Chemistry 201

Reaction Stoichiometry
Limiting Reagents

NC State University

Goals

- Calculate mass of solid reactants/products
- Calculate PVT of gaseous reactants/products
- Construct reaction tables
- Calculate % yield of a reaction
- Determine limiting reactants

Explanation and context

At this stage we are not yet posing the question whether a reaction will go to "completion" or not. We will simply assume that the reaction would produce 100% products if the reactants were present in the correct ratios. When the reactants are not present in the stoichiometric ratios then one of the reactants must be limiting. This is a useful concept and so we will develop it at this stage. But, keep in mind that reactions do not necessarily "go all the way". In reality, there is a chemical equilibrium that exists and may determine that a reaction goes only part way to products before coming to rest (equilibrium). At that point the reactants and products are in a dynamic state of interconversion, but there is no apparent change in the amount of either one. At this point we want to make reaction tables for the purpose of testing stoichiometric ratios.

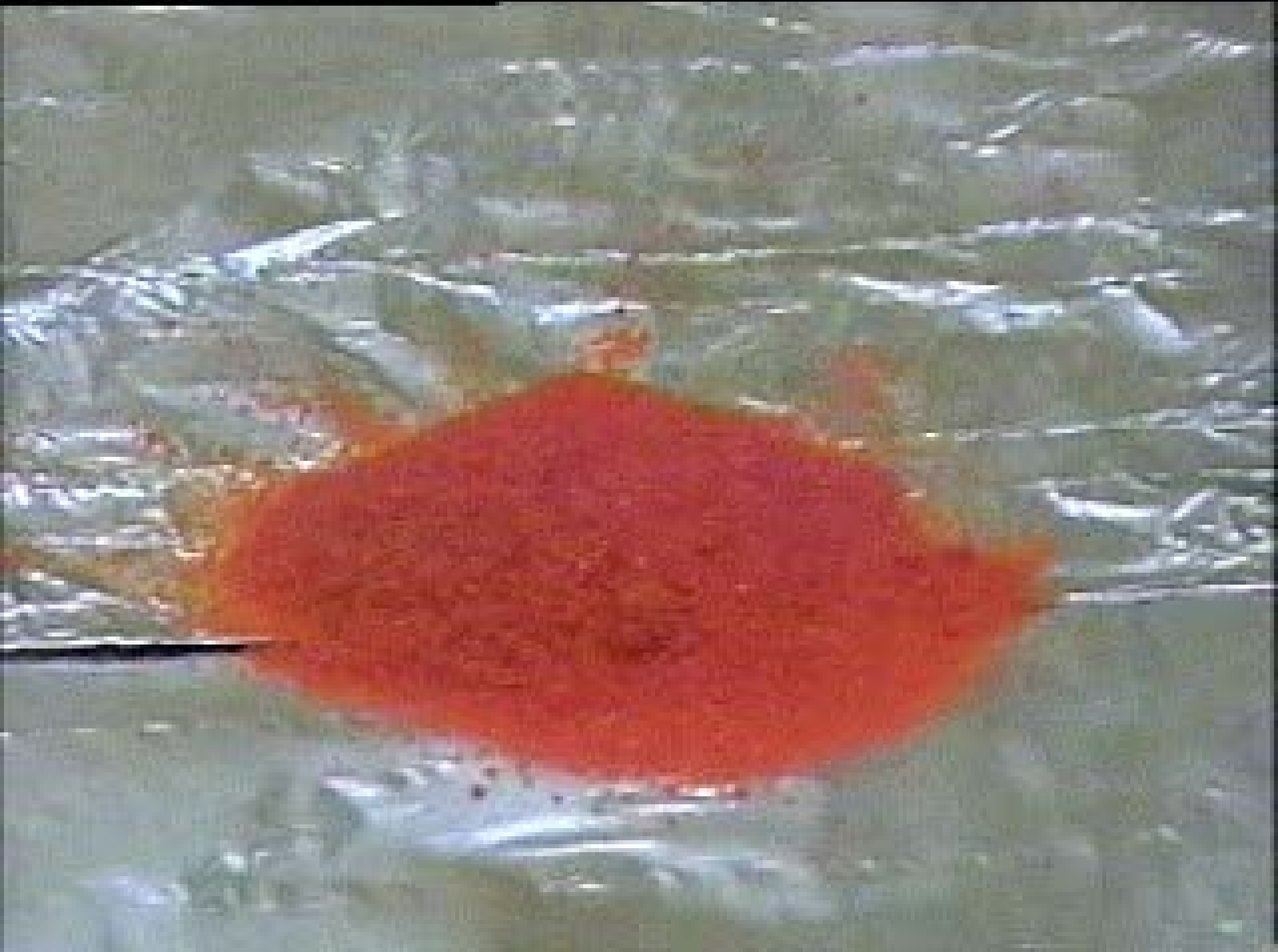
Example problem:
the chromium volcano

When 80.0 g of $(NH_4)_2Cr_2O_7$ decomposes what mass of solid remains?

The chromium volcano

- While the ammonium dichromate decomposes, it gives off orange sparks and throws the green chromium(III) oxide crystals into the air, producing an effect that looks like a miniature volcanic eruption.

- The chromium(III) oxide crystals that are produced are "fluffier" than the original ammonium dichromate crystals, and even though a lot of the mass of the starting materials escapes as vapor, the product looks like a larger amount of material.



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$$(NH_4)_2Cr_2O_7(s) \longrightarrow Cr_2O_3(s) + N_2(g) + 4H_2O(g)$$

Solution: Step 1. Determine the stoichiometric ratio. The solid that remains is Cr_2O_3, which has a 1:1 ratio with $(NH_4)_2Cr_2O_7$. Here we are making the assumption that the reaction proceeds to completion.

