

IH Chemistry and Math Review

Lecture 1

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Equations

$$\text{Mass} = \rho * \text{Vol} \quad \text{SpGr} = \frac{\rho_{\text{liquid}}}{\rho_{\text{water}}} \quad T_R = 460 \text{ }^\circ\text{R} + T_F \quad T_K = 273 \text{ }^\circ\text{C} + T_C$$

$$PV = nRT \quad \frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2} \quad \text{NoMoles} = \frac{\text{Vol}_{\text{cont}}}{\text{AvVol}} \quad \text{NoMoles} = \frac{\text{Mass}}{\text{MW}}$$

$$\text{AvVol} = 24.45 \text{ L} \times \frac{273.16 + T_C}{273.16 + 25C} \times \frac{760\text{mmHg}}{P_{\text{bar}}}$$

$$\text{Vol}_{\text{cont}} = \left(\frac{\text{Conc}_{\text{ppm}}}{10^6 \text{ ppm}} \right) \text{Vol}_{\text{air}} \quad \text{Volume} = \text{NoMoles} \times \text{AvVol}$$

$$\text{Conc}_{\text{mg}/\text{m}^3} = \frac{\text{MW}}{\text{AvVol}} \times \text{Conc}_{\text{ppm}} \quad \text{Conc}_{\text{ppm}} = \frac{\text{AvVol}}{\text{MW}} \times \text{Conc}_{\text{mg}/\text{m}^3} \quad \text{Conc}_{\text{ppm}} = \frac{\text{Vol}_{\text{cont}}}{\text{Vol}_{\text{air}}} \times 10^6 \text{ ppm}$$

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Reference Temperatures and Pressures

STP - Standard Temperature and Pressure

Commonly used for chemical and physical processes.
 0°C (273.15 K, 32F) and 1 atm (101.325 kN/m²,
 101.325 kPa, 14.7 psia, 0 psig, 29.92 in Hg, 760 torr,
 33.95 Ft.H₂O, 407.2 In.W.G, 2116.8 Lbs./Sq.Ft.)

NTP - Normal Temperature and Pressure (OSHA/NIOSH/ACGIH)

25 °C (298.15 K) and 760 mm Hg (101.325 kPa), molar vol = 24.46 L

NTP - Normal Temperature and Pressure (European and U.S. Ventilation)

20 C (293.15 K, 68 F) and 1 atm (101.325 kN/m²,
 101.325 kPa, 14.7 psia, 0 psig, 29.92 in Hg, 760 torr.
 Density 1.204 kg/m³ (0.075 pounds per cubic foot)

SATP - Standard Ambient Temperature and Pressure

Also used in chemistry as a reference with temperature of 25 degC
 (298.15 K) and pressure of 101 kPa.

ISA - International Standard Atmosphere

Reference for aircraft performance
 101.325 kPa, 15 C and 0% humidity.

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Adjusting TLVs to non-NTP conditions

- *Application of TLVs® to Unusual Ambient Conditions.* When workers are exposed to air contaminants at temperatures and pressures substantially different than those at normal temperature and pressure (NTP) conditions (25°C and 760 torr), care should be taken in comparing sampling results to the applicable TLVs®. For aerosols, the TWA exposure concentration (calculated using sample volumes not adjusted to NTP conditions) should be compared directly to the applicable TLVs® published in the *TLVs® and BEIs® book*. For gases and vapors, there are a number of options for comparing air-sampling results to the TLV®, and these are discussed in detail by Stephenson and Lillquist (2001). One method that is simple in its conceptual approach is 1) to determine the exposure concentration, expressed in terms of mass per volume, at the sampling site using the sample volume **not** adjusted to NTP conditions, 2) if required, to convert the TLV® to mg/m³ (or other mass per volume measure) using a molar volume of 24.4® L/mole, and 3) to compare the exposure concentration to the TLV®, both in units of mass per volume.

