CHEN20010 Material and Energy Balances

Compositions of Mixtures

Compositions of Mixtures – Module Learning Outcomes

A student is expected to be able to:

- Define and calculate: mole %, weight %, volume %, mole fractions, mass fractions, ratios, concentrations, partial pressures, average molecular weight of mixtures
- Perform calculations on a component free basis
- Convert between mole fractions and mass fractions

Compositions and Analyses of Mixtures

Chemical engineers rarely work with pure materials. They mostly work with mixtures. Chemical engineers need the ability to accurately and unambiguously define the compositions of any mixtures they work with.

The Coogee Energy plant converts Bass Strait natural gas into methanol.

But what is natural gas?

What is natural gas ?

Natural gas is a hydrocarbon typically found with oil and water in petroleum reservoirs below ground.

Natural gas is a mixture of gases. The composition of the gas varies from location to location.

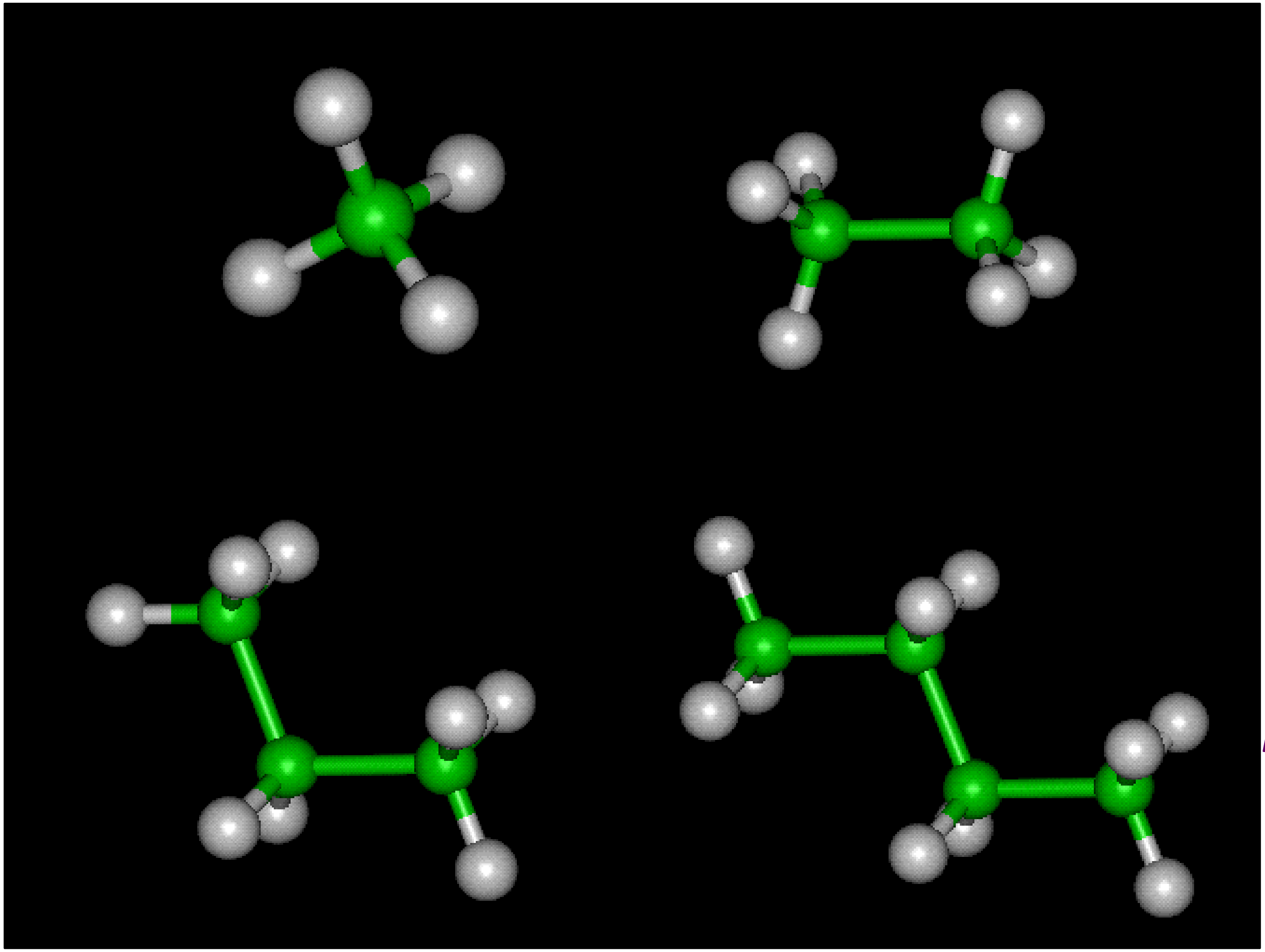
Dry Bass Strait natural gas has a typical composition of:

methane	CH_4	90.7 %
ethane	C_2H_6	5.9 %
propane	C_3H_8	0.6 %
butane	C_4H_{10}	0.1 %
nitrogen	N_2	0.9 %
carbon dioxide	CO_2	1.8 %

But when we refer to %'s are they %'s of the total mass, the total volume, the total number of moles ?

methane

ethane



propane

butane

Compositions and Analyses of Mixtures

Fractional :

$$\frac{\text{amount of A}}{\text{total amount of mixture}}$$

Ratio :

$$\frac{\text{amount of A}}{\text{amount of B}}$$

Component-free :
(B)

$$\frac{\text{amount of A}}{\text{amount of mixture - amount of B}}$$

Compositions and Analyses of Mixtures

Amounts may be MASS, MOLE or VOLUME

Mass fraction :

$$w_i = \frac{\text{mass of } i}{\text{mass of mixture}}$$

$$\%\ {}^{w}/_{w} \quad (\%\text{ by weight}) = 100\, w_i$$

Compositions and Analyses of Mixtures

Mole fraction :

$$x_i = \frac{\text{moles of } i}{\text{total moles}}$$

$$= \frac{w_i / M_i}{\sum_j w_j / M_j}$$

mol % $= 100\ x_i$

Compositions and Analyses of Mixtures

Mass ratio:

$$x_i = \frac{\text{mass A}}{\text{mass B}}$$

Molar ratio:

$$x_i = \frac{\text{mol A}}{\text{mol B}}$$

(for binary mixtures)

Compositions and Analyses of Mixtures

Concentration : $$\frac{\text{mass or mole of A}}{\text{total volume of mixture}}$$

Mass : $$\rho_i = \frac{\text{mass of i}}{\text{total volume of mixture}}$$

Moles : $$C_i = \frac{\text{moles of i}}{\text{total volume of mixture}}$$

e.g. molarity is mol/l

Compositions and Analyses of Mixtures

Volume Concentration (or Volume Fraction)

$$= \frac{\text{volume of component}}{\text{total volume of mixture}}$$

Compositions and Analyses of Mixtures

Volume Concentration (or Volume Fraction)

$$= \frac{\text{volume of component}}{\text{total volume of mixture}}$$

For gases the two volumes must be measured under identical conditions of temperature and pressure.

Compositions and Analyses of Mixtures

Volume Concentration (or Volume Fraction)

$$= \frac{\text{volume of component}}{\text{total volume of mixture}}$$

% $^{v}/_{v}$ = mol % = 100 (volume fraction)

% $^{v}/_{v}$ is mainly used for gases

When the composition of a gas is given it is nearly always expressed as mol %. Where this is not explicitly stated it is usually safe to assume the composition is in mol %.

What is natural gas ?

Dry Bass Strait natural gas has a typical composition of:

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propane	C_3H_8	0.6 %
butane	C_4H_{10}	0.1 %
nitrogen	N_2	0.9 %
carbon dioxide	CO_2	1.8 %

This composition is on a molar basis.

What is natural gas ?

