Atom economy, percentage yield and green chemistry misconception buster

This resource accompanies the article **Teaching atom economy, percentage yield and green chemistry post-16** in *Education in Chemistry* which can be viewed at rsc.li/3CN5ASO. The article provides more ideas, activities and tips for teaching this topic and avoiding misconceptions.

Learning objectives

By the end of this resource, students will be able to:

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.

This resource is designed to identify and target misconceptions at the three main pinch points: calculating percentage yields, calculating atom economies and evaluating sustainability in industrial processes and green chemistry.

How to use the resource

Activity 1 consists of 18 multiple choice questions. Instruct learners to read each question carefully – using the data provided – and tick an answer. There is one correct answer per question. The answer to each question includes an explanation for you to share with learners.

After learners have marked the multiple-choice questions either by peer- or self-assessing, ask them to complete the relevant follow-up tasks to target areas for improvement and increase their understanding of certain topics.

If appropriate, guide learners to follow-up tasks based on misconceptions you have already identified throughout the course or for further practice if they get 18/18 on the quiz. Activity 2 is fully differentiated for learners to target their own misconceptions identified from the multiple-choice quiz.

You can choose to use **task c** separately as it requires students to access research resources.

Extension opportunities

These concepts apply to many industrial processes. One example is in the production of (+)-limonene from orange peel (overview available from FutureLearn at rsc.li/3WY20vZ). As a follow-up activity, get students to read about the process and evaluate whether the new method is more sustainable than conventional methods. The 12 principles of green chemistry, available at rsc.li/4aPzP8h, will guide their thinking.

Encourage students to research further applications of decision-making for industrial processes, if appropriate.

Answers

Activity 1: multiple choice questions

Q.	Answer	Explanation	Activity 2 follow-up task
1.	**B** – 161.0 g	A – You have **halved** the moles, but they are in a 1:1 ratio. C – You have **doubled** the moles, but they are in a 1:1 ratio. D – Incorrect M_r calculation	Complete **task a)**
2.	**C** – The atom economy of the process will always be 100%.	It is highly unlikely for a reaction to have 100% yield, as there will always be inevitable losses during a chemical process. We also have no practical information to enable us to determine the percentage yield. As there is only one product, the atom economy for the reaction will always be 100% – it is determined only from the mass of all the atoms present, not from any procedural impacts.	Complete **task c)**
3.	**C** – 15.4%	A – You have calculated the atom economy for carbon dioxide. B – You have inverted the equation for atom economy. D – You have not multiplied the M_r values by their molar ratio.	Complete **task b)**
4.	**D** – $CH_3COOH + 2H_2 \rightarrow C_2H_5OH + H_2O$	The atom economies for each process are as follows: A = 30.9% B = 51.1% C = 44.0% D = 71.9%	Complete **task b)**

5.	**C** – Carry out the reaction at a suitable temperature to prevent side-reactions.	More steps in a process means there are more chances for product to be lost as it is transferred between vessels. While reducing by-products is beneficial for atom economy, it has no bearing on the yield of product. A reversible reaction can actually lead to a reduction in percentage yield.	Complete **task c)**
6.	**C** – The proportion of reactants that form useful products, as a percentage.	All of the other statements relate to **percentage yield** of a reaction.	Complete **task c)**
7.	**A** – 49.3%	B – You have not used the molar ratios in your calculation. C – You have calculated the atom economy for $NaCl$ instead of $NaOCl$. D – A combination of errors B and C.	Complete **task b)**
8.	**D** – Lower atom economy results in fewer by-products, improving sustainability.	Atom economy is a big driver for sustainability of industrial processes. The higher the atom economy, the more reactant atoms that have been converted into the useful product. High atom economy leads to **less** by-products, less waste and improved sustainability.	Complete **task c)**
9.	**B** – The reaction will always have 100% atom economy.	Percentage yield is driven by the effectiveness of a process in producing product. Despite there being just one product, it does not mean that all reactant has been used up to produce ammonia, especially since the reaction is reversible! Reversible does not necessarily mean unsustainable though. During the Haber process, unreacted gases are recycled back round to the reactor – very sustainable practice. Atom economy is a theoretical measure of the use of atoms within reactions; it is not determined by practical data.	Complete **task c)**
10.	**C** – 68.0 g	A – You haven't used the molar ratio in your calculation. B – Nitrogen is diatomic, so it has an M_r of (14.0 x 2) = 28.0 D – You have used the wrong molar ratio – check again!	Complete **task a)**
11.	**C** – Continually recycle unreacted gases back to the reactor.	Disposal of chemicals in landfill is poor practice in industrial processes. Reaction conditions impact equilibrium yields of product for a reversible	Complete **task c)**

