

Atom economy, percentage yield and green chemistry misconception buster

Learning objectives

- 1 Write equations for percentage yield and percentage atom economy calculations.
- 2 Calculate percentage yield and percentage atom economy given experimental data and chemical equations for processes.
- 3 Interpret and evaluate percentage yields and percentage atom economies for industrial processes.
- 4 Suggest how to improve percentage yields and percentage atom economies for industrial processes.
- 5 Evaluate industrial sustainability given appropriate information.

Introduction

Read each multiple-choice question carefully in Activity 1 and use the diagrams and data provided to tick the correct answer. There is one correct answer per question.

After marking your multiple-choice questions, complete the suggested follow-up tasks to target areas for improvement and increase your understanding of certain topics. The questions cover percentage yield and percentage atom economy calculations, as well as evaluative questions on how to improve industrial processes to make them more sustainable. If you answered a question correctly but you were uncertain or guessed, make sure you complete the relevant follow-up task.

Activity 1: multiple-choice questions

1. The reaction between ethene and steam to produce ethanol is represented by the equation: $\text{C}_2\text{H}_4 + \text{H}_2\text{O} \rightarrow \text{C}_2\text{H}_5\text{OH}$
If 98 g of ethene is used, what is the maximum mass of ethanol that can be produced?
(A_r values: C = 12.0, H = 1.0, O = 16.0)

- A 80.5 g
- B 161.0 g
- C 322.0 g
- D 157.5 g

2. The reaction between ethene and steam to produce ethanol is represented by the equation: $\text{C}_2\text{H}_4 + \text{H}_2\text{O} \rightarrow \text{C}_2\text{H}_5\text{OH}$

Which statement about the process is true?

- A** The percentage yield of the process will always be 100%.
B The theoretical yield of the process will always be less than the actual yield.
C The atom economy of the process will always be 100%.
D The atom economy of the process will always be less than 100%.

3. The hydrogen used in the Haber process is produced from natural gas, containing methane. The equation for this stage of the process is: $\text{CH}_4 + 2\text{H}_2\text{O} \rightarrow \text{CO}_2 + 4\text{H}_2$
Calculate the atom economy for the production of hydrogen.

(A_r values: C = 12.0, H = 1.0, O = 16.0)

- A** 84.6%
B 6.5%
C 15.4%
D 5.9%

4. Which of the following processes has the highest atom economy for the production of ethanol, $\text{C}_2\text{H}_5\text{OH}$ ($M_r = 46.0$).

(A_r values: Na = 23.0, C = 12.0, H = 1.0, O = 16.0, Cl = 35.5, Br = 79.9)

- A** $\text{C}_2\text{H}_5\text{Br} + \text{NaOH} \rightarrow \text{C}_2\text{H}_5\text{OH} + \text{NaBr}$
B $\text{C}_6\text{H}_{12}\text{O}_6 \rightarrow 2\text{C}_2\text{H}_5\text{OH} + 2\text{CO}_2$
C $\text{C}_2\text{H}_5\text{Cl} + \text{NaOH} \rightarrow \text{C}_2\text{H}_5\text{OH} + \text{NaCl}$
D $\text{CH}_3\text{COOH} + 2\text{H}_2 \rightarrow \text{C}_2\text{H}_5\text{OH} + \text{H}_2\text{O}$

5. Which of the following steps could increase the percentage yield of a reaction?

- A** Increase the number of steps in the process.
B Use a process that produces no by-products.
C Carry out the reaction at a suitable temperature to prevent side-reactions.
D Use a process with a reversible reaction.

6. Which of the following statements best describes atom economy?

- A The effectiveness of a process in producing the desired product.
- B The ratio of the actual yield to the theoretical yield, multiplied by 100.
- C The proportion of reactants that form useful products, as a percentage.
- D The amount of reactant successfully converted into product.

7. Consider the following reaction:



What is the atom economy for the production of NaOCl?

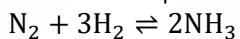
(A_r values: Na = 23.0, C = 12.0, H = 1.0, O = 16.0, Cl = 35.5, Br = 79.9)

- A 49.3%
- B 67.1%
- C 38.7%
- D 52.7%

8. Which statement about sustainability of industrial processes is correct?

- A Lower atom economy results in fewer by-products, improving sustainability.
- B Atom economy has no impact on sustainability.
- C Higher atom economy leads to more waste, reducing sustainability.
- D Higher atom economy means less waste and greater sustainability.