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propane	C_3H_8	0.6 mol %
butane	C_4H_{10}	0.1 mol %
nitrogen	N_2	0.9 mol %
carbon dioxide	CO_2	1.8 mol %

This composition is on a molar basis.

If you had 100 moles of this mixture then you would have 90.7 moles of CH_4, 5.9 moles C_2H_6, 0.6 moles C_3H_8, 0.1 moles C_4H_{10}, 0.9 moles of N_2 and 1.8 moles CO_2.

But in reality, there will be some moisture present in the gas too!

Every 100 moles of dry natural gas might be accompanied by 25.0 moles of water.

Compositions of Mixtures

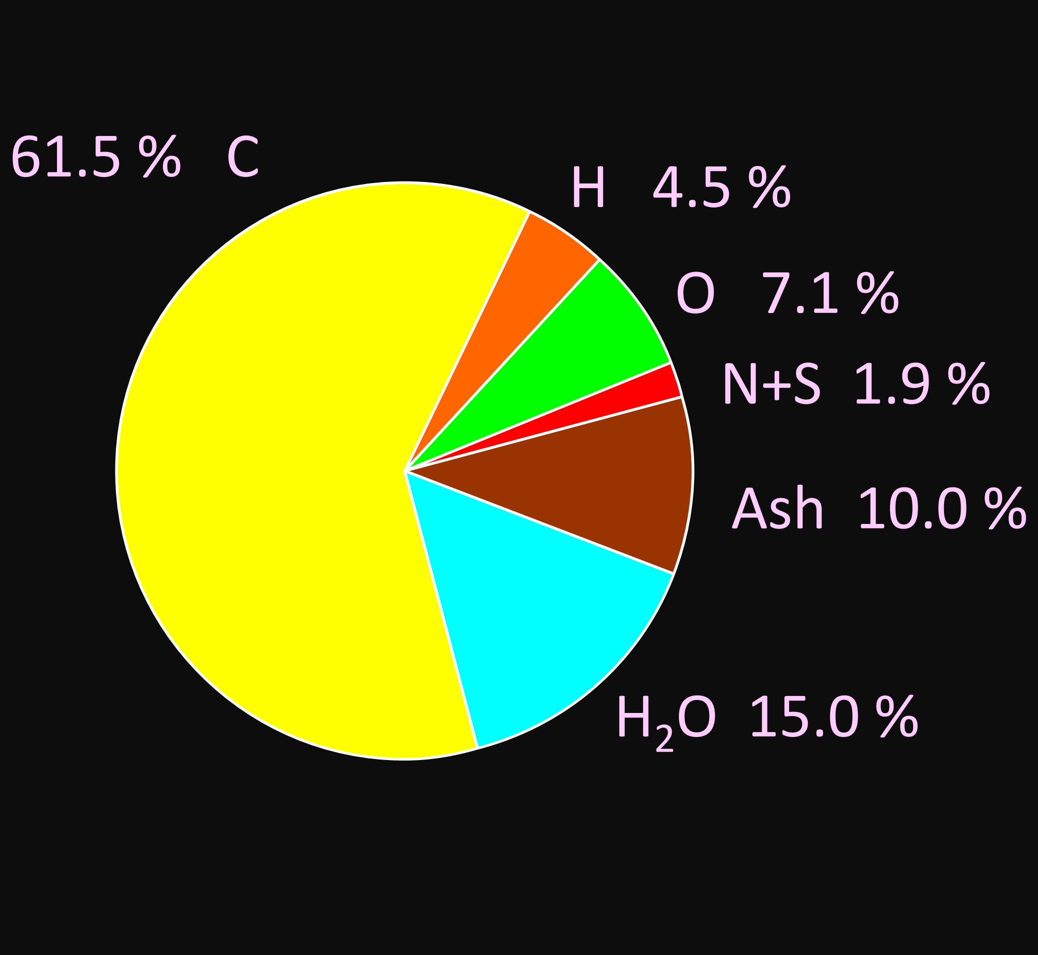
Component-free : One component is omitted from the analysis.

