



تصویب بودجه تفصیلی ۱ سالهای ۱۳۹۵ و ۱۳۹۶ دانشگاه تهران

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Environmental chemistry



Environmental science

- Environmental science in its broadest sense is the science of the complex interactions that occur among the terrestrial, atmospheric, aquatic, living, and anthropological environments
- It includes all the disciplines, such as chemistry, biology, ecology, sociology, and government, that affect or describe these Interactions
- Environmental science will be defined as *the study of the earth, air, water, and living environments, and the effects of technology thereon.*

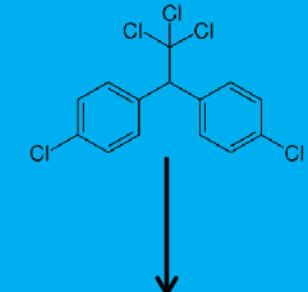
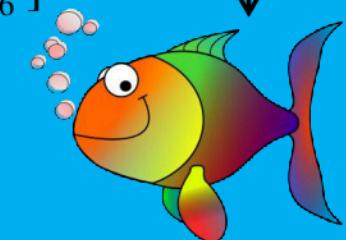
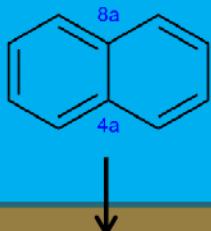
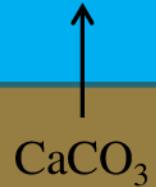
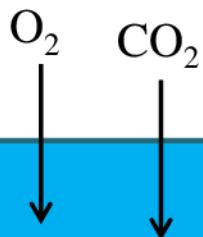
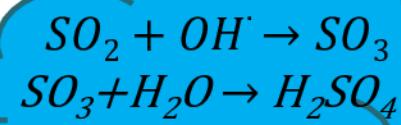


Environmental chemistry

- Environmental chemistry may be defined as *the study of the sources, reactions, transport, effects, and fates of chemical species in water, soil, air, and living environments, and the effects of technology thereon.*
- In recent years many chemists have become deeply involved with the investigation of environmental problems.
- Industries have found that well-trained environmental chemists at least help avoid difficulties with regulatory agencies.
- Some background in environmental chemistry should be part of the training of every chemistry student. The ecologically illiterate chemist can be a very dangerous species. Chemists must be aware of the possible effects their products and processes might have upon the environment.
- Because it deals with natural systems, it is more complicated and difficult than “pure” chemistry.



The Environment





The Environment

- Atmosphere
- Hydrosphere
- Geosphere
- Biosphere
- Anthroposphere

The **anthroposphere** (sometimes also referred as *technosphere*) is that part of the environment that is made or modified by humans for use in human activities

