CHAPTER 2

ATMOSPHERIC CONCENTRATION UNITS

MASS

- Quantity of matter in an object.
- Default SI unit is kilograms (kg)
- Other units
  - Miligrams, micrograms, nanograms (atmospheric concentrations)
  - Pound-mass (1 lb_m = 0.454 kg)

FORCE

- Any influence that causes an object to undergo a certain change in its state (movement, direction, shape, etc.)
- In motion equations
  - Force is the product of mass of the object and its acceleration (Newton's secand law)
- Units
  - Newton (kilogram.meters per second square)
  - Dyn (1 N = 10^5 dyn)
  - Kilogram-force (1 N = 0.10197 kp)
  - Pound-force (1 N = 0.22481 lb_f)

PRESSURE

- The force exerted per unit area in a direction perpendicular to the surface.
- Two reference systems
  - Absolute pressure
    - Total pressure applied to a surface
    - Total atmospheric pressure at sea level is 1 atm
  - Gauge pressure
    - Pressure relative to the local atmospheric pressure
    - Total pressure minus local atmospheric pressure

PRESSURE

- Units
  - Default SI unit is Pa
    - Newtons per square meter (N/m2)
    - Atmospheric pressure at sea level is 101325 Pa
  - Other units
    - Atmospheric pressure unit (atu, atm)
    - bars (mb)
    - psi
    - 1 atm = 1013.25 mb = 101325 Pa
    - 100 Pa = 1 mb
    - 1 atm = 14.7 psi

PRESSURE

- Toricelli experiment
- Mercury
  - 1 atm at sea level = 76 cm Hg = 760 mm Hg
- Water
  - 1 atm at sea level = 10.33 m H2O = 1033 cm H2O
- Other
  - Density of ethanol at 20 C = 789 kg/m3
  - Density of water at 20 C = 998.2 kg/m3
  - Atmospheric pressure in terms of ethanol column?

TEMPERATURE & HEAT

- Heat: Total kinetic energy of all atoms and molecules in a matter
- Temperature: Average kinetic energy of all atoms and molecules in a matter
- Units:
  - Degrees Celcius
    - Water freezes at 0 C, and boils at 100 C
  - Fahrenheit
    - Water freezes at 32 F, and boils at 212 F ➔ slope = 1.8:1.0
  - Kelvin
    - Water freezes at 273 K, and boils at 373 K ➔ slope = 1.0:1.0

VOLUME

- The amount of space occupied by an object
- At any given time space is three-dimensional
  - Each dimension is measured by a length unit.
  - Thus, the default unit is cubic length
- Units
  - Cubic meters, cubic centimeters, liters, mililiters, etc.
  - Cubic foot, cubic inch, gallons, barrel, etc.
  - 1 m3 = 35.315 ft3
- Volume changes by changing temperature and pressure

CONCENTRATION UNITS

- Concentration is the amount of matter (usually pollutant) in unit amount of mixture
- Volumetric concentrations
  - Usually for gaseous components in a mixture
  - Parts per million by volume (ppm or ppmv): number of molecules of a pollutant in a million number of molecules of gaseous mixtures
  - Parts per billion by volume (ppb or ppbv): number of molecules of a pollutant in a billion number of molecules of gaseous mixtures
  - Parts per trillion by volume (ppt or pptv): number of molecules of a pollutant in a trillion number of molecules of gaseous mixtures

CONCENTRATION UNITS

- Volumetric concentrations
  - Partial pressure is most commonly used in air pollution field
  - Partial pressure is a unit of volumetic concentration
  - Example: Partial pressure of benzene in a flue gas is 0.98 mb. What is the ppm concentration? Flue gas pressure is 1013 mb.
    - 0.98 mb / 1013 mb * 1000000 = 993 ppm
  - Comes from ideal gas law.
    - At constant temperature and pressure, volume of a pollutant is proportional to its number of moles in the mixture
  - Concentration is the ratio of volume of gaseous pollutant to the total volume of mixture

CONCENTRATION UNITS

- Volumetric concentrations
  - Example: What is the partial pressure (in mm Hg) of 1350 ppm of toluene in the flue gas at a pressure of 1 atm.
    - 1350 /1000000 * 1 atm * (760 mm Hg / 1 atm) = 1.026 mm Hg
  - Number of moles of a pollutant in unit number of total moles of gaseous mixture is the volumetric concentration of a pollutant.
  - Example: A gaseous mixture of 7000 moles contains a mole of m-xylene? What is the concentration of m-xylene in ppm
    - 1 mole / 7000 moles * 1000000 = 142.9 ppm
  - The atmosphere is roughly a mixture of oxygen (21% by volume) and nitrogen (79% by volume). The concentration of oxygen is 210000 ppm and and of nitrogen is 790000 ppm. Sums up to 1000000 ppm, which is equal to 1.