e.g. coal

	% $^w/_w$	% $^w/_w$, dry
C	61.5	
H	4.5	
O	7.1	
N+S	1.9	
Ash	10.0	
H_2O	15.0	
	100.0	

This means we delete the water component from the analysis and scale up the other components so that their sum is still 100.0

Component-free analysis



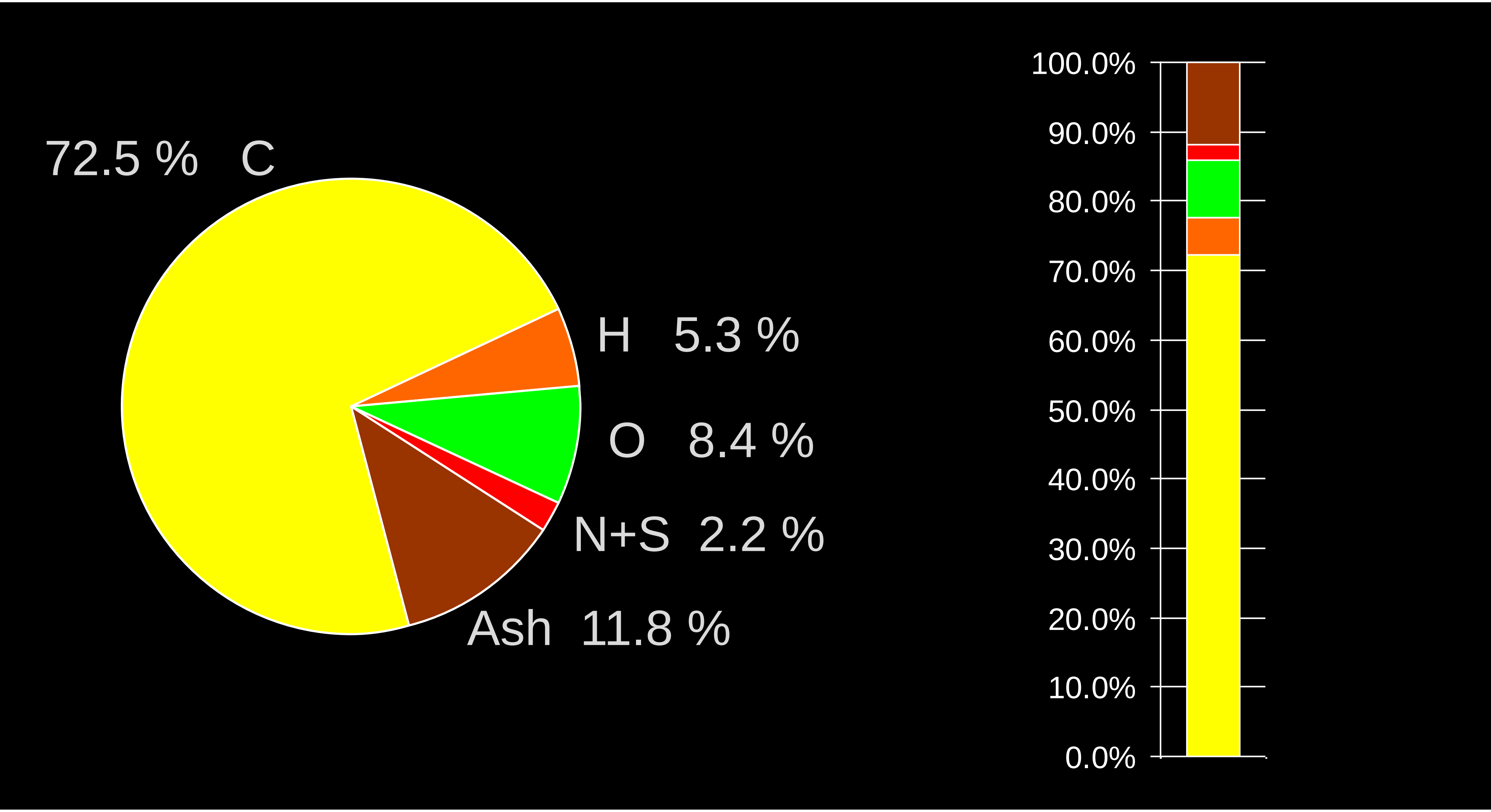
Component-free analysis

Component-free : One component is omitted from the analysis.