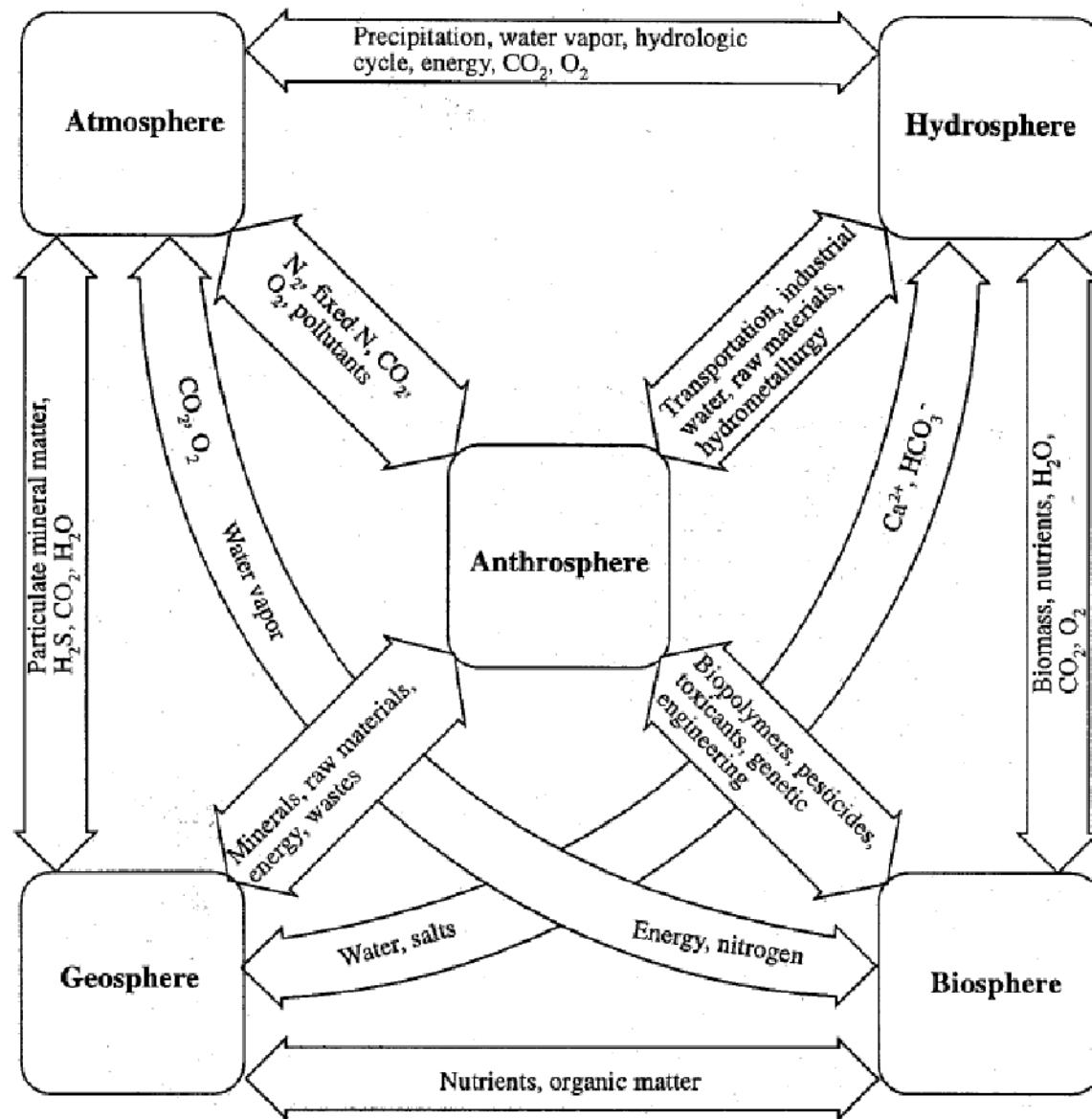


Figure 1.1. Illustration of the close relationships among the air, water, and earth environments with each other and with living systems, as well as the tie-in with technology (the anthrosphere).

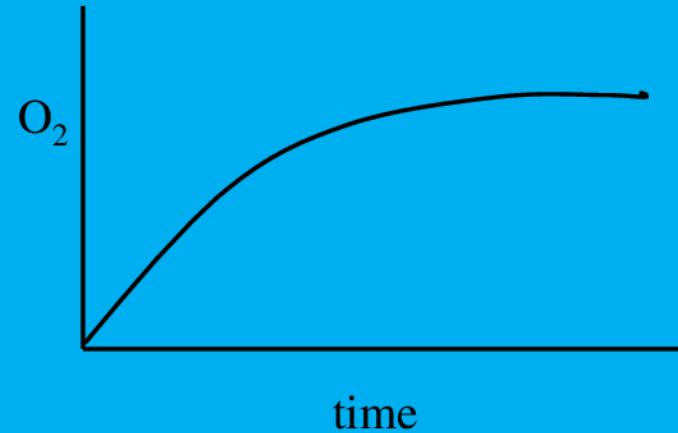
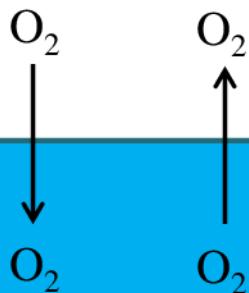
Types of Reactions

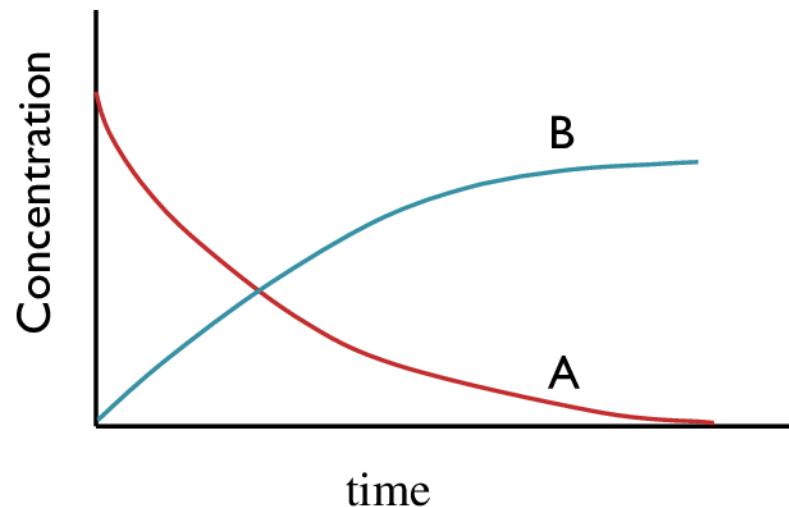
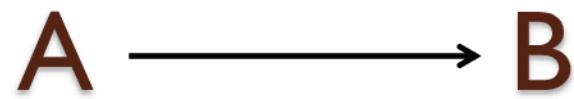
- Acid-Bas reaction
- Oxidation- Reduction reaction
- Complex formation reaction
- precipitation and dissolution
- Gas solubility
- Adsorption
- Biological reaction