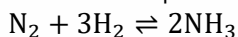
9. The Haber process is used to produce ammonia.



Which statement about the Haber process is true?

- A The percentage yield is high as there is only one product.
- B The reaction will always have 100% atom economy.
- C The reaction is unsustainable because it is reversible.
- D The reaction can never practically attain 100% atom economy.

10. The Haber process is used to produce ammonia.

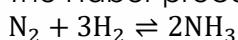


If 56 g of nitrogen is reacted with excess hydrogen, what is the theoretical yield of ammonia?

(A_r values: H = 1.0, N = 14.0)

- A 34.0 g
- B 136.0 g
- C 68.0 g
- D 22.7 g

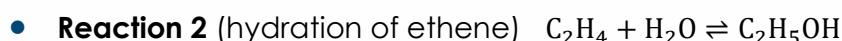
11. The Haber process is used to produce ammonia.



Which of the following would make the industrial process more sustainable?

- A Dispose of chemical waste in landfills.
- B Use a higher pressure.
- C Continually recycle unreacted gases back to the reactor.
- D Carry out the process at a higher temperature.

12. Ethanol can be produced by two processes: fermentation of glucose and hydration of ethene. These processes can be represented by the equations below:



Which statement about the processes is true?

- A Reaction 1 is sustainable because it uses renewable raw materials.
- B Reaction 1 is unsustainable because it produces by-products.
- C Reaction 2 is unsustainable because it only produces one product.
- D Reaction 2 is sustainable because it is reversible.

13. Ethanol can be produced by two processes: fermentation of glucose and hydration of ethene. These processes can be represented by the equations below:

- **Reaction 1** (fermentation of glucose) $\text{C}_6\text{H}_{12}\text{O}_6 \rightarrow 2\text{C}_2\text{H}_5\text{OH} + 2\text{CO}_2$
- **Reaction 2** (hydration of ethene) $\text{C}_2\text{H}_4 + \text{H}_2\text{O} \rightleftharpoons \text{C}_2\text{H}_5\text{OH}$

Which statement about the percentage yields and atom economies is true?

- A Reaction 1 will always have a yield <100% **and** an atom economy <100%.
- B Both reactions always have an atom economy of 100%.
- C Reaction 2 will always have 100% yield and 100% atom economy.
- D Reaction 2 always has a higher yield and a higher atom economy than Reaction 1.

14. Ethanol can be produced by two processes: fermentation of glucose and hydration of ethene. These processes can be represented by the equations below:

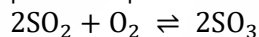
- **Reaction 1** (fermentation of glucose) $\text{C}_6\text{H}_{12}\text{O}_6 \rightarrow 2\text{C}_2\text{H}_5\text{OH} + 2\text{CO}_2$
- **Reaction 2** (hydration of ethene) $\text{C}_2\text{H}_4 + \text{H}_2\text{O} \rightleftharpoons \text{C}_2\text{H}_5\text{OH}$

500 kg of glucose is fermented in **Reaction 1**. Calculate the theoretical yield of ethanol.

(A_r values: C = 12.0, H = 1.0, O = 16.0)

- A 255 kg
- B 128 kg
- C 64 kg
- D 264 kg

15. The **contact process** is important for the production of sulfuric acid. One stage of the process produces sulfur trioxide gas:



The reaction conditions used industrially are: 450°C, 100 kPa, V_2O_5 catalyst.

Using these conditions allows a conversion rate of around 99.5%.

This stage always has an atom economy of 100%. Which statement explains why?

- A The reaction is reversible.
- B There is a high percentage yield of sulfur trioxide.
- C Unreacted sulfur dioxide can be recycled and reused in the process.
- D No by-products are produced.

16. The **contact process** is important for the production of sulfuric acid. Sulfur dioxide is required for the process. This can be made either by burning sulfur in an excess of air or heating sulfide ores (such as pyrite) in an excess of air:

- **Reaction 1** $S + O_2 \rightarrow SO_2$
- **Reaction 2** $4FeS_2 + 11O_2 \rightarrow 2Fe_2O_3 + 8SO_2$

Select the correct atom economies for both processes.