CONCENTRATION UNITS

- Mass concentrations
  - Mass of a pollutant in unit volume of gaseous mixture
  - Units
    - Miligrams per cubic meter
    - Micrograms per cubic meter
    - Nanograms per cubic meter
    - Pounds per cubic foot
    - Pounds per gallon

CONCENTRATION UNITS

- Mass concentrations
  - Can be used to express both particulate and gaseous pollutants
  - Mass of a pollutant does not change with temperature
  - Volume of a gaseous mixture changes with both temperature and pressure
  - Thus, mass concentration changes with both temperature and pressure

CONCENTRATION UNITS

- Conversion between mass and volumetric concentrations
  - 1 ppm = 1 mg/L?
    - Only valid for diluted aqueous solutions
    - Very important
  - In air pollution field, 1 ppm is not equal to 1 mg/L.
  - ppm – mg/m3 conversions are based on ideal gas law
  - Example: 100 ppm benzene, 78 g/mole, 25 C, 1 atm, mg/m3?
  - Example: 650 ppm toluene, 92 g/mole, 100 C, 1 atm, mg/m3?
  - Example: 21% oxygen in atmosphere, 25 C, g/m3?
  - Example: 1200 mg/m3 of toluene, 25 C, 92 g/mole, ppm?
  - Example: 3300 mg/m3 of SO2, 150 C, 64 g/mole, ppm?

FLOWRATE

- Mass flowrate
  - Mass rate of transfer of a matter through a known cross-section per unit time
  - Units
    - Miligrams per second
    - Kilograms per second
    - Tons per year
    - Kilograms per hour
    - Pounds per hour

FLOWRATE

- Volumetric flowrate
  - Volume of a gaseous matter transfered through a known cross-section per unit time
  - Units
    - Cubic meters per second
    - Liters per second
    - Cubic meters per hour
    - Cubic feet per second
    - Cubic feet per hour

FLOWRATE

- Normal and standard conditions
  - Normal conditions: 1 atm, 0 C
  - Standard conditions: 1 atm, 25 C
  - Since volume of a gas changes with temperature and pressure, a standardization is necessary
  - Based on ideal gas law.
  - Units
    - Nm3/s, Nm3/h
    - Acfm = actual cubic foot per minute
    - Scfm = standard cubic foot per minute

FLOWRATE

- Normal and standard conditions
  - Example: Flue gas of 3500 m3/h at 150 C and 1 atm. What is the flowrate under normal conditions?
    - 3500 m3/h * 273 / 423 = 2259 Nm3/h
  - Example: Flue gas with a flowrate of 4000 Nm3/h. What is the actual flowrate at 120 C?
    - 4000 Nm3/h * 393 / 273 = 5758 m/h
  - Example: Flue gas contains 550 mg/m3 of benzene. What is the concentration under normal conditions if flue gas temperature is 230 C?
    - 550 * 303 / 273 = 1013 mg/Nm3

FLOWRATE

- Normal and standard conditions
  - Example: Flue gas contains 475 mg/Nm3 of toluene. Flue gas flowrate is 6500 Nm3/h. Temperature is 160 C. Density of flue gas is 0.812 kg/m3. Toluene: 92 g/mole
  - What is the actual concentration?
    - 475 mg/Nm3 *273/433 = 299.5 mg/m3
  - What is the actual flowrate?
    - 6500 * 433/273 = 10309.5 m3/h
  - What is the mass flowrate of toluene?
    - 475 * 6500 ≈ 299.5 * 10309.5 = 3087500 mg/h = 3.088 kg/h
  - What is the mass flowrate of flue gas?
    - 10309.5 * 0.812 = 8371.3 kg/h

FLOWRATE

- Normal and standard conditions
  - Example (Cont'd): Flue gas contains 475 mg/Nm3 of toluene. Flue gas flowrate is 6500 Nm3/h. Temperature is 160 C. Density of flue gas is 0.812 kg/m3. Toluene: 92 g/mole
  - What is the concentration of toluene in ppm?
    - 0.000475 * 0.082 *273 / 92 = 0.000116 atm = 116 ppm