		reaction but do not necessarily make it more sustainable, particularly if there is a high energy cost associated with the reaction conditions (such as high pressures).	
12.	**A** – Reaction 1 is sustainable because it uses renewable raw materials.	Wherever possible, it is sustainable practice to utilise renewable resources in favour of non-renewables. Production of by-products can reduce atom economy of a process but it is not always a negative if we can make use of the by-products for other processes! Reversible reactions can impact the yield but do not necessarily mean a process is unsustainable.	Complete **task c)**
13.	**A** – Reaction 1 will always have a percentage yield <100% and an atom economy <100%.	Reaction 1 can never have an atom economy of 100%, as there are by-products produced. In practice, a percentage yield of 100% is unattainable practically, as there are inevitable losses during the reactions. Reaction 2 will always have a higher atom economy, as there is only one product. There is no way of knowing that the process will *always* have a higher percentage yield.	Complete **task c)**
14.	**A** – 255 kg	B – You haven't used the molar ratio. C – You have used the wrong molar ratio (divided by 2 instead of multiplying by 2). D – You have calculated the wrong M_r for glucose.	Complete **task a)**
15.	**D** – No by-products are produced.	A reversible reaction has no bearing on the atom economy calculation. Percentage yield and atom economy are separate concepts; they have no impact on each other. While recycling any unreacted reactant is great sustainable practice, it doesn't impact atom economy calculations.	Complete **task c)**
16.	**C** – Reaction 1 = 100%, reaction 2 = 61.6%	A – You have inverted the atom economy equation and not multiplied your final answers by 100 to give a percentage. B – You haven't used the molar ratio when working out atom economy. D – You haven't multiplied by 100 to give a percentage.	Complete **task b)**
17.	**A** – 933 kg	Theoretical yield = 947 kg, which gives an actual yield of 933 kg.	Complete **task a)**

		B – You have the correct theoretical yield but have rearranged the percentage yield equation incorrectly. C – You haven't used the molar ratio to work out the correct theoretical yield. You have also rearranged the percentage yield equation incorrectly. D – You haven't used the molar ratio to work out the correct theoretical yield.	
18.	**C** – 1 and 2 only	Using by-products in other processes or recycling them are important sustainable practices within industry. We must try to avoid sending waste to landfill or contributing to polluting the atmosphere.	Complete **task c)**

Activity 2: follow-up tasks

Follow-up task	Answer
Task a)	**i.** $S + O_2 \rightarrow SO_2$ $n(S)$ = 600 / 32.1 = 18.6915… mol $n(S) = n(SO_2)$ as equal mole ratios in the equation (1:1) mass (SO_2) = 18.6915… x 64.1 = 1198.13… = 1200 kg **ii.** $2SO_2 + O_2 \rightleftharpoons 2SO_3$ $n(SO_2)$ = 18.6915… (as before) $n(SO_2) = n(SO_3)$ as equal mole ratios in the equations (2:2) mass(SO_3) = 18.6915… x 80.1 = 1497.196… = 1500 kg **iii.** $n(SO_3) = n(H_2S_2O_7)$ as equal mole ratios in equation (1:1) = 18.6915… (as before) mass$(H_2S_2O_7)$ = 18.6915 x 178.2 = 3330.8411… = 3330 kg $n(H_2SO_4)$ at the end = 2 x $n(H_2S_2O_7)$ as mole ratio 1:2 = 37.3831… mol mass(H_2SO_4) at the end = 33.3831 x 98.1 = 3667.28972… = 3670 kg **iv.** Percentage yield = [2500 / 3670] x 100 = 68.1% Some points of note: • Since **all** of the masses are in kg, there is no need to convert into g first – this would involve multiplying by 1000 in the first step, only to divide by 1000 again at the end. • All answers are given to an **appropriate degree of accuracy**. The **least** accurate information given in the question was the original mass in grams to 3 s.f. so all answers are given to 3 s.f.

