**Concentrations and Other Units of Measure**  
(Nazaroff & Alvarez-Cohen, Section 1.C.1)

The concept of concentration exists to answer the question:

How much of the “stuff” is there?

*Definition*: The concentration of a substance is the “amount” of it per “amount” of containing material (air, water, soil).

It can be expressed in various units.  
If the containing medium is air for example:

- \( C_A = \frac{\text{mass of } A}{\text{volume of air}} \) — used with mass balances
- \( \{A\} = \frac{\text{moles of } A}{\text{volume of air}} \) — used with chemical reactions
- \( X_A = \frac{\text{mass of } A}{\text{mass of air}} \) — used when air pressure varies
- \( Y_A = \frac{\text{moles of } A}{\text{moles of air}} \) — occasionally handy  
- \( P_A = \frac{\text{partial pressure of } A}{\text{atmospheric pressure}} \) — used for air-water exchange

**Unit conversion**

It is often necessary to switch units, for example, to pass from a chemical reaction in which amounts are most naturally expressed in moles to a mass budget in which amounts are most naturally expressed in grams.

**Rule 1:**  
\[
\text{Mass in grams} = \text{Molecular weight} \times \text{Number of moles}
\]

where

- \( \text{Molecular weight} = \sum \text{Atomic weights} \)

**Examples:**

- \( \text{H}_2\text{O} \): \( MW = 2 \times 1 + 1 \times 16 = 2 + 16 = 18 \) grams per mole
- \( \text{CO}_2 \): \( MW = 1 \times 12 + 2 \times 16 = 12 + 32 = 44 \) grams per mole
- \( \text{H}_2\text{SO}_4 \): \( MW = 2 \times 1 + 1 \times 32 + 4 \times 16 = 2 + 32 + 64 = 98 \) grams per mole
Atomic weights most commonly used in environmental engineering

Hydrogen \( H \) 1
Carbon \( C \) 12 (14 is for radioactive form of \( C \))
Nitrogen \( N \) 14
Oxygen \( O \) 16
Phosphorus \( P \) 31
Sulfur \( S \) 32
Chlorine \( Cl \) 35.45
Calcium \( Ca \) 40

It is helpful to memorize the preceding symbols and atomic numbers.

For other elements, see the Periodic Table of Elements, on the next slide.

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**Periodic Table of Elements**

*Note: Round numbers when they are close to being integers.*

*Examples: Hydrogen \( H = 1 \); Carbon \( C = 12 \); Oxygen \( O = 16 \) but Chlorine \( Cl = 35.45 \).*
Rule 2:

Pressure of a gas is determined from the ideal-gas law
(Nazaroff & Alvarez-Cohen, Section 2.B)

\[ P_A V = n_A RT \]

where \( P_A \) = partial pressure of \( A \), in atm (atmosphere)
\( V \) = volume occupied, in m\(^3\) (entire volume, even if shared with other gases)
\( n_A \) = number of moles of \( A \) in that volume
\( R \) = universal constant
\[ R = 8.205 \times 10^{-5} \text{ atm} \cdot \text{m}^3 / (\text{mol} \cdot \text{K}) = 8.314 \text{ J} / (\text{mol} \cdot \text{K}) \]
\( T \) = absolute temperature, in degrees Kelvin (K)

Recall:

Absolute temperature (K) = temperature in degrees Celsius (°C) + 273.15

When several gases occupy a common volume in a mixture, their partial pressures simply add up to the total pressure, which is usually the atmospheric pressure:

\[ P_{\text{total}} = P_A + P_B + P_C + ... = \frac{RT}{V} \]

Properties of air

Apply ideal-gas law to air.
At standard pressure (\( P = 1 \text{ atm} \)) and temperature (\( T = 15^\circ \text{C} = 288.15 \text{ K} \)), one mole (\( n = 1 \text{ mol} \)) of air occupies a volume \( V \) equal to

\[ V = \frac{nRT}{P} = \frac{(1 \text{ mol})(8.205 \times 10^{-5} \text{ atm} \cdot \text{m}^3/\text{mol} \cdot \text{K})(288.15 \text{ K})}{(1 \text{ atm})} = 0.02364 \text{ m}^3 = 23.64 \text{ L (liters)} = 6.25 \text{ gallons} \]

Also,

Air = mixture of 79% nitrogen + 21% oxygen
\[ \text{MW}_{\text{air}} = (0.79) \text{ MW}_{\text{nitrogen}} + (0.21) \text{ MW}_{\text{oxygen}} \]
\[ = (0.79)(2 \times 14) + (0.21)(2 \times 16) \]
\[ = 22.12 + 6.72 = 28.84 \text{ grams per mole} \]

Actually, the value is 28.95 g/mol because of CO₂ and rare gases (heavier).

This leads to:

\[ \frac{1}{0.02364 \text{ m}^3/\text{mol}} = 42.3 \text{ mol/m}^3 \]
\[ (28.95 \text{ g/mol}) / (23.64 \text{ L/mol}) = 1.22 \text{ g/L} \] at ambient pressure and temperature
Properties of water

Water is a liquid, which may be considered as incompressible in all environmental applications.

