Topic: Chemical calculations

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Content:

Limiting reagent

%Yield

% Purity

- **How do you make a burger?**

How many buns & beef patties, do you think, are required to make 1 burger?

+

- Let's say that I have 6 buns, how many burgers can I make?

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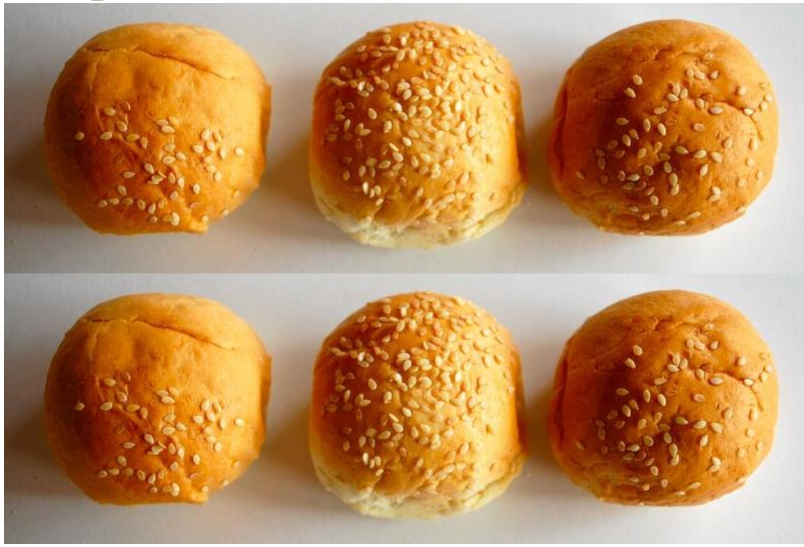
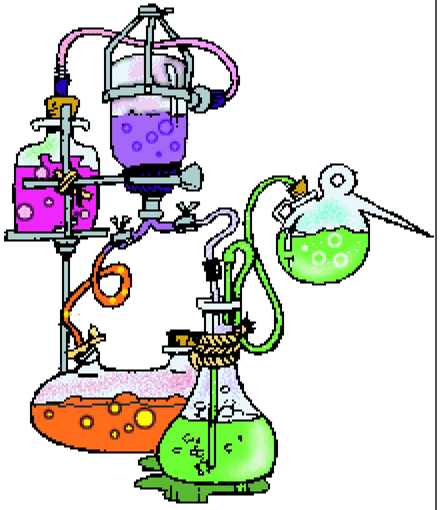
- **Using the same amount of buns**, what if there are only **4 beef** patties available? How many burgers can I make?



Hence, what is the limiting factor?

What is in excess?



This is the same with chemical reactions.

Limiting reactants/reagents

- It is the chemical that is completely consumed in a reaction.
- The reaction stops as soon as the limiting reactant is totally consumed.
- The limiting reactant limits the amount of products formed.
- Check for limiting reactant when the quantities of **two** (or **more**) reactants are given.
- Calculation: Always involves **no. of moles.**

Example 1:

In the Haber process, ammonia is manufactured from nitrogen and hydrogen. A mixture of **5 moles of nitrogen** and **10 moles of hydrogen** were allowed to react according to the following equation:

$$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$$

Which substance is the limiting reagent?

- ***Solution:***

Mole ratio from **balanced equation**:

$$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$$

$$1 \quad : \quad 3 \quad : \quad 2$$

From the **quantities given**:

$$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$$

$$5 \quad : \quad 10$$

No. of moles of NH_3 (Products):

Using mole ratio N_2 = (5 x 2) / 1 = 10 mol.

Using mole ratio H_2 = (10 x 2) / 3 = 6.67 mol.

- The lowest no. of moles produced is the limiting reactants.
- Excess of N_2, limiting reagent/reactant is H_2.

I have some rice seeds. I'm planning on opening a paddy field.

After a period of time…

The amount of plant crop harvested per unit area for a given time → **"products"**

Percentage Yield

Yield → The amount of product obtained from a reaction.

- There are 2 types of yield:

I. Theoretical → The calculated quantity of product that is expected be formed.

II. Actual → The amount of products that is actually obtained in a reaction.

- The % yield is always less than the theoretical yield.
- Percentage yield:

$$\frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100$$

Example 1:

128g of *sulphur dioxide, SO_2*, was reacted with oxygen to produce sulphur trioxide, SO_3. The equation for the reaction is:

$$2SO_2(g) + O_2(g) \rightarrow 2SO_3(g)$$

140g of SO_3 was produced in the reaction. Calculate the percentage yield of the SO_3.

