Quantities
In Chemical Reactions

Mole

Mole: formula weight of a substance (in gram).

12g of C = 1 mol C

23g of Na = 1 mol Na

58.5 g of NaCl = 1 mol NaCl

18 g of H_2O = 1 mol of H_2O

Avogadro's number (6.02×10^{23}): number of formula units in one mole.

1 mole of apples = 6.02×10^{23} apples

1 mole of A atoms = 6.02×10^{23} atoms of A

1 mole of A molecules = 6.02×10^{23} molecules of A

1 mole of A ions = 6.02×10^{23} ions of A

Molar mass (g/mol): mass of 1 mole of substance (in gram) (Formula weight)

molar mass of Na = 23 g/mol

molar mass of H_2O = 18 g/mol

Stoichiometry

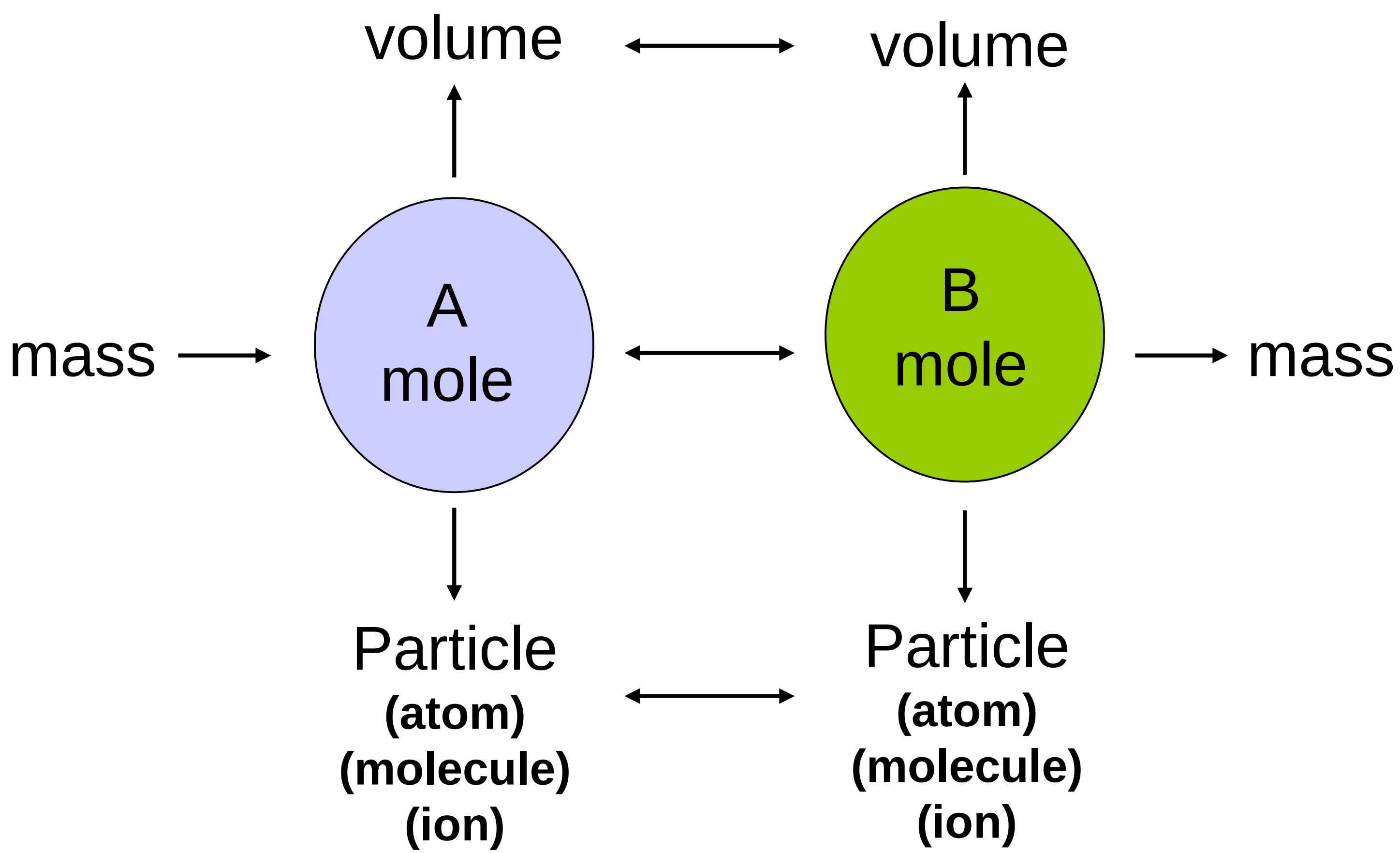
Relationships between amounts of substances in a chemical reaction.

