How much? The amount of chemical change

Reactivity 2.1 · SL and HL

A recipe for a reaction

> A balanced equation is a recipe that counts particles.

- 2 eggs for every 250 g of flour; 6 eggs need 750 g.
- With only 500 g of flour, the flour runs out first.
- This unit: equations $\rightarrow$ masses $\rightarrow$ gases $\rightarrow$ titrations $\rightarrow$ yield.

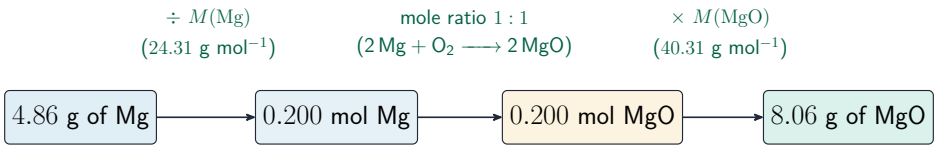
Balancing an equation

1. **Carbon.** $C_3H_8 + O_2 \rightarrow CO_2 + H_2O$. Propane has 3 C, so write $3CO_2$.
2. **Hydrogen.** 8 H on the left, so $4H_2O$
3. **Oxygen last.** $3 \times 2 + 4 = 10$ O, so $5O_2$

Decision

$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$

Reacting masses



Show the **mole ratio** as its own line.

Iron from iron ore

1. **Moles.** $Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$. For 16.0 g Fe_2O_3: $16.0/159.70 = 0.100$ mol.
2. **Ratio 1 : 2.** 0.200 mol Fe
3. **Mass.** 0.200×55.85

Decision

11.2 g of iron

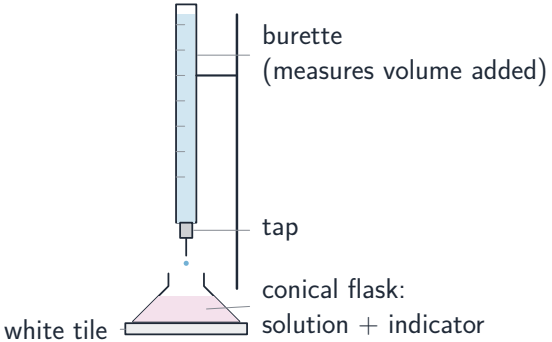
Reacting gas volumes

- 2.50 g $CaCO_3$ with excess HCl gives CO_2.
- 0.0250 mol $CaCO_3$ gives 0.0250 mol CO_2.

$$n = \frac{V}{22.7}$$

V in dm^3 at STP; $0.0250 \times 22.7 = 0.567$ dm^3

Titration



The **titre** is final reading minus initial reading.

Good technique

Rinse with the solution

The **burette**, with the solution it holds.

The **pipette**, with the solution it delivers.

Rinse with water

The conical flask only.

Water there does not change the amount of solute.

Wear appropriate eye protection throughout.

A titration calculation

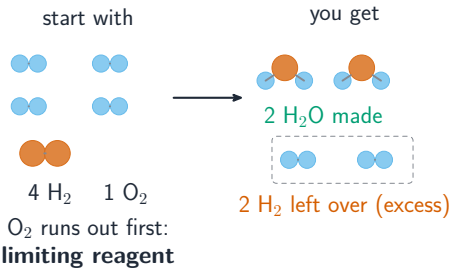
1. **Acid.** 25.00 cm^3 NaOH; 21.50 cm^3 of 0.100 mol/dm^3 H_2SO_4. Acid amount = $0.100 \times 0.02150 = 0.002150$ mol.
2. **Ratio 1 : 2.** $H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O$. Thus 0.004300 mol NaOH.
3. **Concentration.** $0.004300/0.02500 = 0.172$ mol/dm^3 NaOH.

Decision

0.172 mol dm^{-3}

The limiting reactant

$$2\mathbf{H}_2 + \mathbf{O}_2 \rightarrow 2\mathbf{H}_2\mathbf{O}$$



Divide moles by the **coefficient**; the smaller result limits.

Check: which reactant limits?