Solution

Step 1 : Balanced equation	$2SO_2(g) + O_2(g) \rightarrow 2SO_3(g)$
Step 2 : Mole ratio	2 : 2
Step 2.5*: Calculate no. of moles (SO_2)	No. of moles = $\frac{\text{Mass}}{\text{Molar mass or Mr}}$ $= \frac{128\text{ g}}{64\text{ (g)}}$ = <u>2 mol.</u>
Step 3 : Find no. of moles (SO_3)	2 : 2 2 : x No. of moles of SO_3 = $\frac{(2 \times 2)}{2}$ <u>= 2 mol.</u>
Step 4 : Find the mass (SO_3)	Mass = No. of moles X Molar Mass or Mr = 2 mol X 80 (g) = <u>160 g</u>.
Step 5 : Percentage yield (SO_3)	= (Actual / theoretical) X 100% = (140 / 160) X 100% = 87.5%

Example 2

50.0 cm^3 of 0.105 mol/dm^3 aqueous calcium chloride was treated with an excess of aqueous silver nitrate. White silver chloride was precipitated. The precipitate was dried and weighed. A mass of 1.45g was recorded. Calculate the percentage yield.

Solution:

Step 1 : Balanced equation	$2AgNO_3(aq) + CaCl_2(aq) \rightarrow 2AgCl(s) + Ca(NO_3)_2\ (aq)$
Step 2 : Mole ratio	1 : 2
Step 2.5*: Calculate no. of moles ($CaCl_2$)	$\text{Conc. (mol/dm}^3\text{)} = \dfrac{\text{No. of moles (mol)}}{\text{Volume (dm}^3\text{)}}$ No. of moles = Conc. X Volume = 0.105 X (50.0 / 1000) = <u>0.00525 mol.</u>
Step 3 : Find no. of moles (AgCl)	1 : 2 0.00525 : x $\text{No. of moles of AgCl} = \dfrac{(0.00525 \times 2)}{1}$ <u>= 0.0105 mol.</u>
Step 4 : Find the mass (AgCl)	Mass = No. of moles X Molar Mass or Mr = 0.0105 mol X 143.5 (g) = <u>1.51 g</u>.
Step 5 : Percentage yield	= (Actual / theoretical) X 100% = (1.45 / 1.51) X 100% = 96.0%

Percentage Purity

- Sometimes, chemical are not pure and contains impurity.
- It gives the indication of the amount of impurity in a chemical substance.
- Formula for percentage purity:

$$\frac{\text{Mass of pure substance in sample}}{\text{Mass of sample}} \times 100\%$$

How important is it to know the % purity calculation?

"Here's how it works. First we discover the drug and identify the market, then we invent the disease."

- FOR MANY COMPANIES – SUCH AS DRUG & FOOD COMPANIES, THE PURITY OF THE PRODUCT IS EVEN MORE IMPORTANT.
- IMPURITIES CAN KILL!

Example 1

An impure sample of calcium carbonate ($CaCO_3$) contains calcium sulphate as an impurity. When excess hydrochloric acid was added to **6g of the sample**, **1200 cm^3 of gas** was produced (measured at r.t.p.). Calculate **the percentage purity of the calcium carbonate** sample.

Solution:

Step 1 : Balanced equation	$CaCO_3 + 2HCl \rightarrow CaCl_2 + H_2O + CO_2$
Step 2 : Mole ratio	1 : 1
Step 2.5*: Calculate no. of moles (CO_2)	No. of moles = $\frac{\text{Volume of gas}}{\text{Molar volume}}$ $= \frac{1200}{24\ 000}$ = <u>0.05 mol.</u>
Step 3 : Find no. of moles ($CaCO_3$)	1 : 1 0.05 : x No. of moles of $CaCO_3$ = $\frac{(0.05 \times 1)}{1}$ <u>= 0.05 mol.</u>
Step 4 : Find the mass ($CaCO_3$)	Mass = No. of moles X Molar Mass or Mr = 0.05 mol X 100 (g) = <u>5 g</u>.
Step 5 : Percentage purity	= Mass of $CaCO_3$ / Mass of sample X 100%

Example 2:

A **3.21g** sample of <u>copper (II) carbonate </u>was reacted with excess hydrochloric acid. It was found that **480cm^3** of <u>carbon dioxide</u> gas measured at r.t.p. was given off. What is the <u>**percentage purity of the copper (II) carbonate in the given sample**</u>?

[1 mol gas occupies 24.0 dm^3 at r.t.p]

<u>*Solution:*</u>

Step 1 : Balanced equation	$CuCO_3 + 2HCl \rightarrow CuCl_2 + CO_2 + H_2O$
Step 2 : Mole ratio	1 : 1
Step 2.5*: Calculate no. of moles (CO_2)	No. of moles = $\frac{\text{Volume of gas}}{\text{Molar volume}}$ $= \frac{480}{24\ 000}$ = <u>0.02 mol.</u>
Step 3 : Find no. of moles ($CaCO_3$)	1 : 1 0.02 : x No. of moles of AgCl = $\frac{(0.02 \text{ X } 1)}{1}$ <u>= 0.02 mol.</u>
Step 4 : Find the mass ($CaCO_3$)	Mass = No. of moles X Molar Mass or Mr = 0.02 mol X 123.5 (g) = <u>2.47 g</u>.
Step 5 : Percentage purity	= Mass of $CaCO_3$ / Mass of sample X 100%