Look at the Coefficients!

$$2H_2O(l) \rightarrow 2H_2(g) + O_2(g)$$

2	2	1
2 moles	2 moles	1 mole
2 liters	2 liters	1 liter
2 particles	2 particles	1 particle
~~2 grams~~	~~2 grams~~	~~1 gram~~

Stoichiometry

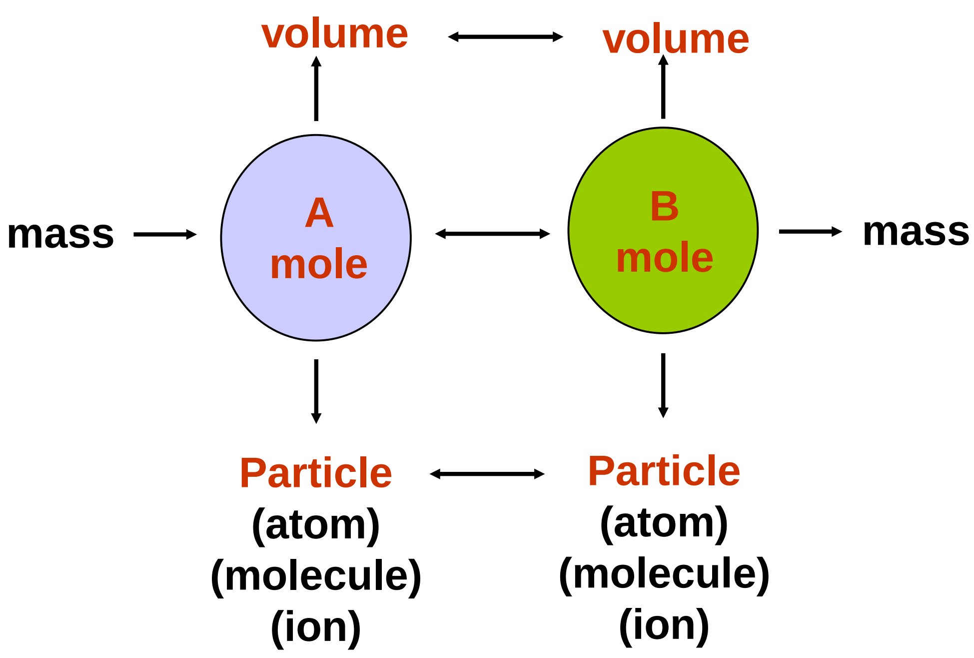


1 Step

Mole A ↔ Mole B

Volume A ↔ Volume B

# of Particles A ↔ # of Particles B



$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

A B

$$23 \text{ mole } CH_4 = ? \text{ moles } H_2O$$

$$23 \text{ mole } CH_4 \left(\frac{2 \text{ moles } H_2O}{1 \text{ mole } CH_4} \right) = 46 \text{ moles } H_2O$$

A B

$$10 \text{ cc } O_2 = ? \text{ cc } CO_2$$

$$10 \text{ cc } O_2 \left(\frac{1 \text{ cc } CO_2}{2 \text{ cc } O_2} \right) = 5 \text{ cc } CO_2$$