	• If you got the answer to one of the parts wrong, don't worry. Continue to mark on, checking each part of the calculation. In an exam, there would be **error carried forward (ecf)** marks available for each part **or** they would give you a value to work with if you had been unable to obtain an answer for previous parts. You may have seen this before in past paper questions.
Task b)	**i.** **Reaction A** %AE = $\frac{(2 \times 1.0)}{12.0+[(2\times1.0)+16.0]} \times 100 = 6.67\%$ **Reaction B** %AE = $\frac{3(2 \times 1.0)}{(2\times27.0)+3[(2\times1.0)+16.0]} \times 100 = 5.56\%$ **Reaction C** %AE = $\frac{(2 \times 1.0)}{(6.9+1.0)+[(2\times1.0)+16.0]} \times 100 = 7.72\%$ Reaction C has the highest atom economy. **ii.** $17.6\% = \frac{3(2 \times 1.0)}{M_r\ of\ reactant\ Y+[(2\times1.0)+16.0]} \times 100$ $0.176 = \frac{6}{M_r\ of\ reactant\ Y+18}$ 0.176 x (reactant Y +18) = 6 M_r of reactant Y + 18 = 34.1 M_r of reactant Y = 16.1 According to the law of conservation of mass, the sum of all the M_rs before and after the reaction should be equal. Sum of M_rs before = 16.1 + [(2 x 1)+16] = 34.1 Sum of M_rs after = M_r of by-product Y + 3(2 x 1) = 34.1 M_r of by-product Y + 6 = 34.1 M_r of by-product Y = 28.1 **iii.** None of the reactions have an atom economy of 100%, since all of the reactions produce by-products. Only reactions which have a single product will have an atom economy of 100%.
Task c)	**i.** The 2-hydroxybenzoic acid must be accurately weighed in order to determine an accurate **theoretical yield**. **ii.** If the warming is stopped too early, not all of the 2-hydroxybenzoic acid may have reacted – the reaction is incomplete. This will lower the percentage yield. If the solution is warmed for too long, side-reactions may occur, lowering the percentage yield of the product. **iii.** If not all of the solid is allowed to precipitate, the percentage yield will be lower than expected as some product will remain in the discarded solution. **iv.** There may be impurities present in the sample or the crystals may not be dry. **v.** Transferring between apparatus leads to inevitable loss of product, leading the percentage yield to be less than 100%. **vi.** Using ethanoyl chloride: %AE = $\frac{180.0}{78.5 + 138.0} \times 100 = 83.1\%$ Using ethanoic anhydride: %AE = $\frac{180.0}{102.0 + 138.0} \times 100 = 75.0\%$ Using ethanoyl chloride has the industrial advantage of having

	a high atom economy – it is a more efficient process. However, the by-product is a **stronger acid** than the ethanoic acid produced when ethanoic anhydride is the starting material. OR Ethanoic anhydride is a cheaper starting material than ethanoyl chloride. OR Ethanoic anhydride is less corrosive than ethanoyl chloride. OR Synthesis using ethanoic anhydride causes less side-reactions (as it is a less vigorous reaction) and hence will produce a higher yield.

Extension task

Suggested ideas

- Using high-powered microwaves uses lower energy processes, which leads to a lower energy cost. It produces double the yield in less time.
- Steam distillation requires more steps – distillation, followed by separation of (+)-limonene from the condensed water vapour using a separating funnel. This will result in more loss of product, lowering the yield. The process using high-powered microwaves does not require this further separation as only the (+)-limonene need be collected.
- The orange peel produced can be converted to biogas once all of the (+)-limonene is removed, which is an economical and greener use of waste materials. Since more (+)-limonene is removed using high-powered microwaves, more of this waste material can be used without contamination with antimicrobial (+)-limonene.