS
  - Arsenopyrite — FeAsS
- ***Oxy-hydroxides***
  - Magnetite — Fe_3O_4
  - Hematite — Fe_2O_3
  - Goethite — FeOOH
  - Ferrihydrite —$Fe(OH)_3$
  - Pyrolusite — MnO_2
  - Manganite — MnOOH
  - Pyrochroite — $Mn(OH)_2$

عناصر اصلی، فرعی در آبهای زیرزمینی

Major Constituents (> 90% of TDS, > 5 mg/L)

- Major Cations: Sodium, Na^+; Magnesium, Mg^{2+}; Calcium, Ca^{2+}
- Major Anions: Chloride, Cl^-; Bicarbonate, HCO_3^-; Sulphate, SO_4^-
- Neutral species: Silicates, SiO_2, $Si(OH)_4$; Carbonic acid, H_2CO_3

Minor Constituents (0.01 - 10 mg/L)

- Minor Cations: Potassium, K^+; Strontium, Sr^{2+}; Iron, Fe^{2+}, Fe^{3+}
- Minor Anions: Nitrate, NO_3^-; Carbonate, CO_3^{2-}; Fluoride, F^-
- Neutral species: Boron, B

مواد ارگانیکی و گازهای محلول در آبهای زیرزمینی

Organic Constituents

- Constituents that contain C except H_2CO_3, HCO_3^-, CO_3^{2-}, CO_2
- Dissolved Organic Carbon (DOC); normally 0.1-10 mg/L but can be as high as 10's mg/L; present as "Humic" and "Fulvic" acids.
- More recently, many organic contaminants: poly-aromatic hydrocarbons (PAH's), TCE, PCE, PCB, and many, many more! - more on this later.

Dissolved Gases

- Most common are: atmospheric gases: N_2, O_2, CO_2; and by-products of biogeochemical processes: CH_4, H_2S, and N_2O.
- H_2S - rotten egg smell; CH_4 - explosion hazards in wells.

دسته مسائل سری اول
در کلاس داده خواهد شد