Limiting Reagent and Percent Yield Activity

How much product can be obtained given that the reaction isn't 100% complete?

The Model: Limiting Reagent

Sulfur dioxide reacts with oxygen to yield sulfur trioxide according to the equation:

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

Suppose there's a flask that initially contains 8 SO_2 molecules and 8 O_2 molecules. The flask is closed so that molecules cannot escape. If the reaction proceeds to the fullest extent, the "before" and "after" freeze frames of the system look like what's in figures 1 and 2.

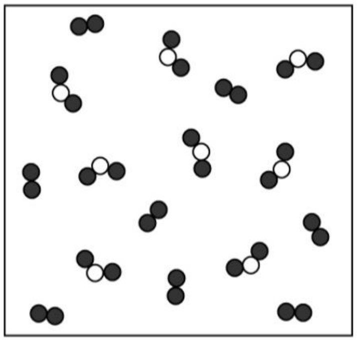


Fig. 1. Before the reaction

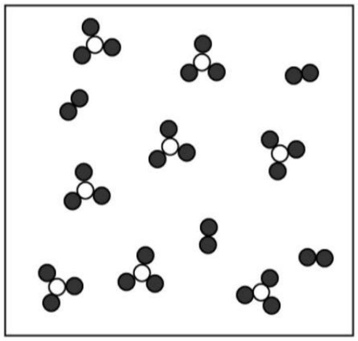


Fig. 2. After the reaction

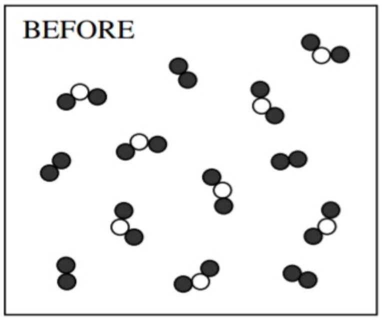
Key Questions

1a. Which reactant remains unreacted in figure 2, the "after" picture? Which reactant was completely consumed during the reaction?

b. Had there been more of a particular reactant, more sulfur trioxide would have been produced. Which reactant limited the production of sulfur trioxide? Why?

c. In your own words, define what a **limiting reagent** is.

2. Suppose the reaction vessel had been set up with the following "before" composition prior to the initiation of the reaction. Sketch what the "after" picture would look like AND identify which species is the limiting reagent and which reagent is in excess.



Limiting reagent ________

Excess reagent ________

AFTER

The Model: Using Moles of Limiting Reagent in Stoichiometry

The above pictures are not realistic because they involve so very few molecules. In a **"real-world"** sample, you are likely to have on the order of 10^{23} molecules.

Consider the following:

Suppose you have a reaction vessel initially containing 13.5 moles of sulfur dioxide and 11.2 moles of oxygen.

$$\text{mol } SO_2 \text{ required to react with all } O_2 = 11.2 \text{ mol } O_2 \times \frac{2\ mol\ SO2}{1\ mol\ O2} = \mathbf{22.4\ mol\ SO_2}$$

Since there aren't 22.4 moles of sulfur dioxide available, we conclude that sulfur dioxide is the limiting reagent and oxygen is the reagent in excess. The numbers of moles of sulfur trioxide and left over oxygen when the reaction is complete are:

mol SO_3 produced: $13.5 \text{ mol } SO_2 \times \frac{2\ mol\ SO3}{2\ mol\ SO2} = \mathbf{13.5\ mol\ SO_3}$

mol O_2 consumed: $13.5 \text{ mol } SO_2 \times \frac{1\ mol\ O2}{2\ mol\ SO2} = \mathbf{6.75\ mol\ O_2}$

mol O_2 remaining: 11.2 mol O_2 initially – 6.75 mol O_2 consumed = **4.45 mol O_2**

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Key Questions

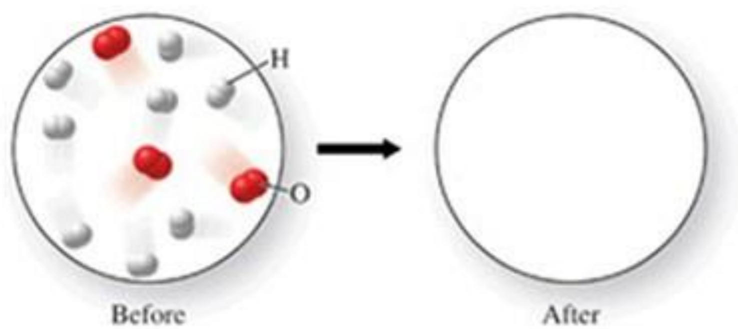
3a. It is the number of moles of the excess reagent / limiting reagent that is used to determine how many moles of each product is produced. **(Circle the correct answer.)**

b. Detail in your own words how one determines the amount of excess reagent that remains unreacted after a reaction is complete. (What is the starting point for calculations? What conversion factors are used? What calculation is necessary to finish the determination?)

EXERCISES

1. The figure shows a molecular-level diagram of reactant molecules for the reaction

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(l)$$



List the number and formulas of the molecules that should be present after the reaction takes place.

