Chem Factsheet

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Atom Economy

To succeed in this topic you need to understand:
- how to calculate the % yield of a reaction
- why % yield is never 100%
- why it is important that the chemical industry does not cause unnecessary environmental damage

After working through this Factsheet you will be able to:
- calculate the atom economy of a reaction
- explain the difference between atom economy and % yield
- understand why atom economy is important

What you should already know

1. ***How do you calculate the % yield of a reaction?***

$$\% \text{ yield} = \frac{\textbf{actual mass of product formed}}{\textbf{theoretical mass of product}} \times 100$$

2. Marie carries out the thermal decomposition of 100 g of calcium carbonate. She weighs the calcium oxide product, and finds that she has made 52 g. ***What is the % yield of her reaction?***

	$CaCO_3$	→	CaO	+	CO_2
mass	100 g		52 g		
molar mass (/g)	100		56		

Moles of $CaCO_3$ to start with
= mass (/g)/Mr = 100/100 = 1 mole $CaCO_3$.
From the equation you would expect 1 mole of $CaCO_3$ to make 1 mole of CaO.
1 mole of CaO has a mass of 56 $gmol^{-1}$, so the theoretical mass of product is 56 g.
Hence, the % yield of the reaction = 52/56 × 100 = 93%.

3. ***Why is % yield never 100%?***
Reactions always have yields lower than 100% for the following reasons: loss of product in transfer and separation, formation of by-products, decomposition of starting materials, incomplete reaction and reversibility.

4. ***What range of % yields might make a reaction economically viable?***
Industrial chemists need their reaction yields to be as high as possible. Generally they will look for reactions with yields above about 75%, so that they do not waste too much starting material. There are of course exceptions where lower yields are acceptable. Some examples include reactions where the product is particularly valuable, or the starting materials are very cheap, or the unused reactants can be recycled and re-used.

What is atom economy?
Atom economy is defined as:

$$\textbf{\% atom economy} = \frac{\textbf{molar mass of } \textbf{\textit{useful}} \textbf{ product}}{\textbf{total molar mass of starting materials}} \times 100$$

Worked example 1
In the thermal decomposition of calcium carbonate to make calcium oxide,
$CaCO_3 \rightarrow CaO + CO_2$
the molar mass of the starting material,
$CaCO_3$ is 40 + 12 + 3(16)g = 100 g.
The useful product is CaO, with a molar mass of 40 + 16 = 56 g.
The atom economy, therefore, is 56/100 × 100 = 56%.

Worked example 2
In the blast furnace, iron oxide reacts with carbon monoxide to make iron.
The equation for the reaction is $Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$.

The total molar mass of the starting materials is:
(2×56) + (3×16) + 3(12+16) =244 g

The molar mass of the useful product (iron) is **2** × 56 = 112 g.
Hence, the % atom economy = 112/244 = 46%.

Why is atom economy important?

The atom economy of a reaction determines its efficiency, in terms of how many atoms of starting materials are usefully converted to product. This is an important measure of the environmental friendliness of a reaction. It is less wasteful and therefore more 'green' to have a reaction where all the atoms of the starting material are converted to useful product, rather than a reaction where most of the atoms are converted to useless by-products.

Consider the three reactions shown in Table 1 and check that you agree with the % atom economies. The addition reaction has an atom economy of 100%, showing that this is the least wasteful of the three, since all the starting atoms are converted to useful product. Addition reactions always have atom economies of 100%, and are therefore environmentally valuable. Remember, though, that an atom economy of 100% tells us nothing about the yield of the reaction.

Table 1: Reaction types and atom economy

Equation	Reaction type	Useful product	% Atom economy
$CH_3Cl + NaOH \rightarrow CH_3OH + NaCl$	Substitution	CH_3OH	35%
$2Al_2O_3 \rightarrow 4Al + 3O_2$	Decomposition	Al	53%
$C_2H_4 + HCl \rightarrow C_2H_5Cl$	Addition	C_2H_5Cl	100%

Other environmental considerations

Atom economy is not the only measure of the environmental friendliness of a reaction. Other factors include:
- The % yield
- The availability, source and toxicity of the starting materials, especially there renewability
- The temperature and pressure used during the reaction since higher values use more energy
- Reaction reversibility
- The use of toxic solvents, reagents or catalysts
- The ease of separation of the useful product from the reaction mixture

Practice Questions

1. Explain how each of these factors contributes to the 'greenness' of a chemical reaction:
   (a) atom economy
   (b) % yield
   (c) temperature
   (d) use of a catalyst
   (e) the source of the starting materials

2. Calculate the % atom economy of each of these reactions. The useful products are highlighted in bold.
   (a) $S + O_2 \rightarrow \mathbf{SO_2}$
   (b) $TiO_2 + 2Mg \rightarrow \mathbf{Ti} + 2MgO$
   (c) $TiO_2 \rightarrow \mathbf{Ti} + O_2$
   (d) $C_2H_4 + H_2O \rightarrow \mathbf{C_2H_5OH}$
   (e) $C_{10}H_{22} \rightarrow C_2H_4 + \mathbf{C_8H_{18}}$
   (f) $C_{10}H_{22} \rightarrow \mathbf{C_2H_4} + \mathbf{C_8H_{18}}$

3. Explain the difference in your answers to 2(e) and 2(f).

4. The reactions in 2(b) and 2(c) show two ways of extracting titanium. Which would you choose? What else might you need to know before deciding?

5. Ammonia is synthesised in the Haber Process:
   $N_2 + 3H_2 \rightleftharpoons 2NH_3$

   (a) What is the atom economy of this reaction (you should be able to work this out without doing any calculations)?
   (b) What does the symbol $\rightleftharpoons$ mean?
   (c) What effect does this have on the % yield of the reaction?

Answers

1. (a) **atom economy**
   A measure of how many atoms of starting material are converted to useful product. Reactions with high atom economies use fewer natural resources and create less waste.

   (b) **% yield**
   A measure of the actual amount of useful product formed in a reaction. Reactions with high yields convert starting materials to products with low waste, inefficiency or the need for awkward separations.

   (c) **temperature**
   Low temperature reactions use less energy.

   (d) **use of a catalyst**
   Catalysts cause the reaction to follow a different reaction route with a lower activation energy, allowing the reaction to be carried out at a reduced temperature. However, some catalysts contain toxic metals (e.g. platinum, mercury) which could cause damage to ecosystems if released into the environment.

   (e) **the source of the starting materials**
   Many feedstock chemicals are derived from crude oil, a non-renewable resource. Chemists are working hard to find alternative, renewable sources of starting materials, such as plant sugars.

2. (a) 100%, (b) 38%, (c) 65%, (d) 100%, (e) 80%, (f) 100%.

3. In 2(e), only one of the products is useful, while in 2(f), they both are. This shows that it is both environmentally and economically beneficial to make use of all the products of a reaction (cracking, in this example).

4. 2(c) has a higher atom economy, and therefore might be the best choice. However, it would also depend on factors such as % yield, the reaction temperature, and ease of separation of the titanium from the other product.

5. (a) 100%
   (b) The reaction is reversible.
   (c) In reversible reactions, the % yield will probably be low since the products decompose to the starting materials. In the Haber Process, the high economic value of the product compensates for the low yield.

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