Your turn

$2Al + 3Cl_2 \rightarrow 2AlCl_3$. Start with 0.200 mol Al and 0.200 mol Cl_2. Which reactant limits?

A. Neither limits, because the amounts are equal.

B. Aluminium limits.

C. Chlorine limits.

D. The heavier reactant limits.

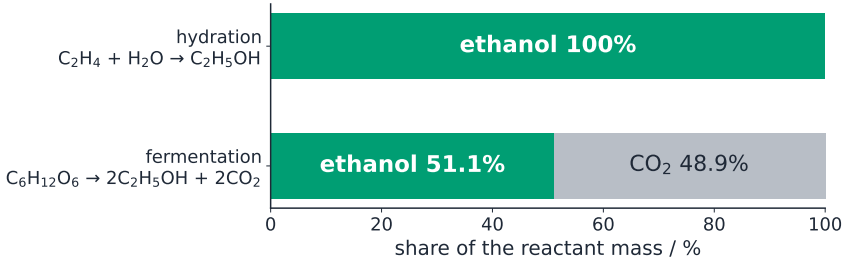
Percentage yield

- **Theoretical yield** comes from the **limiting reactant**.
- Losses, side reactions and equilibrium lower the yield.

$$\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

$AlCl_3$, $14.2/17.8 \times 100 = 79.8\%$

Atom economy



This hydration equation places all stoichiometric reactant mass in ethanol.

A closed-system mass balance includes escaped gas

Closed boundary

Count all reactants and products, including gases.

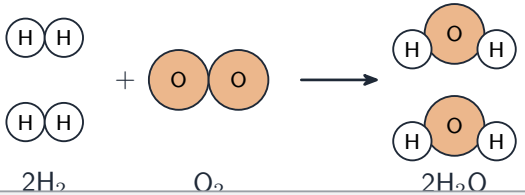
$Ca^{2+} + CO_3{}^{2-} \rightarrow CaCO_3$: net charge zero on both sides.

Open flask

Escaping CO_2 lowers the flask-plus-contents mass.

The gas still contains the carbon and oxygen atoms.

A balanced equation as particles



each side: 4 H atoms and 2 O atoms
change the coefficients, never the formulae

Atoms are rearranged, never made or lost

Keep unrounded values through the ratio

1. **Given.** 11.0 g C_3H_8; M=44.11 g/mol. $C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$.
2. **Amount.** O_2 required $= 5 \times 11.0/44.11 = 1.24688\ldots$ mol.
3. **Mass.** Multiply by 32.00 g/mol: 39.9002… g $\rightarrow$ 39.9 g.

Decision

Do not use 1.25×32.00 and then report 39.9.

Compare a hot gas mixture at the same conditions

1. **Invented case.** 40.0 cm^3 H_2 + 30.0 cm^3 O_2 at 400 K, 100 kPa; ideal gases, water remains vapour.
2. **Reaction.** $2H_2 + O_2 \rightarrow 2H_2O$. Consume 40.0 cm^3 H_2 and 20.0 cm^3 O_2.
3. **Final gases.** 40.0 cm^3 $H_2O(g)$ plus 10.0 cm^3 O_2 = 50.0 cm^3 at the same T,p.

Decision

Condensation or a change in T,p changes this gas-volume conclusion.

Endpoint and equivalence are different conditions

Equivalence

Stoichiometric amounts match the balanced reaction ratio.

It is defined by amounts, rather than a particular colour.

Endpoint

An observed **indicator** change used to stop delivery.

A poor indicator can give repeatable but biased titres.

Subtract readings before selecting titres

Run	**Initial / cm^3**	**Final / cm^3**	**Titre / cm^3**
rough	0.00	22.10	22.10
1	22.10	43.65	21.55
2	0.00	21.45	21.45
3	21.45	42.95	21.50

Quantify reading uncertainty and identify bias

1. **Readings.** Each has stated maximum uncertainty 0.05 cm^3. Difference: maximum 0.10 cm^3.
2. **Percentage.** $0.10/21.50 \times 100 = 0.47\%$ of the **titre**.
3. **Separate bias.** An initially empty **burette** tip can consume apparent delivered volume without reaching the flask.