A) $2H_2O + 6H_2 + 2O_2$ B) $3H_2O + 5H_2 + O_2$ C) $4H_2O + 4H_2 + O_2$
D) $6H_2O + 2H_2 + O_2$ E) $6H_2O + 2H_2$

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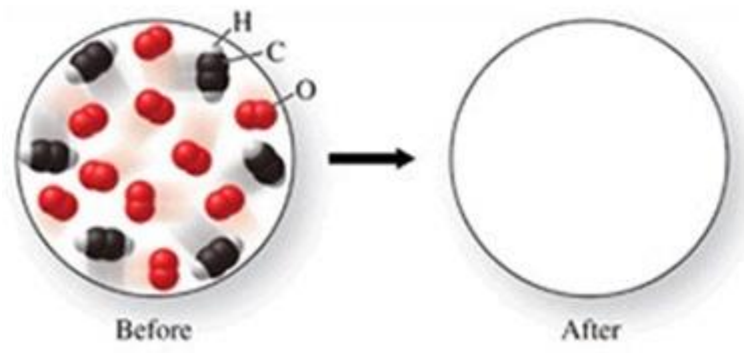
2. The figure shows a molecular-level diagram of reactant molecules for the reaction:

$$2C_2H_2(g) + 5O_2(g) \rightarrow 4CO_2(g) + 2H_2O(g)$$



List the number and formulas of the molecules that should be present after the reaction takes place.

A) $4CO_2 + 2H_2O$

B) $4CO_2 + 2H_2O + 2C_2H_2$

C) $4CO_2 + 2H_2O + 2C_2H_2 + 5O_2$

D) $6CO_2 + 3H_2O + 3O_2$

E) $8CO_2 + 4H_2O + 2C_2H_2$

3. Metal hydrides react with water to form hydrogen gas and the metal hydroxide. For example:

$$SrH_2(s) + 2\ H_2O(l) \rightarrow Sr(OH)_2(s) + 2H_2\ (g)$$

You wish to calculate the mass of hydrogen gas that can be prepared from 5.63 g of strontium hydride and 4.80 g of water.

a.) If all of the strontium hydride reacts, how many moles of hydrogen gas will be produced?

b.) If all of the water reacts, how many moles of hydrogen gas will be produced?

c.) Which reactant is the limiting reactant? Explain.

d.) Calculate how many grams of hydrogen can be produced.

4. Freon-12 (CCl2F2) is synthesized by the reaction between carbon tetrachloride and antimony (III) fluoride at a temperature slightly above room temperature. Balance the following chemical equation (Hint: Balance F first.):

$$\_\_\_ \ CCl_4(l) + \_\_\_ \ SbF_3(s) \rightarrow \_\_\_ \ CCl_2F_2(g) + \_\_\_ \ SbCl_3(s)$$

Suppose 5.0 mol of antimony (III) fluoride is added to 10.0 mol of carbon tetrachloride. (Hint: Show via calculation which reactant is the limiting reagent.) How many moles of each species (CCl_4, SbF_3, CCl_2F_2, and $SbCl_3$) are there at the end if the reaction is 100% complete?

5. Calcium nitrate and ammonium fluoride react to form calcium fluoride, dinitrogen monoxide, and water vapor. What mass of each substance is present after 16.8 g of calcium nitrate and 17.50 g of ammonium fluoride react completely?

The Model: Percent Yield

When you bake a cake, some of the cake batter is left in the bowl in which it was mixed. When chemical reactions take place, losses of reactants and products due to transference make the obtained quantity of product less than what would be predicted based on the number of moles of the limiting reagent. Many reactions do not proceed 100% (i.e., products recombine to form the original reactants). Also some reactions result in unexpected "side products", which account for some of the mass that could have been found in the desired product. All of these errors lead to the **actual yield** (what is obtained) being less than the **theoretical yield** (that which is based on stoichiometry). The actual yield and theoretical yield are related by the **percent yield** of the reaction:

$$\%\ \boldsymbol{yield} = \frac{\boldsymbol{actual\ yield}}{\boldsymbol{theoretical\ yield}}\ \boldsymbol{x\ 100}\ \%$$

Exercises

6. What is the percent yield of a reaction in which 200. g of phosphorus trichloride reacts with excess water to form 128 g of HCl and aqueous phosphorous acid, H_3PO_3?

7. In order to synthesize nylon, adipic acid ($H_2C_6H_8O_4$ = 146.0 g/mol) must first be synthesized. Adipic acid is produced commercially by oxidizing cyclohexane (C_6H_{12}) at an elevated temperature:

$$2\ C_6H_{12}(l) + 5\ O_2(g) \rightarrow 2\ H_2C_6H_8O_4(l) + 2\ H_2O(g)$$

Such a synthesis typically takes place with a percent yield of 77.0%. If 1.00 kg of adipic acid is the goal, what is the minimum number of moles of oxygen gas that need to be passed through a body of liquid cyclohexane? (Ask yourself: "Is the mass „1.00 kg" an actual yield or a theoretical yield?")

8. Hydrogen fluoride may be produced by reacting calcium fluoride with sulfuric acid.

$$CaF_2\ (s) + H_2SO_4\ (aq) \rightarrow 2\ HF\ (g) + CaSO_4\ (s)$$

Suppose 29.2 g of calcium fluoride (Molar mass = 78.08 g/mol) is added to 48.3 g of sulfuric acid (98.09 g/mol). (Which reactant is the limiting reagent?) If 13.9 g of hydrogen fluoride (20.01 g/mol) are obtained, what is the percent yield for the synthesis?