Green chemistry, atom economy and sustainable development

Learning objectives

1. Understand what sustainable development is and the role of green chemistry in advancing it.
2. Explain the importance of percentage yield and atom economy for sustainable development.
3. Calculate the percentage yield and atom economy of a chemical process given relevant data.

Introduction

Around the world, millions of people live in poverty. Many don't have access to healthcare and even in richer communities, education and healthcare could be better.

To improve this, countries need to grow their economies, but economic growth can cause pollution and harm the environment. The challenge is to grow in a way that helps people today without damaging the planet for future generations. This is called **sustainable development**, and it is becoming more important as the world's population grows.

One way the chemical industry is helping sustainable development is through **green chemistry**. One of the principles of green chemistry is to avoid producing harmful substances instead of making them and then cleaning them up later.

Green chemistry is:

- safer
- uses fewer raw materials
- often cheaper than traditional methods.

There are three main ways to make chemical processes greener:

- Use safer starting materials
- Use gentler conditions, such as better catalysts and safer solvents
- Use methods with fewer steps and less waste.

Questions

1. Explain why it is better to avoid pollution and making harmful substances than to make them and clean them up later.

2. Why might using a catalyst (or a more efficient catalyst) make a chemical process greener?

Percentage yield

Most of the chemical industry is concerned with changing one material (a raw material) into a more useful and valuable substance (the product). This process can have several steps and is called a chemical synthesis.

Scientists and engineers want to make as much product as possible from the raw materials they use.

They can measure how successful a process is by calculating the **yield**. This shows how much product is actually made compared to how much could be made.

The percentage yield of a reaction is calculated using the equation:

$$\%\text{ yield} = \frac{\text{mass of product actually made}}{\text{maximum mass of product that could be made}} \times 100$$

3. In a chemical synthesis of calcium oxide, calcium carbonate is heated in an oven. The equation for the reaction is:

	$CaCO_3$	$\rightarrow$ CaO	+ CO_2
Relative formula mass:	100	56	44
Reacting mass:	100 kg	56 kg	44 kg

If 100 kg of $CaCO_3$ is heated, the maximum mass of each product that could be made is shown above as the reacting mass.

If when 50 kg of calcium carbonate is heated, 21 kg of calcium oxide is made, calculate the percentage yield of the reaction.

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4. To make sulfur dioxide, sulfur is burned in oxygen:

$$S + O_2 \rightarrow SO_2$$

If, when 8 g of sulfur is used, 14 g of sulfur dioxide is produced, calculate the percentage yield of the reaction.

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Atom economy

Yield is useful, but it does not tell the whole story. This is because yield is calculated by looking at only one reactant and one product.

Green chemistry aims to use as much of the raw materials as possible to make the final product and to produce as little waste as possible.

Sometimes, a reaction can have a high yield but still create a lot of waste. This means it has a low **atom economy**.

To make a process more environmentally friendly, scientists need to think about both yield and atom economy.

Look again at the reaction from **Q3**:

$$CaCO_3 \rightarrow CaO + CO_2$$

If we split up the formulas, we can look at what happens to each atom in the reaction. The atoms shown in **bold** end up in the product we want (the calcium oxide), the rest do not.

$$\mathbf{Ca}\ C\ \mathbf{O}\ O\ O \rightarrow Ca\ O + C\ O\ O$$

From the original atoms, one C atom and two O atoms are wasted – they are not in the final, desired product.

For a balanced chemical equation, green chemists use atom economy to measure how much of the reactants end up in the desired product.

It can be calculated by the equation:

$$\%\ \text{atom economy} = \frac{\text{relative formula mass of desired product}}{\text{total relative formula mass of all reactants}} \times 100$$

Where relative formula mass refers to the total relative formula mass of all the atoms in the final desired product or reactants.

So, for this example:

$$\%\ \text{atom economy} = \frac{M_r \text{ of CaO (the desired product)}}{M_r \text{ of } CaCO_3} \times 100$$

Relative atomic masses: $C = 12$, $O = 16$, $Ca = 40$.

$$\%\ \text{atom economy} = \frac{40 + 16}{40 + 12 + (3 \times 16)} \times 100 = 56\%$$

How to calculate atom economy step-by-step

- **Step one:** Write out the balanced symbol equation.
- **Step two:** Calculate the relative formula mass of the desired product (the relative atomic mass of all the atoms in the desired product). Remember to account for any numbers in front of the symbols indicating that multiples of that product are produced.
- **Step three:** Calculate the total relative formula mass of all reactants (the relative atomic mass of all the atoms going into the reaction).
- **Step four:** Apply the formula:

$$\% \textbf{ atom economy} = \frac{\textbf{relative formula mass of desired product}}{\textbf{total relative formula mass of all reactants}} \times \mathbf{100}$$

5. Calculate the atom economy for the reaction in **Q4**.

$$S + O_2 \rightarrow SO_2$$

6. Iron is extracted from its ore, iron oxide, using carbon:

$$2Fe_2O_3 + 3C \rightarrow 4Fe + 3CO_2$$

Calculate the atom economy of this reaction.

7. Titanium can be extracted from its ore by two different methods.

Method 1 uses a more reactive metal to displace the titanium:

$$TiO_2 + 2Mg \rightarrow Ti + 2MgO$$

Method 2 is electrolysis of the ore. The overall reaction for this method is:

$$TiO_2 \rightarrow Ti + O_2$$

(a) Calculate the atom economy for each reaction.

(b) Explain which method is greener and what other information you might want to know before making a final decision.

(c) Oxygen is a useful product and can be sold.

What is the atom economy of the electrolysis if the oxygen is collected and sold? Explain your answer.

8. Alkanes can be cracked to form alkenes.

Decane, can be cracked to form two products, ethene C_2H_4 and octane C_8H_{18}.

$$C_{10}H_{22} \rightarrow C_2H_4 + C_8H_{18}$$

(a) If only the alkene (ethene) can be sold, state the atom economy of this process.

(b) If both products can be sold, state the atom economy.

(c) Explain why your answers to (a) and (b) are different.

9. The key reaction in the Haber process for making ammonia, NH_3 is:

$$N_2 + 3H_2 \rightleftharpoons 2NH_3$$

(a) State the atom economy of this reaction.

(b) Explain what the $\rightleftharpoons$ symbol suggests about the likely yield of this reaction.

10. Explain why using reactions with high atom economies is important for sustainable development.