STACK GAS CORRECTIONS

- With respect to oxygen concentration
  - To prevent dilution of industrial stack gases with ambient air
  - Legislations set emission standards for 3% oxygen or 6% oxygen
  - Correction:

$$C_C = C_m \frac{21-R}{21-M}$$

  - C_c = concentration of pollutant with respect to reference oxygen
  - C_m = concentration of pollutant measured in stack gas
  - R = Percent reference oxygen
  - M = Actual percent oxygen concentration measured in stack gas

STACK GAS CORRECTIONS

- With respect to oxygen concentration
  - Example: Flue gas contains 450 mg/Nm3 of m-xylene and 6% oxygen. What is the m-xylene concentration wrt 3% oxygen?
    - 450 * (21-3) / (21-6) = 540 mg/Nm3
  - Example: Flue gas contains 1200 ppm of benzene and 5.4% of oxygen. What is the benzene concentration wrt 3% oxygen?
    - 1200 * (21 – 3) / (21 – 5.4) = 1385 ppm

STACK GAS CORRECTIONS

- With respect to humidity
  - Legislations usually set emission standards based on dry flue gas
  - Correction: $$C_C = C_m \frac{100}{100 - H}$$
  - H = Percent humidity measured in stack gas
  - Example: Sulfur dioxide concentration in flue gas is 950 mg/Nm3. Humidity is 4.7%. What is the concentration on a dry basis?
  - 950 * 100 / (100-4.7) = 997 mg/Nm3

STACK GAS CORRECTIONS

- With respect to temperature
  - Legislations usually set emission standards based on normal conditions, that's 0 C
  - Correction:

$$C_C = C_m \frac{T_m}{T_S}$$

  - T_m = Measured temperature of stack gas in Kelvin
  - T_S = Normal temperature in Kelvin (273 K)
  - Example: Sulfur dioxide concentration in flue gas is 840 mg/m3. Temperature is 230 C. What is the normal concentration?
  - 840 * 503 / 273 = 1548 mg/Nm3

STACK GAS CORRECTIONS

- With respect to pressure
  - Legislations usually set emission standards based on normal conditions, that's 1 atm or 1013 mb
  - Correction:

$$C_C = C_m \frac{P_S}{P_m}$$

  - P_m = Measured pressure of stack gas
  - P_S = Normal pressure
  - Example: Sulfur dioxide concentration in flue gas is 840 mg/m3. Pressure is 1022 mb. What is the normal concentration?
  - 840 * 1013 / 1022 = 832 mg/m3

EXAMPLE

- A flue gas contains 1400 ppm of m-xylene. The flue gas flowrate is 6700 m3/h at 120 C and a pressure of 1023 mb. The oxygen concentration in the flue gas is 5.6% and humidity is 3.8%. The emission standard for m-xylene is 500 mg/Nm3 on a dry basis based on 3% oxygen. M-xylene: 106 g/mole. Density of flue gas under normal conditions is 1.25 kg/m3.
- What is the flue gas flowrate under normal conditions?
  - 6700 m3/h * (273 / 393) * (1023 / 1013) = 4700 Nm3/h
- What is the actual concentration of m-xylene?
  - $1400/10^6$ * 106 / 0.082 / 393 = 0.004605 g/L = 4605 mg/m3

EXAMPLE

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- What is the concentration under normal conditions?
  - 4605* (393 / 273) * (1013 / 1023) = 6564 mg/Nm3
- What is the concentration under normal conditions on a dry basis?
  - 6564 * 100 / (100 – 3.8) = 6823 mg/Nm3

EXAMPLE

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- What is the concentration under normal conditions on a dry basis, corrected with respect to 3% reference oxygen?
  - 6564 mg/Nm3 * (21-3) / (21-5.6) = 7975 mg/Nm3
- What is the mass flowrate of m-xylene?
  - 6564 mg/Nm3 * 4700 Nm3/h = 3.085 * 10^7 mg/h = 30.85 kg/h

EXAMPLE

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- What is the molar flowrate of flue gas if its molar mass is 28.27 g/mole?
  - 5875 kg/h / (28.27 kg/kmole) = 207.82 kmole / h
- Check the ppm concentration of m-xylene?
  - 0.291 kmole/h / 207.82 kmole/h = 0.0014 kmole/kmole = 1400 ppm

EXAMPLE

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- Check if the industry meets emission standard?
  - 7975 mg/Nm3 > 500 mg/Nm3 ➔ Fails