e.g. coal

	% $^{w}/_{w}$	% $^{w}/_{w}$, dry
C	61.5	
H	4.5	
O	7.1	
N+S	1.9	
Ash	10.0	
H_2O	15.0	
	100.0	

Composition on a dry basis



Component-free analysis

Component-free : One component is omitted from the analysis.

e.g. coal

	% $^w/_w$	% $^w/_w$, dry	% $^w/_w$, dry, ash-free
C	61.5	72.5	
H	4.5	5.3	
O	7.1	8.4	
N+S	1.9	2.2	
Ash	10.0	11.8	
H_2O	15.0		
	100.0	100.0	

This means we delete the water and ash components from the analysis and scale up the other components.

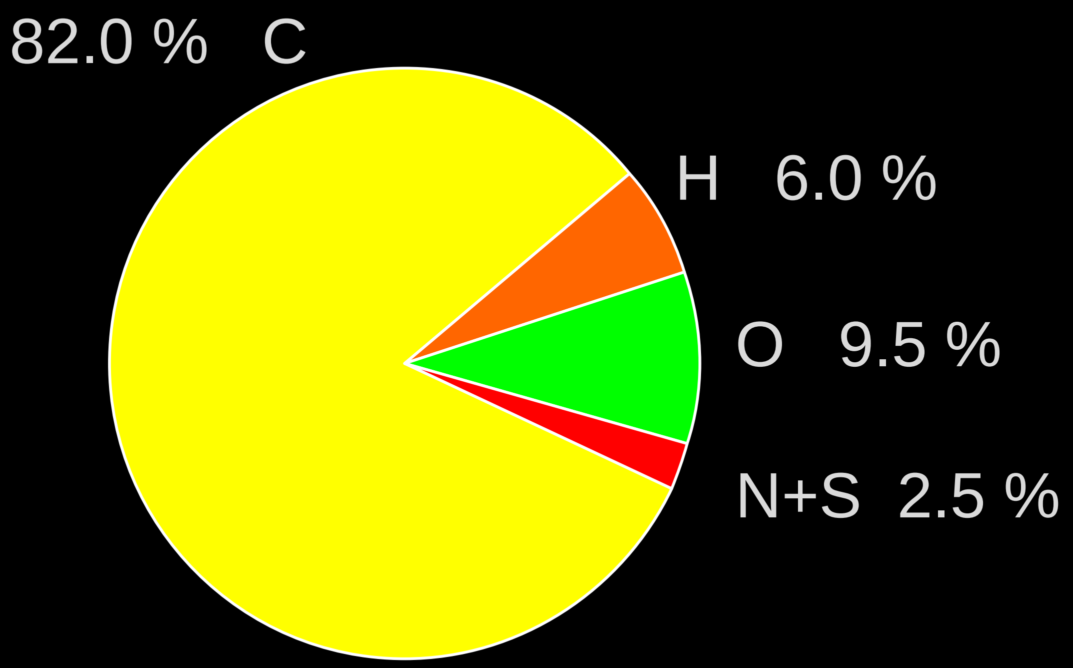
Component-free analysis

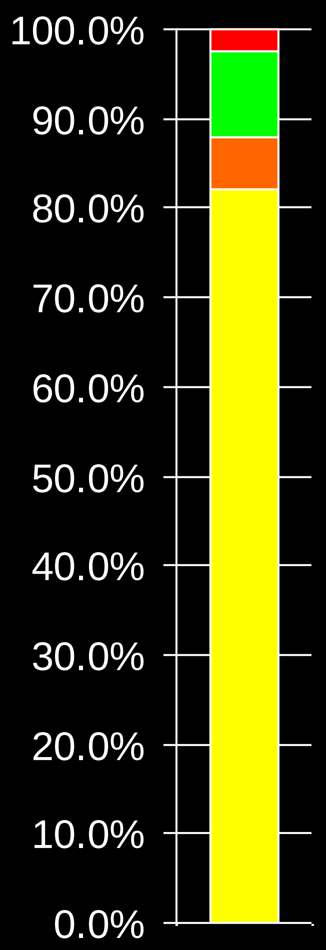
Component-free : One component is omitted from the analysis.