A B

$$2{\times}10^{26} \text{ molecules } H_2O = ? \text{ molecules } O_2$$

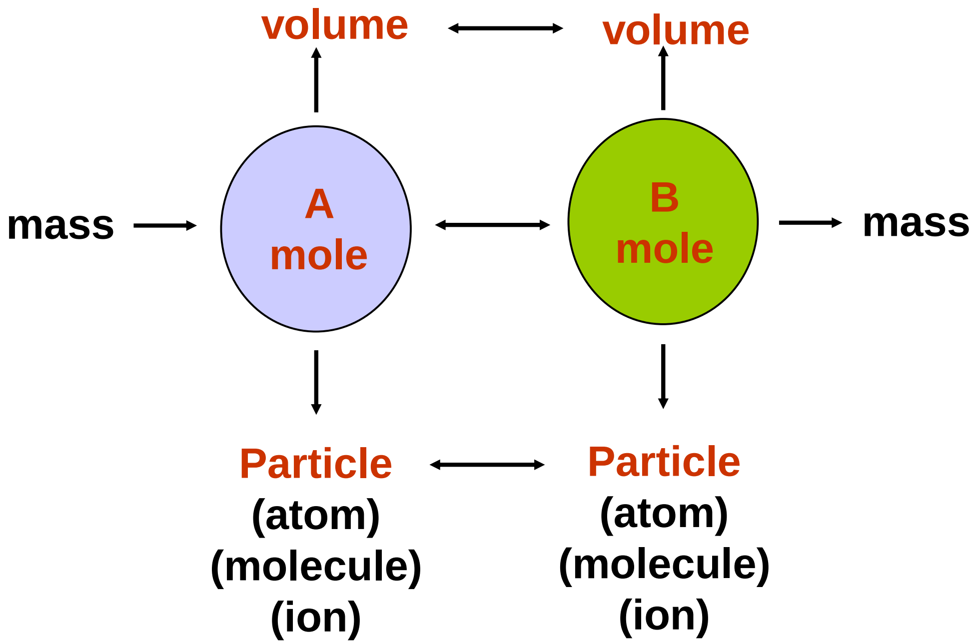
$$2{\times}10^{26} \text{ molecules } H_2O \left(\frac{2 \times (6.02{\times}10^{23} \text{ molecules } O_2)}{2 \times (6.02{\times}10^{23} \text{ molecules } H_2O)} \right) = 2{\times}10^{26} \text{ molecules } O_2$$

2 Steps

Mole A ↔ Volume B

Mass A ↔ Mole B or Volume A

# of Particles A ↔ Mole B or Volume A



$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

A B

$32\text{ g } CH_4 = \text{? moles } CO_2$

$$32\text{ g } CH_4 \left(\frac{1\text{ mole } CH_4}{16\text{ g } CH_4}\right)\left(\frac{1\text{ mole } CO_2}{1\text{ mole } CH_4}\right) = 2.0\text{ mole } CO_2$$

A A

$40.\text{ g } CH_4 = \text{? L } CH_4$

$$40.\text{ g } CH_4 \left(\frac{1\text{ mole } CH_4}{16\text{ g } CH_4}\right)\left(\frac{22.4\text{ L } CH_4}{1\text{ mole } CH_4}\right) = 56\text{ L } CH_4$$

STP: **1 mole of substance (gas) = 22.4 L = 22400 cc (cm^3 or mL)**

A B

$5\text{ moles } CO_2 = \text{? molecules } O_2$

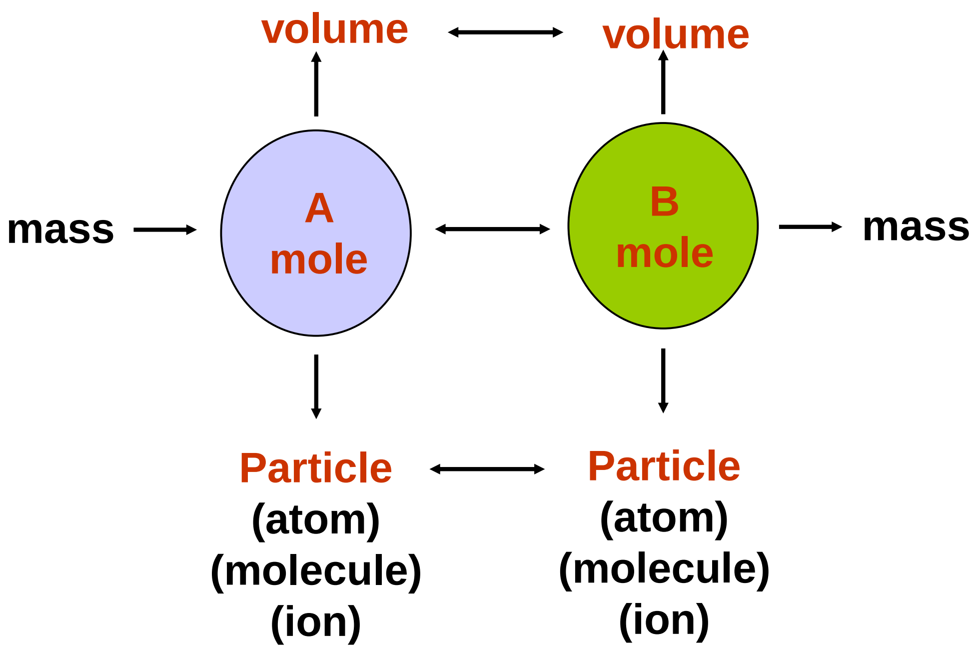
$$5\text{ moles } CO_2 \left(\frac{2\text{ mole } O_2}{1\text{ mole } CO_2}\right)\left(\frac{6.02\times10^{23}\text{ molecules } O_2}{1\text{ mole } O_2}\right) = 6\times10^{24}\text{ molecules } O_2$$