Numbers for water are:

\[ \text{H}_2\text{O} \rightarrow \text{MW} = 2\times1 + 1\times16 = 18 \rightarrow 18.0 \text{ g/mol} \]

Density = 997 g/L (Think: 1 kg per liter)

Combine the above:

\[ \frac{997 \text{ g/L}}{18.0 \text{ g/mol}} = 55.4 \text{ mol/L} \]

Summary of unit conversion

1 mole weighs MW grams and occupies V liters

- moles \rightarrow MW \rightarrow grams
- \[ \text{V} \rightarrow \text{MW/V} \]
- moles to grams: multiply by MW
- moles to liters: multiply by V
- liters to grams: multiply by \( \frac{\text{MW}}{\text{V}} \) if gas; use density if liquid
Common abbreviations

- %: percent 1 part in 100
- ‰: per mil 1 part in 1000
- ppm: part per million 1 part in $10^6$
- ppb: part per billion 1 part in $10^9$
- ppt: part per trillion 1 part in $10^{12}$

Convention: The “part” stands for “mass” in water but for “moles” in air.

Air Example:

Today’s carbon dioxide concentration in the atmosphere is reported to be about 409 ppm.

This means that there are 409 moles of CO₂ per million moles of air.

In-class exercise

Knowing that the total mass of the atmosphere is $4.99 \times 10^{15}$ metric tons,

And that the current CO₂ concentration is 409 ppm,

How many tons of CO₂ are there in the atmosphere?

Then, what is the partial pressure of CO₂ in the atmosphere?

How much weight has been added on your shoulders since the CO₂ concentration rose from its pre-industrial level of 270 ppm?
Stoichiometry
(Nazaroff & Alvarez-Cohen, Section 3.A)

Stoichiometry is the application of mass balance to chemical transformation. In short, atoms are conserved, and when combinations of atoms disintegrate, new combinations form with the same atoms. No loss, no gain.

Example: Oxidation of glucose

\[
\text{C}_6\text{H}_{12}\text{O}_6 + (???) \text{O}_2 \rightarrow (???) \text{CO}_2 + (???) \text{H}_2\text{O}
\]

First, equilibrate the C’s and H’s before and after:

\[
\text{C}_6\text{H}_{12}\text{O}_6 + (???) \text{O}_2 \rightarrow 6 \text{CO}_2 + 6 \text{H}_2\text{O}
\]

Thus, we need 6x2 + 6x1 = 18 O’s on the right; already 6 on left, need 12 more:

\[
\text{C}_6\text{H}_{12}\text{O}_6 + 6 \text{O}_2 \rightarrow 6 \text{CO}_2 + 6 \text{H}_2\text{O}
\]

Use of stoichiometry to make material budgets

Take oxidation of glucose again:

\[
\text{C}_6\text{H}_{12}\text{O}_6 + 6 \text{O}_2 \rightarrow 6 \text{CO}_2 + 6 \text{H}_2\text{O}
\]

From this, we note that it takes

\[
6 \text{ molecules of oxygen (O}_2) \rightarrow 1 \text{ molecule of glucose (C}_6\text{H}_{12}\text{O}_6)\]

Thus, 6 moles of oxygen are needed to oxidize 1 mole of glucose.

MW of oxygen = 2x16 = 32 g/mol
MW of glucose = 6x12 + 12x1 + 6x16 = 72 + 12 + 96 = 180 g/mol

So, it takes 6x32 = 192 grams of oxygen to oxidize 180 grams of glucose.

Check values on the right:
Production is 6 moles of carbon dioxide (CO\textsubscript{2}) \rightarrow 6x(12+32) = 6x44 = 264 grams
6 moles of water (H\textsubscript{2}O) \rightarrow 6x(2+16) = 6x18 = 108 grams
Total on right = 264 + 108 = 372 grams
while total on left is = 180 + 192 = 372 grams.
In-class problems

Combustion of butane: \( \text{C}_4\text{H}_{10} \)

Formation of ambient ozone (O\(_3\)), by three successive reactions:

\( \text{NO}_2 \) splits into NO and atomic O

O combines with oxygen to make ozone

Ozone reacts with NO to produce O\(_2\) and NO\(_2\)

Answers:

\( \text{C}_4\text{H}_{10} + 6.5\ \text{O}_2 \rightarrow 4\ \text{CO}_2 + 5\ \text{H}_2\text{O} \) (208 grams of oxygen needed to burn 58 grams of butane)

\( \text{NO}_2 \rightarrow \text{NO} + \text{O} \)

\( \text{O} + \text{O}_2 \rightarrow \text{O}_3 \) (46 grams of nitrogen dioxide produces 48 grams of ozone)

\( \text{O}_3 + \text{NO} \rightarrow \text{O}_2 + \text{NO}_2 \)

Precision and Accuracy

(Nazaroff & Alvarez-Cohen, Section 1.C.7)

In engineering generally and especially in environmental matters, no quantity can be known perfectly well. There will always be some error attached to the measurement or to the calculated value.

**Precision** indicates how well the measurement is made. Repeated measurements yield similar values, but there may be a **bias** in the measuring technique.

**Accuracy** describes how close a measurement actually gets to the true value.