(M_r values: $SO_2 = 64.1$, $FeS_2 = 120.0$, $Fe_2O_3 = 159.6$)

(A_r values: $S = 32.1$, $O = 16.0$, $Fe = 55.8$)

- A Reaction 1 = 1%, reaction 2 = 1.6%
- B Reaction 1 = 100%, reaction 2 = 42.2%
- C Reaction 1 = 100%, reaction 2 = 61.6%
- D Reaction 1 = 1%, reaction 2 = 0.62%

17. The **contact process** is important for the production of sulfuric acid. This can be made either by burning sulfur in an excess of air or heating sulfide ores (such as pyrite) in an excess of air:

- **Reaction 1** $S + O_2 \rightarrow SO_2$
- **Reaction 2** $4FeS_2 + 11O_2 \rightarrow 2Fe_2O_3 + 8SO_2$

650 kg of oxygen is used for reaction 2. Given that a 98.5% yield is attained, calculate the actual yield of SO_2 in kg for reaction 2.

(M_r values: $SO_2 = 64.1$, $FeS_2 = 120.0$, $Fe_2O_3 = 159.6$)

(A_r values: $S = 32.1$, $O = 16.0$, $Fe = 55.8$)

- A 933 kg
- B 961 kg
- C 1320 kg
- D 1280 kg

18. Industrial processes often produce by-products. There are many options for these by-products, including:

1. using them as a starting material to produce other useful products
2. recycling them where possible
3. sending them to landfill
4. neutralising them (if needed) and releasing them into the air

Which of the statements, 1–4, increase the sustainability of a process?

- A 1 only
- B 1, 2, and 4
- C 1 and 2 only
- D All of the above, 1–4

Activity 2: follow-up tasks

Your teacher will give you the answers and explanations to the multiple-choice questions. Using your responses to Activity 1, complete the suggested follow-up tasks to target areas for improvement and increase your understanding.

Area for improvement	Follow-up task
<p>Percentage yield calculations You should be able to:</p> <ul style="list-style-type: none"> calculate the theoretical yield of a product from a given mass of reactant use balanced equations to calculate percentage yields for reactions 	<p>Percentage yields are practical measures which compare the actual yield obtained in a chemical process with the maximum theoretical yield calculated from the balanced chemical equation.</p> <p>Calculating percentage yields is an important skill. Some key points to remember:</p> <ul style="list-style-type: none"> The amount of product obtained in a chemical reaction is called the yield. To calculate the theoretical yield of a product, you use the mass of reactant and the balanced equation for the reaction. The percentage yield is then calculated by: $\text{Percentage yield} = \frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100$ <p>Task a)</p> <p>The contact process is an important industrial process used to make sulfuric acid. There are three main stages to the process. (M_r values: $\text{SO}_2 = 64.1$, $\text{SO}_3 = 80.1$, $\text{H}_2\text{S}_2\text{O}_7 = 178.2$ A_r values: $\text{S} = 32.1$, $\text{O} = 16.0$, $\text{Fe} = 55.8$)</p> <ol style="list-style-type: none"> The first stage of the contact process involves producing sulfur dioxide: $\text{S} + \text{O}_2 \rightarrow \text{SO}_2$ If 600 kg (3 s.f.) of sulfur is used, calculate the maximum theoretical yield of sulfur dioxide which could be produced. The sulfur dioxide produced in stage 1 goes on to react with oxygen in a reversible reaction: $2\text{SO}_2 + \text{O}_2 \rightleftharpoons 2\text{SO}_3$ Use your yield from part i to determine the maximum theoretical yield of sulfur trioxide, SO_3. Give your answer to an appropriate degree of accuracy.