3 Steps

Mass A ↔ Mass B

Mass A ↔ Volume B or # of Particles B

# of Particles A ↔ Volume B



$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

A B

46.0 g CH_4 = ? g H_2O

$$46.0\text{ g }CH_4\left(\frac{1\text{ mole }CH_4}{16\text{ g }CH_4}\right)\left(\frac{2\text{ mole }H_2O}{1\text{ mole }CH_4}\right)\left(\frac{18\text{ g }H_2O}{1\text{ mole }H_2O}\right) = 104\text{ g }H_2O$$

Limiting Reagents

$$N_2(g) + O_2(g) \rightarrow 2NO(g)$$

	$N_2(g)$	$O_2(g)$	$2NO(g)$
Stoichiometry:	1 mole	1 mole	2 moles
Before reaction:	1 mole	4 moles	
After reaction:	0 mole	3 moles	2 moles

Limiting Reagents

$$N_2(g) + O_2(g) \rightarrow 2NO(g)$$

Stoichiometry:	1 mole	1 mole	2 moles
Before reaction:	1 mole	4 moles	
After reaction:	0 mole	3 moles	2 moles

Used up first **Left over**

Limiting Reagents

Limiting reagent

$$N_2(g) + O_2(g) \rightarrow 2NO(g)$$

	$N_2(g)$	$O_2(g)$	$2NO(g)$
Stoichiometry:	1 mole	1 mole	2 moles
Before reaction:	1 mole	4 moles	
After reaction:	0 mole	3 moles	2 moles

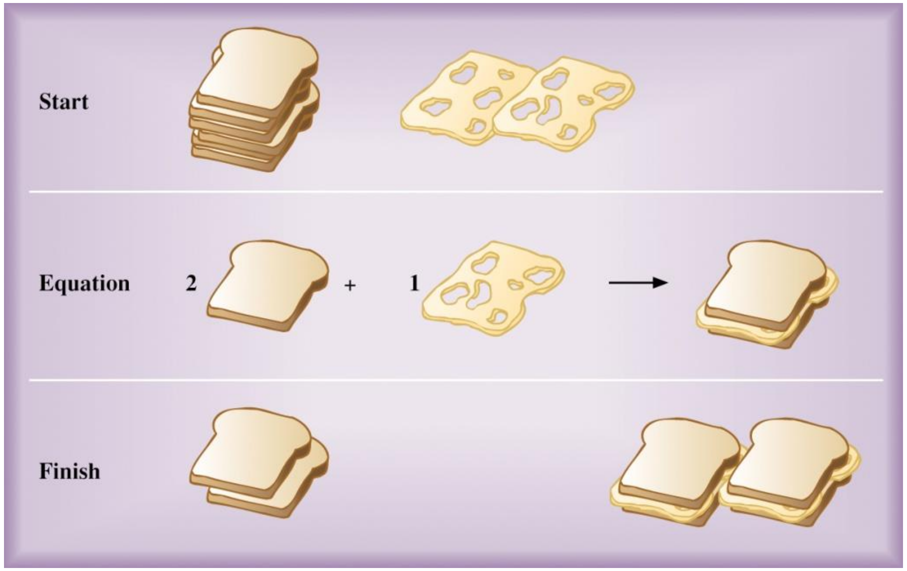
Used up first

Left over

Limiting Reagents

Limiting reagent: is the reactant that is used up first.