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Solution: Step 2.Calculate the relative mass of ammonium chromate and chromium oxide.

$(NH_4)_2Cr_2O_7 = 8(1) + 2(14) + 2(52) + 7(16)$

$= 252$ g/mol

$Cr_2O_3 = 2(52) + 3(16) = 152$ g/mol

The ratio is 152/252 = 0.60, so the mass is

(80.0 grams)(0.60) = 48 grams

Systematic method for determining yield

If we examine a typical reaction:

$$(NH_4)_2Cr_2O_7(s) \longrightarrow Cr_2O_3(s) + N_2(g) + 4H_2O(g)$$

We can give a systematic procedure for determining the yield of a product. Intrinsically, the yield is a molar yield, which is usually given in percentage. If one is given the mass of the starting material (as we were previously), one may calculate the mass of the product first using the stoichiometry and relative molar mass, but this takes the number of moles into account.

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We can give a systematic procedure for determining the yield of a product.

Step 1. Determine the number of moles of the reactant.

Step 2. Determine the stoichiometric ratio (i.e. how many moles of product are formed per mole of reactant).

Step 3. Convert the product moles to grams.

Determining reaction yield

What is the yield of the reaction if 80.0 g of $(NH_4)_2Cr_2O_7$ decomposes to form 32.0 g of Cr_2O_3?

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$(NH_4)_2Cr_2O_7(s) \longrightarrow Cr_2O_3(s) + N_2(g) + 4H_2O(g)$

Solution: Step 1. Calculate the number of moles of reactant: molar mass of $(NH_4)_2Cr_2O_7$ = 252 g/mol

$$n = \frac{m}{M} = \frac{80.0\ grams}{252\ g/mol} = 0.317\ moles$$

2. Step 2. The stoichiometric ratio is 1:1

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Determining reaction yield

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Solution: Step 3. The theoretical yield of Cr_2O_3 is 48.0 Grams. Therefore, the reaction yield is:

$$\%Yield = \frac{actual\ grams}{theoretical\ grams}100\% = \frac{32.0\ grams}{48.0\ grams}100\% = 67\%$$

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Determining the volume of a gaseous product

When 80.0 g of $(NH_4)_2Cr_2O_7$ decomposes what volume of N_2 is produced at 25 ^oC and 1 atm?