e.g. coal

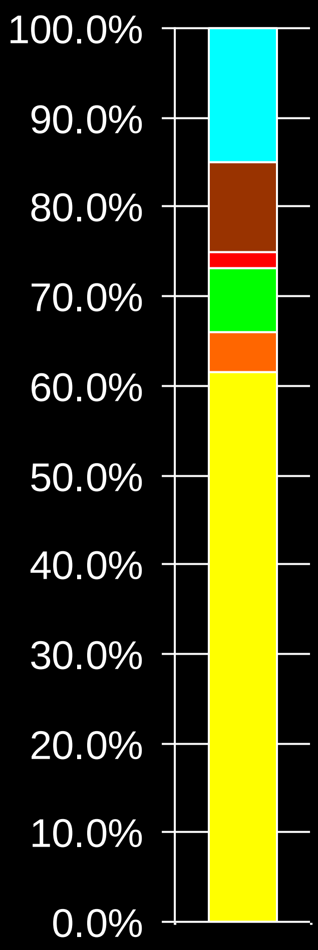
	% $^w/_w$	% $^w/_w$, dry	% $^w/_w$, dry, ash-free
C	61.5	72.5	
H	4.5	5.3	
O	7.1	8.4	
N+S	1.9	2.2	
Ash	10.0	11.8	
H_2O	15.0		
	100.0	100.0	100.0

Composition on a dry, ash-free basis

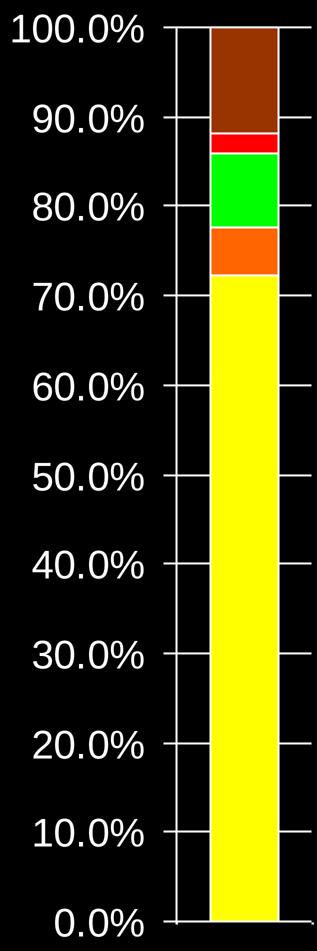




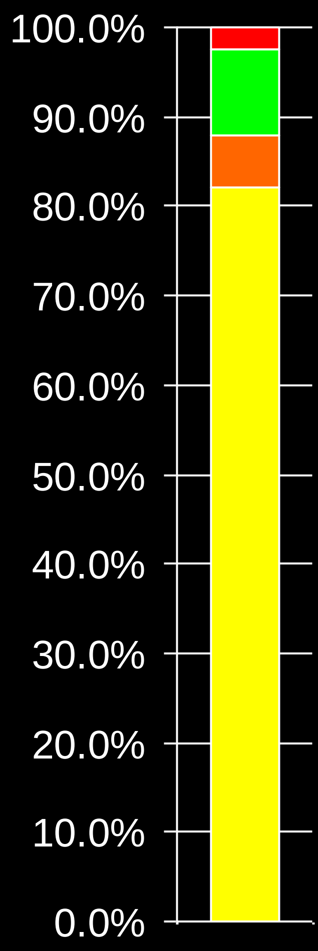
Original Data



Dry Basis



Dry, Ash-Free Basis



Average Molecular Weights of Mixtures

$$\left(\begin{array}{c} \text{Average} \\ \text{Molecular} \\ \text{Weight} \end{array} \right) = \sum_{\substack{\text{all} \\ \text{components}}} \left(\text{mol fraction}_i \times \text{Mol. Weight}_i \right)$$

Example : If a mixture has a composition of 17 mol % HCl, 51 mol % H_2O and 32 mol % HNO_3, what is the average molecular weight of the mixture ?