Decision

A small range of repeated titres does not remove a shared bias.

Scale an aliquot back to the prepared sample

1. **Invented preparation.** Sample made to 250.0 cm^3; a 25.00 cm^3 aliquot reacts 1:1 with 0.00200 mol titrant.
2. **Aliquot.** Analyte amount = 0.00200 mol in the pipetted portion.
3. **Full sample.** 250.0/25.00 = 10.0 aliquots, so 0.0200 mol in the prepared solution.

Decision

Do not apply the tenfold amount factor twice.

A solution mixture has a new final volume

1. **Invented inputs.** 25.0 cm^3 $CaCl_2$ at 0.120 M: 0.00300 mol Ca^{2+}. 40.0 cm^3 Na_2CO_3 at 0.0500 M: 0.00200 mol carbonate.
2. **Precipitate.** $Ca^{2+} + CO_3{}^{2-} \rightarrow CaCO_3$. Carbonate limits; $0.00200 \times 100.09 = 0.200$ g solid.
3. **Remaining calcium.** 0.00100 mol / (0.0250+0.0400) dm^3 = 0.0154 mol/dm^3.

Decision

Assume complete precipitation, additive volumes and negligible dissolved solid.

Yield and atom economy answer different questions

Yield

Actual desired product / theoretical desired product $\times 100$.

An apparent value above 100% can reveal wet or impure product.

Atom economy

Desired product mass / all stoichiometric reactant mass $\times 100$.

Does not measure solvent, energy, toxicity, actual conversion or cost.

Infer sample purity from a dry gas amount

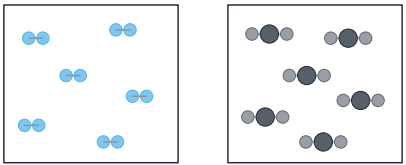
1. **Invented case.** 1.25 g impure limestone gives 0.227 dm^3 dry CO_2 at STP; only $CaCO_3$ generates gas, and collection is complete.
2. **Amount and mass.** $0.227/22.7 = 0.0100$ mol $CaCO_3$; $\times 100.09 = 1.0009$ g $CaCO_3$.
3. **Purity.** $1.0009/1.25 \times 100 = 80.1\%$. CO_2 loss biases the inferred purity downwards.

Decision

Wet gas requires the CO_2 partial pressure, rather than the total pressure.

Equal volumes, equal molecules

same volume, same temperature and pressure

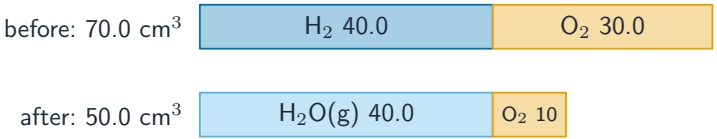


hydrogen, H_2 carbon dioxide, CO_2

the same **number** of molecules (6 each), even though CO_2 is bigger

> At the same temperature and pressure

Gas volumes before and after



$2H_2 + O_2 \rightarrow 2H_2O(g)$
H_2 limits; 20.0 O_2 used
same 400 K and 100 kPa

cooling to condense the water would change the gas volume

Hydrogen is limiting; 10 cm^3 of oxygen is left

Exam tips

> Yield compares masses; **atom economy** compares the equation.

- Balance first; change only the coefficients.
- Convert cm^3 to dm^3; 22.7 dm^3/mol applies at 273.15 K and 100 kPa.
- Leave out the rough **titre**.

Check yourself

Try these

Balance $Al + O_2 \rightarrow Al_2O_3$.

Find H_2 volume at STP from 0.654 g Zn and excess acid; use M(Zn)=65.38 g/mol and 22.7 dm^3/mol.

$2H_2 + O_2 \rightarrow 2H_2O$. Start with 4.00 g H_2 and 16.0 g O_2; use molar masses 2.02 and 32.00 g/mol. Find what limits.

For $CH_4 + H_2O \rightarrow CO + 3H_2$, use 16.05, 18.02 and 2.02 g/mol to find atom economy for H_2.