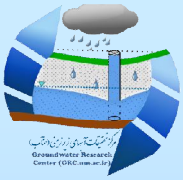


مرکز تحقیقات آبهای زیرزمینی (متآب)

Groundwater Research Center (GRC)

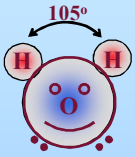
هیدروژئوشیمی و کیفیت منابع آب

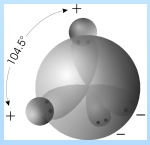
Groundwater Geochemistry

فصل اول

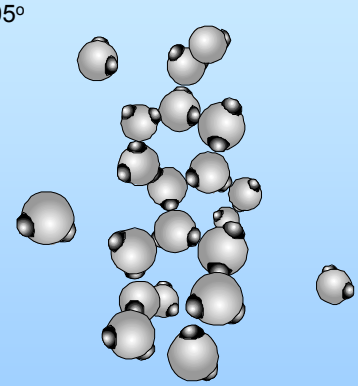
خصوصیات آب (Water Characteristics)

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.



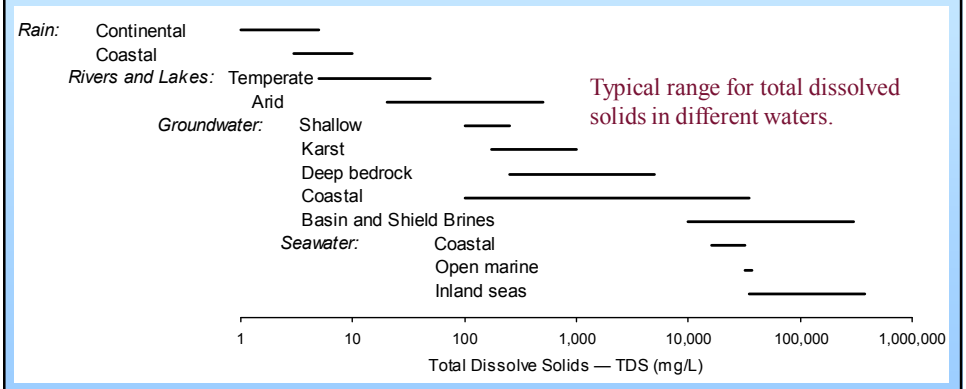
Hydrogen bonding and the tetrahedral structure of water

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).



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

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

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

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

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)

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

(Important note) نکته مهم

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 $m \cong M$

epm ≅ meq/L

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 **Tl** 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