	<p>iii. The sulfur trioxide undergoes further reactions to produce the desired product, sulfuric acid. It is first dissolved in some sulfuric acid to produce fuming sulfuric acid, $\text{H}_2\text{S}_2\text{O}_7$:</p> $\text{H}_2\text{SO}_4 + \text{SO}_3 \rightarrow \text{H}_2\text{S}_2\text{O}_7$ <p>This can then be further reacted to produce sulfuric acid:</p> $\text{H}_2\text{S}_2\text{O}_7 + \text{H}_2\text{O} \rightarrow 2\text{H}_2\text{SO}_4$ <p>Use your yield from part (ii) to calculate the maximum theoretical yield of fuming sulfuric acid and hence the theoretical yield of sulfuric acid at the end of the process. Give your answer to an appropriate degree of accuracy.</p> <p>iv. If the actual yield of sulfuric acid was 2500 kg, calculate the percentage yield. Give your answer to an appropriate degree of accuracy.</p>
<p>Atom economy calculations You should be able to:</p> <ul style="list-style-type: none"> calculate the A_r and M_r of substances in an equation use balanced equations to calculate the atom economy for reactions 	<p>Atom economy is a purely theoretical measure of the mass of atoms which end up in our useful product and is therefore a measure of how efficient the process is. Some key points to remember:</p> <ul style="list-style-type: none"> Use your periodic table to find the A_r and M_r for different substances. Be particularly careful about diatomic elements and larger, more complex molecules. The molar ratio must be included in these calculations – you must use a balanced chemical equation when carrying out these calculations! Atom economy (%) = $\frac{M_r \text{ of the desired product}}{\text{Total } M_r \text{ values of all the reactants}} \times 100$ A process which produces only one product will therefore always have 100% atom economy. <p>Task b)</p> <p>Many chemical reactions produce hydrogen. Four such reactions, A–D, are given below.</p> <p>Reaction A: $\text{C} + \text{H}_2\text{O} \rightarrow \text{CO} + \text{H}_2$</p> <p>Reaction B: $2\text{Al} + 3\text{H}_2\text{O} \rightarrow \text{Al}_2\text{O}_3 + 3\text{H}_2$</p> <p>Reaction C: $\text{LiH} + \text{H}_2\text{O} \rightarrow \text{LiOH} + \text{H}_2$</p> <p>Reaction D: $\text{Reactant Y} + 3\text{H}_2\text{O} \rightarrow \text{By-product Z} + 3\text{H}_2$</p> <p>Hydrogen is a useful product and is being investigated as a viable alternative to fossil fuels.</p> <p>i. Which reaction, from A–C, has the highest atom economy?</p>

	<p>ii. The atom economy of reaction D is 17.6%. Find the M_r of reactant Y and hence, the M_r of by-product Z.</p> <p>iii. Explain why none of these reactions have an atom economy of 100%.</p>
<p>Green chemistry and sustainability in industrial processes</p> <p>You should be able to:</p> <ul style="list-style-type: none">• explain why chemists aim to design processes with high percentage atom economy• identify factors which may impact the yield of a chemical process	<p>Atom economy and percentage yield calculations are important because:</p> <ul style="list-style-type: none">• Processes with a high atom economy are a huge advantage in industry: they make efficient use of reactants, giving economic, ethical and environmental advantages.• Percentage yield calculations use practical data to determine the effectiveness of a process in producing product. It is important that you can pick out why an actual yield may vary from a theoretical yield.• When comparing industrial advantages of processes, it is important to consider raw materials, by-products and atom economies. <p>Task c)</p> <p>Read the instructions for preparing salicylic acid (The preparation of 2-hydroxybenzoic acid rsc.li/41ndpFV) and answer the questions below.</p> <ol style="list-style-type: none">i. During stage 1, the sample of 2-hydroxybenzoic acid must be weighed accurately. Why is this?ii. Step 4 of stage 1 requires the solution to be warmed for a further five minutes. One student stops this stage too early. Another student stops this stage too late. Explain the potential impacts of these procedural errors.iii. During stage 2, it is important to wait until precipitation appears complete. How might it impact the percentage yield if this step is stopped too early?iv. Why might the yield of aspirin appear higher than expected?v. State one other reason why the percentage yield could be less than 100%.

vi. Aspirin can be prepared by acylation reactions, using either ethanoyl chloride or ethanoic anhydride:



Calculate the atom economy of each process.

(M_r values: $\text{CH}_3\text{COCl} = 78.5$, $(\text{CH}_3\text{CO})_2\text{O} = 102.0$, $\text{HOC}_6\text{H}_4\text{COOH} = 138.0$, $\text{CH}_3\text{COOC}_6\text{H}_4\text{COOH} = 180.0$)

Give one industrial advantage of each process.

Extension task

Read the article **Limonene and orange peel** from FutureLearn available at rsc.li/3WY20vZ.

Identify the industrial advantages of using microwaves to extract (+)-limonene using high-powered microwaves, compared to the conventional methods of steam distillation. You may find it helpful to refer to **The 12 principles of green chemistry** (RSC) available at rsc.li/4aPzP8h

Research further applications to find out how atom economy guides decision-making for industrial processes and how the twelve principles of green chemistry are applied to chemical engineering – there are **many** applications!