Limiting reagents can control a reaction:



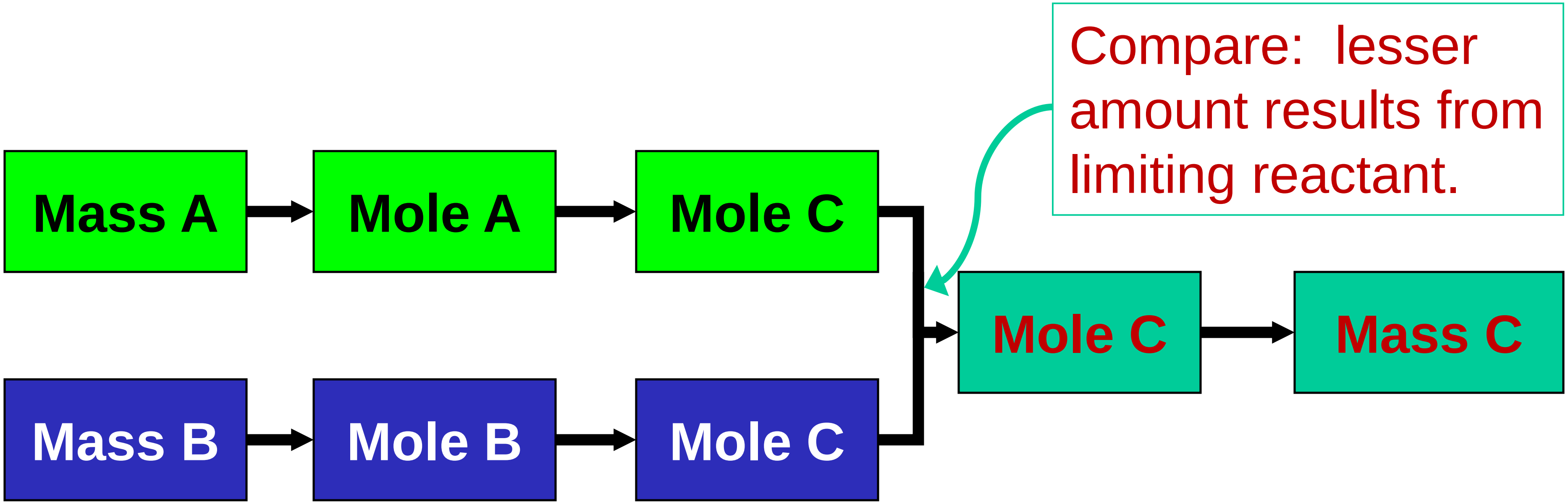
$$N_2(g) + O_2(g) \rightarrow 2NO(g)$$

Limiting Reagents

- To solve these problems, follow these steps:

$$A + B \rightarrow C + D$$

  - Convert reactant A to moles of C (or D).
  - Convert reactant B to moles of C (or D).
  - Compare moles of C (or D) produced by A and B.



Limiting Reagents

Example:

$$2\ Al(s) + 3\ Cl_2(g) \rightarrow 2\ AlCl_3(s)$$

A chemist combines 10.0 g of each reactant. Which is the limiting reagent?

$$10.0\text{ g Al} \times \frac{1\text{ mol Al}}{26.98\text{ g Al}} \times \frac{2\text{ mol AlCl}_3}{2\text{ mol Al}} = \mathbf{0.371\ mol\ AlCl_3}$$

$$\boxed{10.0\text{ g Cl}_2} \times \frac{1\text{ mol Cl}_2}{70.9\text{ g Cl}_2} \times \frac{2\text{ mol AlCl}_3}{3\text{ mol Cl}_2} = \boxed{\mathbf{0.0940\ mol\ AlCl_3}}$$

The *smallest* number is the result of the limiting reactant. So, **Cl_2 is the limiting reactant**.