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Avogadro's Volume: molar volume of any gas

At 0C, 760 mmHg, AvVol = 22.414 L

At 20C, 760 mmHg , AvVol = 24.055 L

At 25C, 760 mmHg , AvVol = 24.465 L

At 70F, 760 mmHg , AvVol = 24.146 L

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Density

- Density (ρ) is the amount of matter contained in a unit volume of a substance
- $\rho = \text{Mass/Volume}$
- Reference density: water
 - English - 8.345 lb/gal
 - Metric - 1 g/mL_{liq}

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Specific gravity

The ratio of the weight or mass of a given substance, at a specified temperature, to that of an equal volume of another reference substance

Reference of liquid or solid is water
Reference of gases is air or H₂

$$SpGr = \frac{\rho_{liquid}}{\rho_{water}}$$

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Problem 1

- Find the specific gravity of acetone if the density is 6.54 lb/gal.

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Problem 1 solution

$$SpGr = \frac{\rho_{liquid}}{\rho_{water}} = \frac{6.54 \text{ lb/gal}}{8.33 \text{ lb/gal}} = 0.79$$

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Problem 2

- Find the density in lb/gal of carbon disulfide if the SpGr is 1.26.

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Problem 2 solution

$$SpGr = \frac{\rho_{liquid}}{\rho_{water}}$$

- Find the density in lb/gal of carbon disulfide if the SpGr is 1.26.

$$\begin{aligned}\rho_{CS_2} &= SpGr_{CS_2} \times \rho_{H_2O} \\ &= 1.26 \times 8.33 \text{ lb/gal} \\ &= 10.5 \text{ lb/gal}\end{aligned}$$

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Problem 3

- Given the specific gravity of carbon disulfide is 1.26, what is the mass of 75 ml of CS₂?

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Problem 3 solution

- Given the specific gravity of carbon disulfide is 1.26, what is the mass of 75 ml of CS₂?

$$\begin{aligned}\text{Mass of CS}_2 &= \rho * \text{Vol}_{\text{liq}} \\ &= \text{SpGr}_{\text{CS}_2} \times \rho_{\text{H}_2\text{O}} * \text{Vol}_{\text{liq}}\end{aligned}$$

$$\begin{aligned}\text{Mass of CS}_2 &= 1.26 \times 1.00 \frac{\text{g}}{\text{ml}} \times 75 \text{ ml} \\ &= 94.5 \text{ g}\end{aligned}$$

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Problem 4

- If 94.5 g of CS₂ were vaporized, how much vapor would be produced?

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Problem 4 solution

$$\text{Volume} = \text{NoMoles} \times \text{Vol} / \text{mole}$$

$$\text{Mass} = \text{NoMoles} \times \text{MassPerMole}$$

- If 94.5 g of CS₂ were vaporized, how much vapor would be produced @25C and sea level?
- Solution: Determine number of moles
Based on the molar volume determine the total volume

$$\text{AvVol} = 24.45 \times \frac{273.16 + T_c}{273.16 + 25C} \times \frac{760 \text{ mmHg}}{P_{\text{bar}}} = 24.45 \text{ L} / \text{mole}$$

$$\text{NoMoles} = \frac{\text{Mass}}{\text{MW}} = \frac{94.5 \text{ g}}{(12 + 2 \times 32) \text{ g} / \text{mole}} = \frac{94.5 \text{ moles}}{76} = 1.243 \text{ moles}$$

$$\text{Volume} = \text{NoMoles} \times \text{AvVol} = 1.234 \text{ moles} \times 24.45 \text{ L} / \text{mole}$$

$$= 30.4 \text{ L}$$

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Problem 5

- If that volume of vapor were to be diluted with 10 m³ of clean air, what would the concentration be in PPM?

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Problem 5 solution

If that volume of vapor were to be diluted with 10 m³ of clean air, what would the concentration be in PPM?

$$\begin{aligned} \text{Conc}_{ppm} &= \frac{\text{Vol}_{cont}}{\text{Vol}_{air}} \times 10^6 \text{ ppm} \\ &= \frac{30.3L}{30.3L + 10m^3 \times 1000 \frac{L}{m^3}} \times 10^6 \text{ ppm} = 3030 \text{ ppm} \end{aligned}$$

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Problem 6

- What is the mass, in mg, of CS₂ in a 10 Liter sample of air collected at 25° C, if the concentration of CS₂ in the sample is 500 PPM?