MW (HCl) = 36.5 MW (H_2O) = 18.0 MW (HNO_3) = 63.0

Average Molecular Weights of Mixtures

Conversions between Mole Fractions and Mass Fractions

Example 1 : Mass fractions ⇨ Mole fractions

A hydrocarbon mixture has a composition of 3.9 % $^{w}/_{w}$ H_2, 40.2 % $^{w}/_{w}$ CH_4 and 55.9 % $^{w}/_{w}$ C_2H_6. What is its composition on a molar basis ?

	MW	Mass (g)	Moles	Mole fraction
H_2	2.0			
CH_4	16.0			
C_2H_6	30.0			

Conversions between Mole Fractions and Mass Fractions

These calculations were performed assuming the total mass of the mixture was 100.0 g. Do the results change if a different total mass is used?

Let's use 1000.0 g.

	MW	Mass (g)	Moles	Mole fraction
H_2	2.0			
CH_4	16.0			
C_2H_6	30.0			
		1000		

The composition we calculate is independent of the basis of calculation, i.e., the amount of mixture.

Conversions between Mole Fractions and Mass Fractions

Example 2 : Mole fractions ⇨ Mass fractions

A gas mixture has a composition of 27.0 mol % CO_2, 21.0 mol % CO and 52.0 mol % He. What is its composition on a mass basis ?

	MW
CO_2	44.0
CO	28.0
He	4.0

Conversions between Mole Fractions and Mass Fractions

Conversions between Mole Fractions and Mass Fractions

Example 3 : Molar basis ⇨ Dry, weight basis

The composition of air after it has been exhaled from the human body is typically 16.0 mol % O_2, 75.9 mol % N_2, 0.9 mol % Ar, 4.4 mol % CO_2 and 2.8 mol % H_2O. Express this composition on a dry, mass basis.

Conversions between Mole Fractions and Mass Fractions

Example 3 :

	MW	Moles
O_2	32.0	16.0
N_2	28.0	75.9
Ar	39.9	0.9
CO_2	44.0	4.4
H_2O	18.0	2.8
		100.0

Conversions between Mole Fractions and Mass Fractions

Example 4 : Mole fractions ⇨ Mass fractions

Dry Bass Strait natural gas has a composition of 90.7 mol % CH_4, 5.9 mol % C_2H_6, 0.6 mol % C_3H_8, 0.1 mol % C_4H_{10}, 0.9 mol % N_2 and 1.8 mol % CO_2. What is its composition on a mass basis ?

	MW
CH_4	16.0
C_2H_6	30.0
C_3H_8	44.1
C_4H_{10}	58.1
N_2	28.0
CO_2	44.0

Conversions between Mole Fractions and Mass Fractions

Compositions and Analyses of Mixtures

Gas Partial Pressures

Dalton's Law :

$$\sum_{\substack{\text{all} \\ \text{components}}} (\text{ partial pressure }) = \text{total pressure}$$

$$\sum (\, pp \,) = P_T$$

For any component of a gas mixture :

$$PP_i = x_i \, P_T$$

Compositions and Analyses of Mixtures

Gas Partial Pressures

For any component of a gas mixture :

$$PP_i = x_i P_T$$

Consider air with the composition : 79 mol % N_2
21 mol % O_2

$$\left(\begin{array}{c}\text{Partial pressure of } N_2 \text{ on a day when} \\ \text{the total pressure is 102.1 kPa}\end{array}\right)$$

$$= 0.79 \times 102.1 = 80.7 \text{ kPa}$$

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