Limiting Reagents

2. What mass of product is produced (in g)?

$$2\ Al(s) + 3\ Cl_2(g) \rightarrow 2\ AlCl_3(s)$$

$$0.0940\ \text{mol}\ AlCl_3 \times \frac{133.33\ \text{g}\ AlCl_3}{1\ \text{mol}\ AlCl_3} = \boxed{\mathbf{12.54\ g\ AlCl_3}}$$

3. What species are present in the final mixture?

$AlCl_3$*(s)* and some left-over Al*(s)* are present.

Limiting Reagents

4. How much Al*(s)* remains?

$$2\ Al(s) + 3\ Cl_2(g) \rightarrow 2\ AlCl_3(s)$$

Limiting reagent

$$10.0\ g\ Cl_2 \times \frac{1\ mol\ Cl_2}{70.9\ g\ Cl_2} \times \frac{2\ mol\ Al}{3\ mol\ Cl_2} \times \frac{26.98\ g\ Al}{1\ mol\ Al} = \mathbf{2.54\ g\ Al}$$

(reacted)

- 10.0 g original – 2.54 g used = **7.46 g Al*(s)*** remains

Limiting Reagents

Example:

$$C_3H_8(g) + 5\ O_2(g) \rightarrow 3\ CO_2(g) + 4\ H_2O(g)$$

1. A chemist combines 10.0 g of each reactant. Which is the limiting reagent?

2. What mass of each product is produced (in g)?

3. What species are present in the final mixture?

Limiting Reagents

$$C_3H_8(g) + 5\ O_2(g) \rightarrow 3\ CO_2(g) + 4\ H_2O(g)$$

1. A chemist combines 10.0 g of each reactant. Which is the limiting reagent?

$$10.0\ g\ C_3H_8 \times \frac{1\ mol\ C_3H_8}{44.09\ g\ C_3H_8} \times \frac{3\ mol\ CO_2}{1\ mol\ C_3H_8} = \mathbf{0.680\ mol\ CO_2}$$

$$\boxed{10.0\ g\ O_2} \times \frac{1\ mol\ O_2}{32.00\ g\ O_2} \times \frac{3\ mol\ CO_2}{5\ mol\ O_2} = \boxed{\mathbf{0.188\ mol\ CO_2}}$$

The *smallest* number is the result of the limiting reactant. So, **O_2 is the limiting reactant**.

Limiting Reagents

$$C_3H_8(g) + 5\ O_2(g) \rightarrow 3\ CO_2(g) + 4\ H_2O(g)$$

2. What mass of each product is produced (in g)?

$$0.188 \text{ mol } CO_2 \times \frac{44.01 \text{ g } CO_2}{1 \text{ mol } CO_2} = \boxed{\mathbf{8.27 \text{ g } CO_2}}$$

$$10.0 \text{ g } O_2 \times \frac{1 \text{ mol } O_2}{32.00 \text{ g } O_2} \times \frac{4 \text{ mol } H_2O}{5 \text{ mol } O_2} \times \frac{18.016 \text{ g } H_2O}{1 \text{ mol } H_2O} = \boxed{\mathbf{4.50 \text{ g } H_2O}}$$

Limiting reagent

3. What species are present in the final mixture?

$CO_2(g)$, $H_2O(g)$ and some remaining $C_3H_8(g)$.

Limiting Reagents

Example:

$$CS_2(l) + 3\ O_2(g) \rightarrow CO_2(g) + 2\ SO_2(g)$$

- You have 1.55 g of $CS_2(l)$ and excess $O_2(g)$. What mass of each product forms?

$$1.55\text{ g } CS_2 \times \frac{1\text{ mol } CS_2}{76.15\text{ g } CS_2} \times \frac{1\text{ mol } CO_2}{1\text{ mol } CS_2} \times \frac{44.01\text{ g } CO_2}{1\text{ mol } CO_2} = \boxed{\mathbf{0.896\text{ g } CO_2}}$$

$$1.55\text{ g } CS_2 \times \frac{1\text{ mol } CS_2}{76.15\text{ g } CS_2} \times \frac{2\text{ mol } SO_2}{1\text{ mol } CS_2} \times \frac{64.07\text{ g } SO_2}{1\text{ mol } SO_2} = \boxed{\mathbf{2.61\text{ g } SO_2}}$$

Percent Yield

Percentage yield: a comparison of actual to theoretical yield.

$$\text{Percent yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100\%$$

actual yield: **mass of product formed (exprimental determination)**

theoretical yield: **mass of product that should form according to limiting reactant calculation. (according to stoichiometry)**

Note: percentage yields can be calculated using units of either moles or grams.

