ENVIRONMENTAL CHEMISTRY

- Stoichiometry

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Environmental Chemistry

- Almost every pollution problem (and solution) has a chemical basis
- Arise from chemical transformation/reactions of compounds
- Effects of chemical properties of waste

Environmental Chemistry

√ **To understand and control natural systems, we must understand chemical and biochemical reactions**

- Biodegradation of hazardous wastes
- Greenhouse gases
- Ozone hole and urban ozone
- Acid deposition
- Water pollution
- Air pollution

Definitions

- **Atom** (Gr. “unbreakable”): basic structural unit
- **Protons** (+1): positively charged particle
  - Determines atomic number
- **Neutron** (0): no charge
  - With protons, determines atomic mass unit (AMU)
- **Electrons** (-1): negatively charge particle
  - Determine chemical properties
- **Atomic Weight**: mass of atom in AMU
  - e.g. Carbon weighs 12 amu (6 protons, 6 neutrons)
- **Isotopes**: atoms with same number of protons and different number of neutrons
- **Molecule**: combination of atoms (covalent bonds)
- **Molecular weight**: sum of atomic weights
  - e.g. MW of methane, CH_4 = 1(12) + 4(1) = 16 g/mole
- **Mole**: Avogadro’s number of molecules (6.0221413×10^{23})

$$\text{Number of moles} = \frac{\text{mass}}{\text{molecular weight}}$$

Chemical Reactions Stoichiometry

✓ **Stoichiometry** (Gr. stoikheion = element):
Study of quantitative relationships between reacting species and products

- Basis for material balances (inputs/outputs) for chemical processes

- First step: balance reaction equation by balancing the key element being oxidized or reduced (e.g., C)

e.g., combustion of methane with oxygen (to get energy)

$$CH_4 + O_2 \rightarrow CO_2 + H_2O$$

- Need more H on RHS, more O on LHS
- By trial and error
  - Balance C (OK)
  - Balance H (double water to get H)
  - Balance O (double oxygen to get O)

Stoichiometry

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

- In units of mass:
  - 1 mol CH_4 = 16 g
  - 1 mol of O_2 = 2*16 = 32 g
  - 1 mol of CO_2 is 12+2*16 = 44 g
  - 1 mol of water is 18g

Examples

- Combustion of pentane

$$C_5H_{12} + O_2 \rightarrow CO_2 + H_2O$$

- Use limestone to neutralize SO_2
  - Limestone is $CaCO_3$
  - Product is gypsum $CaSO_4$

$$CaCO_3 + \quad SO_2 + \quad O_2 \quad \rightarrow \quad CaSO_4 + \quad CO_2$$

Example

- If 50 g of pentane were combusted, how many grams of water would be formed?

Write a balanced equation

50 g of pentane is how many moles?

Example

- 0.83 mM glucose solution ($C_6H_{12}O_6$) is completely biodegraded to CO_2 and water. How much oxygen is required (mg/L)?

Example (solution)

- Write a balanced equation

- Find MW of each component
  - Glucose – 180 g/mol
  - Oxygen – 32 g/mol
  - Carbon Dioxide – 44 g/mol
  - Water – 18 g/mol

- Calculate O_2 requirement on a mass basis

$$C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$$

Example (solution)

- We have 0.83×10^{-3} M of glucose:

Oxygen Demand

- This oxygen demand calculated in the previous example is **theoretical oxygen demand**:
  - The oxygen needed to fully oxidize organic material to carbon dioxide and water

- There is also **biochemical oxygen demand**:
  - The actual amount of oxygen required for oxidation (stabilization) of organic wastes carried out by bacteria

- BOD ≤ TOD (since some carbon is converted to cell material rather than fully oxidized all the way to CO_2, and some carbons are non-biodegadable)
  - We will discuss BOD and other oxygen demands later in the course

Example

- Energy consumption in North America is 85 x 10^{18}J/yr.

  If all energy came from a fuel with composition C_2H_3 and an energy content of 43 x 10^6 J/kg,

  At what rate would CO_2 be emitted?

Example (solution)

- Write a balanced equation

reactants & products: $C_2H_3 + O_2 \rightarrow CO_2 + H_2O$

balance C, H, O_2:

- What mass of fuel is used in a year?

- Use MWs to calculate mass of CO_2 emitted

  - C_2H_3: 2(12) + 3(1) = 27 g/mol
  - CO_2: 1(12) + 2(16) = 44 g/mol

Example (solution)

Stoichiometry of Some Important Reactions

- Aerobic biodegradation of benzene in an aquifer

  $C_6H_6 + 7.5O_2 \rightarrow 6CO_2 + 3H_2O$

- Biodegradation of sewage in activated sludge

  $C_{10}H_{19}O_3N + 12.5O_2 \rightarrow 10CO_2 + 8H_2O + NH_3$

- Acid mine drainage

  $FeS_2 + 3.5O_2 + H_2O + 2H^+ \rightarrow Fe^{+2} + 2H_2SO_4$

- Nitrification

  $NH_3 + 2O_2 \rightarrow NO_3^- + H_2O + H^+$