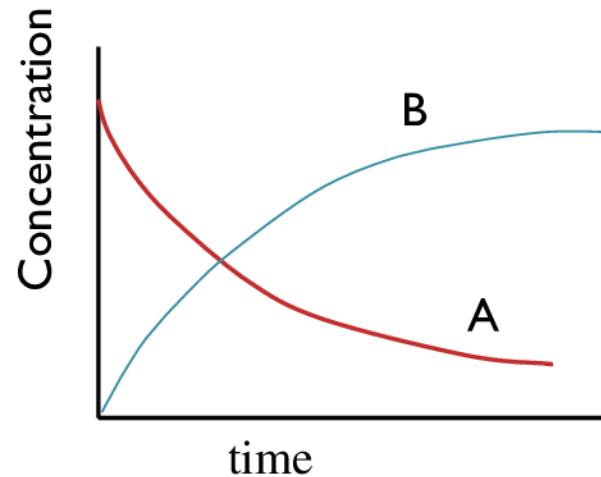
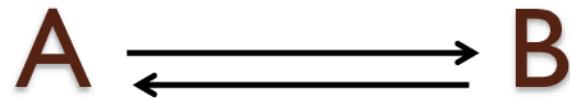
Symbols used in chemical equations

Symbol	Description	Comments
→	Irreversible reaction	Single arrow points from the reactants to the products, e.g., $A + B \rightarrow C$
↔	Reversible reaction	Double arrows used to show that the reaction proceeds in the forward or reverse direction, depending on the solution characteristics
[]	Brackets	Concentration of a chemical constituent or compound in mol/L
{ }	Braces	Activity of a chemical constituent or compound
(s)	Solid phase	Used to designate chemical component present in solid phase, e.g., precipitated calcium carbonate, $\text{CaCO}_3(\text{s})$
(l)	Liquid phase	Used to designate chemical component present in liquid phase, e.g., liquid water, $\text{H}_2\text{O}(\text{l})$
(aq)	Aqueous (dissolved)	Used to designate chemical component dissolved in water, e.g., ammonia in water, $\text{NH}_3(\text{aq})$
(g)	Gas	Used to designate chemical component present in gas phase, e.g., chlorine gas, $\text{Cl}_2(\text{g})$
→ ^x	Catalysis	Chemical species, represented by x, catalyzes reaction, e.g., cobalt (Co) is the catalyst in the reaction $\text{SO}_3^{2-} + \frac{1}{2}\text{O}_2 \xrightarrow{\text{Co}} \text{SO}_4^{2-}$
↑	Volatilization	Arrow directed up following a component is used to show volatilization of given component, e.g., $\text{CO}_3^{2-} + 2\text{H}^+ \rightleftharpoons \text{CO}_2(\text{g}) \uparrow + \text{H}_2\text{O}$
↓	Precipitation	Arrow directed down following a component is used to show precipitation of given component, e.g., $\text{Ca}^{2+} + \text{CO}_3^{2-} \rightleftharpoons \text{CaCO}_3(\text{s}) \downarrow$

Equilibrium







$$R_f = k_f [A]$$

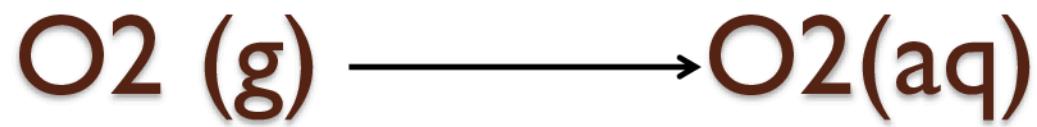
$$R_b = k_b [B]$$

$$R_f = R_b$$

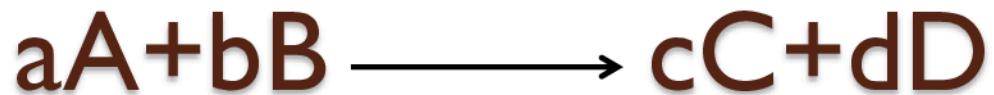
$$k_f [A] = k_b [B]$$

$$\frac{k_f}{k_b} = \frac{[B]}{[A]}$$

$$\frac{k_f}{k_b} = K_{eq} = \frac{[B]_{eq}}{[A]_{eq}}$$



$$K_{eq} = \frac{DO}{PO_2}$$



$$\frac{[C]^c[D]^d}{[A]^a[B]^b} = K_c \quad (5-32)$$

where

K_c = equilibrium constant (subscript c used to signify
equilibrium constant based on species concentration)

