14–16 years

Green chemistry, atom economy and sustainable development

ROYAL SOCIETY OF CHEMISTRY

Education
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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.

Sustainable development

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.

Green chemistry

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

How do you think chemists could adapt chemical processes to make them greener?

Green chemistry

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. Explain why using a catalyst might make a chemical process faster.

Unscaffolded questions

Percentage yield

Most of the chemical industry is about 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:

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

Calculating percentage yield

Worked example

Ethanol is produced by the reaction of ethene and water.

	ethene	+	water	→	ethanol
	C_2H_4	+	H_2O	→	CH_3CH_2OH
Relative formula mass (M_r)	28		18		46
Reacting masses	28 kg		18 kg		46 kg

When 28 kg of ethene is reacted with an excess of water, the maximum mass of ethanol that can be made is 46 kg.

Calculate the percentage yield if only 32 kg of ethanol is actually made.

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

$$\%\ \text{yield} = \frac{32\ \text{kg}}{46\ \text{kg}} \times\ 100 = \mathbf{70\%}$$

Calculating percentage yield

Ethanol is produced by the reaction of ethene and water.

	ethene	+	water	→	ethanol
	C_2H_4	+	H_2O	→	CH_3CH_2OH
M_r	28		18		46
Reacting masses	28 kg		18 kg		46 kg

When 84 kg of ethene is reacted with an excess of water, 124 kg of ethanol is produced. What is the percentage yield of the reaction?

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

$$\begin{array}{c}\text{Maximum mass of ethanol that could} \\ \text{be made from 84 kg of ethene}\end{array} = \frac{84\text{ kg}}{28\text{ kg}} \times 46\text{kg} = 138\text{kg}$$

$$\% \text{ yield} = \frac{124\text{ kg}}{138\text{ kg}} \times 100 = \mathbf{89.9\%}$$

Questions

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

$$CaCO_3 \rightarrow CaO + CO_3$$

Reacting mass: 100 kg 56 kg 44 kg

If 100 kg of $CaCO_3$ is heated, the maximum mass of calcium oxide that can be made is 56 kg (shown 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.

a) What is the maximum mass of calcium oxide that could be made when 50 kg of $CaCO_3$ is heated?

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

Use this equation:

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

Questions

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

	S	$+$	O_2	$\rightarrow$	SO_2
Reacting mass:	32 g		32 g		64 g

If 32 g of sulfur is burned in oxygen, the maximum mass of sulfur dioxide that can be produced is 64 g.

a) If, when 32 g of sulfur is burned only 48 g of sulfur dioxide is produced, calculate the percentage yield.

b) In a different reaction, 8 g of sulfur is burned in oxygen and 14 g of sulfur dioxide is produced.

c) Calculate the percentage yield of this reaction.
HINT: first calculate the maximum mass of sulfur dioxide that could be produced from the 8 g of sulfur.

Questions

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_3
Relative formula mass (M_r)	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.

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?

HINT: first calculate the maximum mass of sulfur dioxide that could be produced from 8 g of sulfur.

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.

Atom economy

Consider the reaction for making calcium oxide, CaO:

$$CaCO_3 \rightarrow CaO + CO_2$$

If we split up the formulas, we can look at what happens to each atom in the reaction.

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

The atoms shown in **bold** end up in the product we want (the calcium oxide), the rest do not.

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

Atom economy

For any given balanced symbol equation, green chemists define atom economy as:

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

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

The higher the atom economy of a reaction, the more of the reactant atoms that end up in the desired product. The less waste there is.

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:

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

Calculating atom economy

Hydrogen gas, H_2 can be made from the reaction of water with coke (a form of carbon). The equation for the reaction is:

$$C + H_2O \rightarrow H_2 + CO$$

Calculate the atom economy of the process for making hydrogen.

Relative atomic masses: $H = 1, C = 12, O = 16$.

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

$$= \frac{M_r \text{ of } H_2}{M_r \text{ of } C + M_r \text{ of } H_2O} \times 100 = \frac{2 \times 1}{12 + [(2 \times 1) + 16]} \times 100$$

$$= \frac{2}{30} \times 100 = 6.7\%$$

Worked example

Calculating atom economy

Worked example

Nitric acid, HNO_3 is made by the reaction:

$$2NH_3 + 4O_2 + H_2O \rightarrow 3H_2O + 2HNO_3$$

Calculate the atom economy of the process for making nitric acid.

Relative atomic masses: $H = 1, N = 14, O = 16.$

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

Mass of desired product ($2HNO_3$) = 2 × [1 + 14 + (3 × 16)] = 126

Total mass of all reactants ($2NH_3 + 4O_2 + H_2O$) = (2 × 17) + (4 × 32) + 18 = 180

$$\%\ \text{atom economy} = \frac{126}{180} \times 100 = \mathbf{70\%}$$

Questions

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

$$S + O_2 \rightarrow SO_2$$

Relative atomic masses: O = 16, S = 32

a) Calculate the mass of the desired product, $SO_{2.}$

b) Calculate the total mass of all reactants, $S + O_{2.}$

c) Calculate the atom economy for the reaction. Use the equation:

$$\%\ \text{atom economy} = \frac{M_\text{r}\ \text{of desired product}}{\text{total}\ M_\text{r}\ \text{of all reactants}} \times 100$$

Questions

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.

Relative atomic masses: C = 12, O = 16, Fe = 56

a) Mass of the desired product ($4Fe$) =

b) Total mass of all reactants ($2Fe_2O_3 + 3C$) =

c) % atom economy =

Scaffolded questions

Questions

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:

$$TiO_2 \rightarrow Ti + O_2$$

Relative atomic masses: O = 16, Mg = 24, Ti = 48

a)

i. Calculate the atom economy for **method 1**.

ii. Calculate the atom economy for **method 2**.