Percent Yield

Example:

- Analysis for sulfate (SO_4^{2-}) uses barium cation (Ba^{2+}).

$$SO_4^{2-}(aq) + BaCl_2(aq) \rightarrow BaSO_4(s) + 2\ Cl^-(aq)$$

- If a sample containing 1.15 g of SO_4^{2-} is reacted with excess barium chloride, how much $BaSO_4$ should form? If a chemist actually collects 2.02 g $BaSO_4$, what is the percent yield?

Percent Yield

How much $BaSO_4$ should form?

$$SO_4^{2-}(aq) + BaCl_2(aq) \rightarrow BaSO_4(s) + 2\ Cl^-(aq)$$

$$1.15\text{ g } SO_4^{2-} \times \frac{1\text{ mol } SO_4^{2-}}{96.07\text{ g } SO_4^{2-}} \times \frac{1\text{ mol } BaSO_4}{1\text{ mol } SO_4^{2-}} \times \frac{233.37\text{ g } BaSO_4}{1\text{ mol } BaSO_4} = \mathbf{2.79\ g}\ BaSO_4$$

- If a chemist actually collects 2.02 g $BaSO_4$, what is the percent yield?

$$P.Y.\% = \frac{2.02\text{ g } BaSO_4}{2.79\text{ g } BaSO_4} \times 100\% = \mathbf{72.4\ \%}$$

At-Home Practice

- **Practice problem:** A chemist reacts 7.67 g of H_2 gas with 30.46 g of O_2 gas. What is the theoretical yield of water in grams? (Limiting reactant calculation.)
- The actual experimentally measured amount is only 28.6 g of H_2O. What is the percent yield?
- Next lecture, our clicker questions will be:
  - ❖ What is the theoretical yield?
  - ❖ What is the percent yield?

Heat of reaction

$$2HgO(s) + \text{heat (energy)} \rightarrow 2Hg(l) + O_2(g)$$

Endothermic reaction

$$C_3H_8(s) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l) + \text{heat (energy)}$$

Exothermic reaction

All combustion reactions are exothermic.

Enthalpy

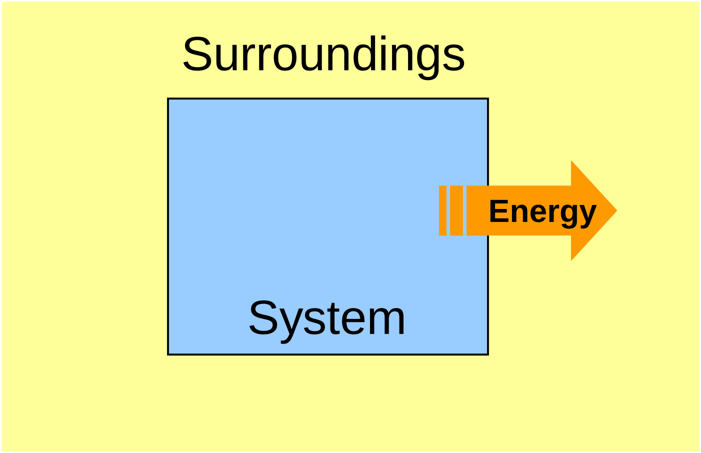
Enthalpy (Thermochemistry): heat of chemical reactions.

For a reaction in constant pressure,
the change of enthalpy is equal to energy that flows as heat.