[] = concentration of species, mol/L

a, b, c, d = stoichiometric coefficients of species A, B, C, D,
respectively



$$\frac{[\text{H}^+][\text{HCO}_3^-]}{[\text{H}_2\text{CO}_3]} = K_c = 5.0 \times 10^{-7}$$

$$\text{p}K = -\log_{10} K$$

$$\text{p}K_c = -\log_{10} K_c = -\log_{10}(5.0 \times 10^{-7}) = 6.3$$

TABLE | 9.4 K_a AND pK_a VALUES FOR SELECTED ACIDS

Name	Formula	K_a	pK_a
Hydrochloric acid	HCl	1.0×10^7	-7.00
Phosphoric acid	H_3PO_4	7.5×10^{-3}	2.12
Hydrofluoric acid	HF	6.6×10^{-4}	3.18
Lactic acid	$CH_3CH(OH)CO_2H$	1.4×10^{-4}	3.85
Acetic acid	CH_3CO_2H	1.8×10^{-5}	4.74
Carbonic acid	H_2CO_3	4.4×10^{-7}	6.36
Dihydrogenphosphate ion	$H_2PO_4^-$	6.2×10^{-8}	7.21
Ammonium ion	NH_4^+	5.6×10^{-10}	9.25
Hydrocyanic acid	HCN	4.9×10^{-10}	9.31
Hydrogencarbonate ion	HCO_3^-	5.6×10^{-11}	10.25
Methylammonium ion	$CH_3NH_3^+$	2.4×10^{-11}	10.62
Hydrogenphosphate ion	HPO_4^{2-}	4.2×10^{-13}	12.38



The amount of matter is expressed by

- Mass (g)
- Volume (L)
- Mole (mol)
- Equivalent (eq)

Mole

- $1 \text{ mol} = 6.02 \times 10^{23}$ of anything
- Or a package containing 6.02×10^{23} of anything
- The mass of this package is named molar mass: M (g/mol)
- $\text{mol} = \frac{g}{M}$

periodic table

*Lanthanide series

**Actinide series

lanthanum 57 La 138.91	cerium 58 Ce 140.12	praseodymium 59 Pr 140.91	neodymium 60 Nd 144.24	promethium 61 Pm [145]	samarium 62 Sm 150.36	euroium 63 Eu 151.96	gadolinium 64 Gd 157.25	terbium 65 Tb 158.93	dysprosium 66 Dy 162.50	holmium 67 Ho 164.93	erbium 68 Er 167.26	thulium 69 Tm 168.93	yterbium 70 Yb 173.04
actinium 89 Ac [227]	thorium 90 Th 232.04	protactinium 91 Pa 231.04	uranium 92 U 238.03	neptunium 93 Np [237]	plutonium 94 Pu [244]	americium 95 Am [243]	curium 96 Cm [247]	berkelium 97 Bk [247]	californium 98 Cf [251]	einsteinium 99 Es [252]	fermium 100 Fm [257]	mendeleyevium 101 Md [258]	nobelium 102 No [259]

Equivalent

- One mole of positive charge
 - One mole of negative charge
 - One mole of H^+
 - One mole of OH^-
-
- 1 mol Fe^{3+} = 3 mol positive charge = 3 eq
 - 1 mol H_2SO_4 = 2 mol H^+ = 2 eq

Equivalent mass: E (g/eq)

- The mass of one equivalent
- M(H₂SO₄): 98 g/ mol
- E (H₂SO₄): 49 eq/g
- M(Ca²⁺): 40 g/ mol
- E(Ca²⁺): 20 g/ eq
- M(CaCO₃): 100 g/ mol
- E(CaCO₃): 50 g/ mol
- $E = \frac{M}{n}$



Concentration

- $Molarity = mol/L$
- $Normality = eq/L$
- $ppm = mg/L \text{ or } mg/kg \text{ or } \mu l/l$
- $ppb = \mu g/L \text{ or } \mu g/kg \text{ or } nl/l$
- mg/m^3