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Solution: 1. Calculate the number of moles of reactant: molar mass of $(NH_4)_2Cr_2O_7$ = 252 g/mol

$$n = \frac{m}{M} = \frac{80.0\ grams}{252\ g/mol} = 0.317\ moles$$

2. Use the ideal gas law to calculate the volume:

$$V = \frac{nRT}{P} \qquad V = \frac{(0.317\ mol)\left(0.08206\ \frac{Latm}{molK}\right)(298K)}{1\ atm}$$

V = 7.75 L

Determining reactant mass

What mass of $(NH_4)_2Cr_2O_7$ is required to produce 4.50 L of N_2 at 2.00 atm and 100.^oC?

$$(NH_4)_2Cr_2O_7(s) \longrightarrow Cr_2O_3(s) + N_2(g) + 4H_2O(g)$$

Solution: 1. Calculate the number of moles using the ideal gas law

$$n = \frac{PV}{RT} = \frac{(2\ atm)(4.5\ L)}{\left(0.08206\ \frac{Latm}{molK}\right)(373K)}$$

Therefore, n = 0.294 moles

2. Calculate the mass of 0.294 moles (given that the stoichiometry ratio is 1:1 for $(NH_4)_2Cr_2O_7:N_2$:

m = nM = (0.294 moles)(252 g/mol) = 74 grams

Determining the limiting reagent

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Solution:

The reaction is

$$SiCl_4 + 2\,Mg \rightarrow Si + 2\,MgCl_2$$

Determining the limiting reagent

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Step 1. Determine the limiting reagent.

$$n_{SiCl_4} = \frac{5.0\ g}{165.8 \frac{g}{mol}} = 0.0302\ moles$$

$$n_{Mg} = \frac{9.0\ g}{24.3 \frac{g}{mol}} = 0.370\ moles$$

Determining the limiting reagent

When 5.0 g of $SiCl_4$ react with 9.0 g of Mg, what is the theoretical yield of Si?

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The reaction is

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Step 2. Compare to the mole ratio to the stoichiometric ratio.

$$\frac{n_{Mg}}{n_{SiCl_4}} = \frac{0.370 moles}{0.0302\,moles} = 12.2$$

The mole ratio is Mg: $SiCl_4$ is 2. Therefore, Mg is in excess. $SiCl_4$ is the limiting reagent.

Determining the limiting reagent

When 5.0 g of $SiCl_4$ react with 9.0 g of Mg, what is the theoretical yield of Si?

Step 3. Use the number of moles of the limiting reagent to calculate the grams of product that can theoretically be obtained (theoretical yield).
Step 4. The ratio of SiCl4 to Si is 1:1 so the maximum number of moles of Si is 0.0302.
The mass of Si is:

$$m_{SiCl_4} = (0.0302\,mol)\left(28\frac{g}{mol}\right)$$

which corresponds to 0.846 grams of Si.
This is the theoretical yield.

How much Mg would remain unreacted?

How much Mg would remain unreacted?

Solution:

Step 1. Determine the number of moles Mg that actually reacted. The mole ratio is 2:1 so

$$n_{Mg} = (2)(0.0302\,moles)$$

or 0.0604 moles.

Step 2. Determine the number of moles that are unreacted

$$n_{Mg} = 0.370\,mol - \ 0.0604\,mol$$

which corresponds to 0.3096 moles of Mg.

Step. 3 Determine the mass to be 7.53 grams.

$$m_{Mg} = (0.31\,mol)\left(24.3\ \frac{gm}{mol}\right) = 7.53\ gm$$

Chemical equilibrium means that the reaction may not result in 100% yield

At this point, we cannot whether these reactions will proceed to completion. That depends on the equilibrium constant, and we have not calculated that yet. The yields calculated here are theoretical yields, i.e. the yield that would be obtained if the equilibrium is in favor of products.

We will show that the equilibrium constant can be calculated from tabulated values of the free energy for the reactants and products.