$$\Delta H_p = \text{heat}$$

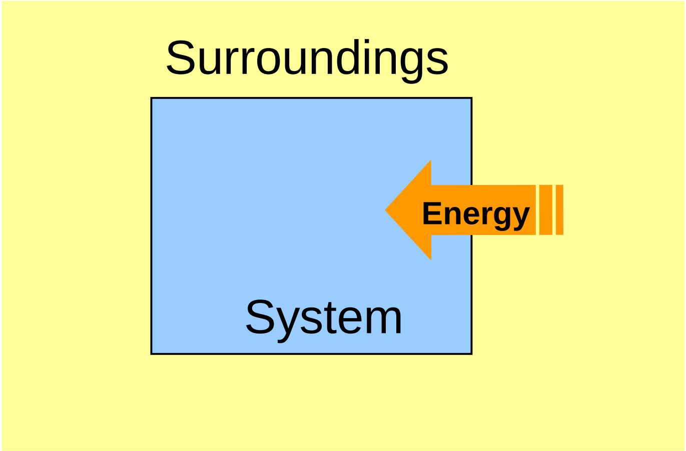
Constant pressure

Enthalpy



Exothermic

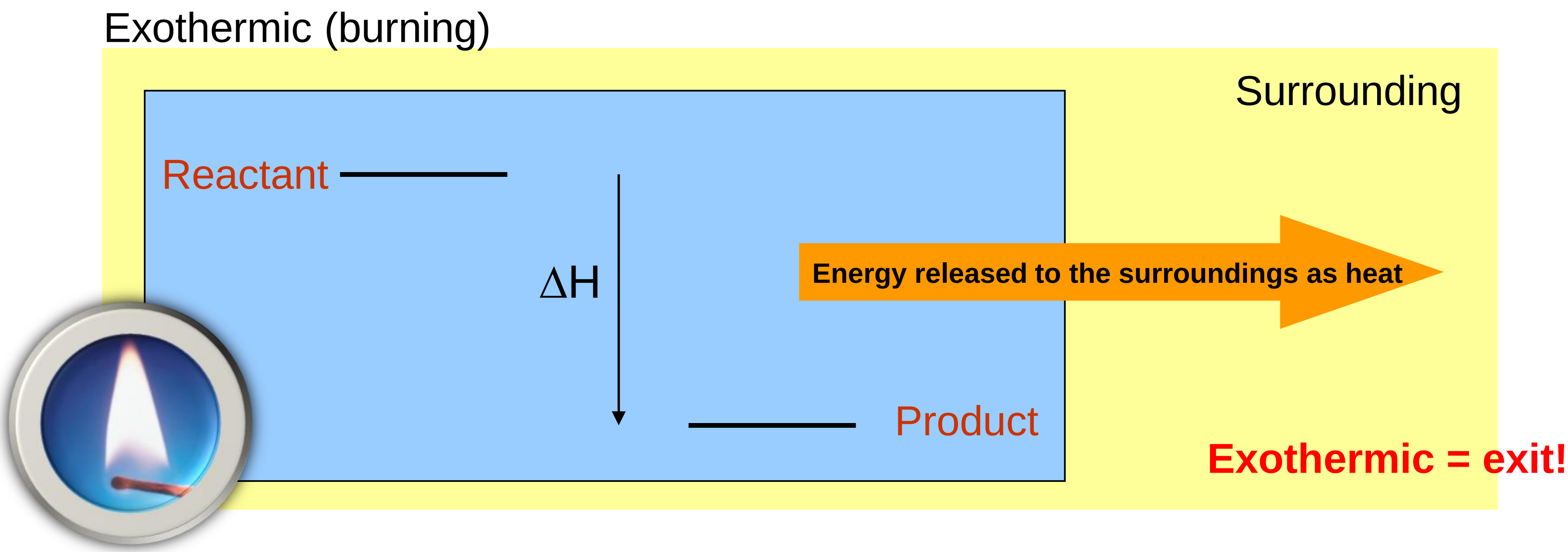
Exothermic: ΔH is negative.
(heat flows out of the system).



Endothermic

Endothermic: ΔH is positive.
(heat flows into the system).

Heat of reaction



In endothermic condition, products have the higher energy level than reactants.

Enthalpy

Practice:

$$S(s) + O_2(g) \rightarrow SO_2(g) \quad \Delta H = -296 \text{ kJ}$$

- Calculate the quantity of heat released when 2.10 g of sulfur is burned in oxygen at constant pressure.

$$2.10 \text{ g S} \times \frac{1 \text{ mol S}}{32.26 \text{ g S}} = 0.0655 \text{ mol S}$$

$$0.0655 \text{ mol S} \times \frac{-296 \text{ kJ}}{1 \text{ mol S}} = \mathbf{-19.4 \text{ kJ}}$$

Use the ΔH value like a conversion factor.

Gram → Mole → kJ