The concentration of Benzene in air is 5 mg/m³. convert it to the unit of ppm

- M(Benzene): 78.11 g/mol
- 1mol= 78.11 g
- 1mol=22.4 l
- ? $\mu l = 1l \times \frac{1 m^3}{1000l} \times \frac{5 mg}{1 m^3} \times \frac{1 g}{1000 mg} \times \frac{1 mol}{78.11 g} \times \frac{22.4 l}{1 mol} \times \frac{1 \times 10^6 \mu l}{1l} = 1.43 \mu l$
- $ppm = \frac{mg}{m^3} \times \frac{22.4}{M}$



Stoichiometry

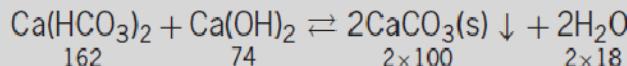
A quantitative relationship that defines the relative amount of each reactant consumed and each product generated during a chemical reaction.

Example 5-2 Determination of product mass using stoichiometry

For the reaction shown in Eq. 5-22, estimate the amount of $\text{CaCO}_3(\text{s})$ that will be produced from the addition of calcium hydroxide to water containing 50 mg/L $\text{Ca}(\text{HCO}_3)_2$. Use a flow rate of 1000 m³/d and determine the quantity of $\text{CaCO}_3(\text{s})$ in kilograms per day. Assume that the reaction proceeds in the forward direction to completion.

Solution

1. Write the chemical equation and note the molecular weight of the reactants and products involved in the reaction. The molecular weights are written below each species in the reaction.



2. Determine the molar relationship for the disappearance of $\text{Ca}(\text{HCO}_3)_2$ and formation of $\text{CaCO}_3(\text{s})$:

$$\left[\frac{2 \text{ mol CaCO}_3(\text{s})}{1 \text{ mol Ca}(\text{HCO}_3)_2} \right] \left[\frac{100 \text{ g CaCO}_3(\text{s})}{\text{mol CaCO}_3(\text{s})} \right] \left[\frac{1 \text{ mol Ca}(\text{HCO}_3)_2}{162 \text{ g Ca}(\text{HCO}_3)_2} \right]$$
$$= 1.23 \frac{\text{g CaCO}_3(\text{s})}{\text{g Ca}(\text{HCO}_3)_2}$$

Therefore, for each gram of $\text{Ca}(\text{HCO}_3)_2$ removed, 1.23 g of $\text{CaCO}_3(\text{s})$ will be produced.

3. Compute the mass of $\text{CaCO}_3(\text{s})$ that will be produced each day.
 - a. Determine the mass of $\text{Ca}(\text{HCO}_3)_2$ removed each day:

$$\begin{aligned}\text{Ca}(\text{HCO}_3)_2 \text{ removed} &= (0.050 \text{ g/L})(1000 \text{ m}^3/\text{d})(1000 \text{ L/m}^3) \\ &= 50,000 \text{ g/d}\end{aligned}$$

b. Estimate the amount of $\text{CaCO}_3(\text{s})$ produced each day:

$$\begin{aligned}\text{CaCO}_3(\text{s}) \text{ produced} &= [50,000 \text{ g Ca(HCO}_3)_2/\text{d}] \\ &\times [1.23 \text{ g CaCO}_3(\text{s})]/[\text{g Ca(HCO}_3)_2](1 \text{ kg}/10^3 \text{ g}) \\ &= 61.5 \text{ kg CaCO}_3(\text{s})/\text{d}\end{aligned}$$

Comment

In addition to estimating the amount of $\text{CaCO}_3(\text{s})$ produced, it is also possible to estimate the amount of calcium hydroxide that must be added to water to bring about this reaction. However, due to the nonideal nature of water treatment processing, the amount of calcium hydroxide that is required will exceed the stoichiometric amount, which is the minimum amount needed.

Ionic strength

$$I = \frac{1}{2} \sum_i C_i Z_i^2 \quad (5-37)$$

I = ionic strength of solution, mol/L(M)

C_i = concentration of species i, mol/L(M)

Z_i = number of replaceable hydrogen atoms or their equivalent
(for oxidation-reduction reactions, Z is equal to the change
in valence)

$$I = (2.5 \times 10^{-5}) (\text{TDS})$$

where TDS = total dissolved solids, mg/L



Calculate Ionic strength of a solution containing CaCl_2 100 mg/L

- $$\frac{\text{mol}}{\text{L}} = \frac{\text{mg/L}}{\text{M}} \times 10^{-3}$$