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

c) Oxygen is a useful product and can be sold. Explain the atom economy of the electrolysis if the oxygen is collected and sold.

Questions

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}.

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

Relative atomic masses: H = 1, C = 12

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.

Questions

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:

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Calculate the atom economy of this reaction.

Unscaffolded questions

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a) Calculate the atom economy for each reaction.

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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.

Answers

Unscaffolded answers

1. Various answers are possible, including:
   - Not all pollution may be cleared up
   - Energy will be wasted producing unwanted materials
   - It is better not to produce hazardous materials at all then there is no danger of them being spilled or falling into the wrong hands
2. Using a catalyst (or more efficient catalyst) may mean that the process can be carried out at a lower temperature, which saves energy. It may also increase the yield of one product over that of another, unwanted one.
3. (21/28) × 100 = 75%
4. Maximum mass of SO_2 that could be produced = 16 g

Percentage yield = (14/16) × 100 = 87.5%

Answers

Unscaffolded answers

5. Atom economy = 100%

6. $$\frac{(4 \times 56)}{2 \times [(56 \times 2) + (3 \times 16)] + (3 \times 12)} \times 100 = \frac{224}{356} \times 100 = 62.9\%$$

7.

a) Displacement: 48/([48 + (2 ×16)] + (2 × 24)) ×100 = 48/128 × 100 = 37.5 %

Electrolysis: 48/(48 + (2 ×16)) ×100 = 48/80 × 100 = 60%

b) The greener process appears to be electrolysis. Before finally deciding, it might be important to know how much energy is used in each process, what (if any) solvents are used and what the yield for each reaction is.

c) Atom economy = 100% because both products are now useful, so all the reactants have been converted into useful products and there is no waste.

Answers

8.

a) $$\frac{[(2 \times 12) + (4 \times 1)]}{[(10 \times 12) + (22 \times 1)]} \times 100 = \frac{28}{142} \times 100 = 19.7\%$$

b) Atom economy = 100%

c) If only one product can be sold, then the rest is wasted; if both can be sold then there is no waste product and the atom economy is greater.

9.

a) Atom economy = 100%

b) The reversible reaction symbol ($\rightleftharpoons$) suggests that the reaction is unlikely to have a very high yield.

Answers

10. Answers include:

    - more efficient use of resources
    - less waste
    - less pollution
    - less energy used

    These things are important for sustainable development because they all help to make sure that we leave the planet healthy for future generations and do not use up all the available resources.

Answers

1. Various answers are possible, including:
   - Not all pollution may be cleared up
   - Energy will be wasted producing unwanted materials
   - It is better not to produce hazardous materials at all then there is no danger of them being spilled or falling into the wrong hands
2. Using a catalyst (or more efficient catalyst) may mean that the process can be carried out at a lower temperature, which saves energy. It may also increase the yield of one product over that of another, unwanted one.
3.

   a) 28 kg

   b) $(21/28) \times 100 = 75\%$

Answers

4.

a) Percentage yield = (48/64) × 100 = 75%

b) Maximum of SO_2 that could be made = 16 g

c) Percentage yield = (14/16) × 100 = 87.5%

5.

a) M_r of SO_2 = 32 + (2 × 16) = 64

b) M_r of $S + O_2$ = 32 + (2 × 16) = 64

c) Atom economy = (64/64) × 100 = 100%

6. M_r of desired product ($4Fe$) = 4 × 56 = 224

Total M_r of all reactants ($2Fe_2O_3 + 3\,C$) = (2 × 160) + (3 × 12) = 356

% atom economy = (224/356) × 100 = 62.9%

Answers

7.

a) **Method 1**: $\frac{48}{[48 + (2 \times 16)] + (2 \times 124)} \times 100 = \frac{48}{128} \times 100 = 37.5\%$

Method 2: $\frac{48}{48 + (2 \times 16)} \times 100 = \frac{48}{80} \times 100 = 60\%$

b) The greener process appears to be electrolysis. Before finally deciding, it might be important to know how much energy is used in each process, what (if any) solvents are used and what the yield for each reaction is.

c) Atom economy = 100% because both products are now useful, so all the reactants have been converted into useful products and there is no waste.

8.

a) $\frac{[(2 \times 12) + (4 \times 1)]}{[(10 \times 12) + (22 \times 1)]} \times 100 = \frac{28}{142} \times 100 = 19.7\%$

b) Atom economy = 100%

c) If only one product can be sold, then the rest is wasted; if both can be sold then there is no waste product and the atom economy is greater.

Answers

9.

a) Atom economy = 100%

b) The reversible reaction symbol (⇌) suggests that the reaction is unlikely to have a very high yield.

10. Answers include:

- more efficient use of resources
- less waste
- less pollution
- less energy used

These things are important for sustainable development because they all help to make sure that we leave the planet healthy for future generations and do not use up all the available resources.

Scaffolded answers

Find out more

To find out more about how chemists can contribute to sustainable development have a look at the following articles:

- **Life cycle assessment of fast-food containers** (rsc.li/48PcLEY)
  How can life cycle assessments help compare the environmental impact of fast-food containers?

- **Fixing fashion** (rsc.li/2Jdg7HU)
  What can we do to reduce the environment impact of our clothes throughout their life cycle?

- **Why the world urgently needs more chemists** (rsc.li/4eT6BYp)
  How can learners make a difference by pursuing a career in chemistry?