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Problem 6 solution

What is the mass, in mg, of CS₂ in a 10 Liter sample of air collected at 25° C, if the concentration of CS₂ in the sample is 500 PPM?

- 1) Calculate the volume of pure CS₂ needed to produce 500 PPM in 10 L.
- 2) Determine number of moles in that volume.
- 3) Determine mass from the number of moles and the gram molar (GMW) weight.

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$$Conc_{ppm} = \frac{Vol_{cont}}{Vol_{air}} \times 10^6 ppm$$

Problem 6 solution - continued

What is the mass in mg of CS₂ in a 10 Liter sample of air collected at 25° C, if the concentration of CS₂ in the sample is 500 PPM?

- 1) Calculate the volume of pure CS₂ needed to produce 500 PPM in 10 L.

$$Vol_{cont} = \left(\frac{Conc_{ppm}}{10^6 ppm} \right) Vol_{air} = \left(\frac{500 ppm}{10^6 ppm} \right) 10L = 5 \times 10^{-3} L$$

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Problem 6 solution - continued

What is the mass in mg of CS₂ in a 10 Liter sample of air collected at 25° C, if the concentration of CS₂ in the sample is 500 PPM?

- 1) Calculate the volume of pure CS₂ needed to produce 500 PPM in 10 L. Vol = 5x10⁻³ L
- 2) Determine number of moles in that volume.

$$\text{NoMoles} = \frac{\text{Vol}_{cont}}{\text{Vol}_{one\ mole}} = \frac{5 \times 10^{-3} \text{ L}}{24.4 \text{ L/mole}} = 2.05 \times 10^{-4}$$

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Problem 6 solution - continued

What is the mass in mg of CS₂ in a 10 Liter sample of air collected at 25° C, if the concentration of CS₂ in the sample is 500 PPM?

- 2) Number of moles in that volume = 2.05x10⁻⁴ moles
- 3) Determine mass from the number of moles and the MW.

$$\text{MW}_{\text{CS}_2} = 12 + 2 \times 32 = 76 \text{ g/mole} = 76000 \text{ mg/mole}$$

$$\text{Mass} = \text{NoMoles} \times \text{WtPerMole}$$

$$= \text{NoMoles} \times \text{MW} / \text{mole}$$

$$= 2.05 \times 10^{-4} \text{ moles} \times 76000 \text{ mg / mole} = 15.6 \text{ mg}$$

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$$AvVol = 24.45 L \times \frac{273.16 + T_C}{273.16 + 25C} \times \frac{760 mmHg}{P_{bar}}$$

Equations to convert from ppm to mg/m³

$$Conc_{ppm} = \frac{AvVol}{MW} \times Conc_{mg/m^3}$$

$$Conc_{mg/m^3} = \frac{MW}{AvVol} \times Conc_{ppm}$$

When converting values expressed as an element (e.g., as Fe, as Ni), the molecular weight of the element should be used, not that of the entire compound.

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Absolute Temperature

- Degree Rankin (°R)- English

$$T_R = 460 \text{ } ^\circ\text{R} + T_F$$

- Degree Kelvin (°K) – metric

$$T_K = 273 \text{ } ^\circ\text{C} + T_C$$

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General Gas Law

$$PV = nRT$$

$$PV = nRT$$

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$$

- Permits the determination of the value of any of the three basic characteristics of the gas/vapor being evaluated that result from changes to one or both of the other two characteristics.

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STP volume correction for NTP

$$\frac{P_1 \times V_1}{T_1} = \frac{P_2 \times V_2}{T_2}$$

$$V_2 = \frac{T_2}{P_2} \times \frac{P_1 \times V_1}{T_1}$$

$$V_2 = V_1 \times \left(\frac{T_2}{T_1} \right) \times \left(\frac{P_1}{P_2} \right)$$

$$V_2 = 22.25 \text{ L} \times \left(\frac{298^\circ\text{K}}{273^\circ\text{K}} \right) \times \left(\frac{760 \text{ mm Hg}}{760 \text{ mm Hg}} \right)$$

$$V_2 = 24.5 \text{ L at } 25^\circ\text{C and } 760 \text{ mm Hg}$$

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