Introduction

We've discussed in class how we can relate the pressure, temperature, and volume of a gas to the number of moles of gas molecules present. This is a very practical relationship, as it is difficult to deal with measuring out specific masses of a gas to use in a chemical reaction. Imagine trying to weigh out 15 grams of oxygen gas on one of our analytical balances!

Since we know that the volume of a gas is proportional to the number of moles of gas present, we often discuss gas amounts using a volume - often, the volume of the gas at STP (0 ^oC, 1 atm pressure). We can use the **ideal gas equation**, though, to relate the number of moles of gas to the gas volume at **any** condition.

Stoichiometry problems involving gases

We discussed stoichiometry previously. All the concepts from then are still valid now, but we will deal with gaseous species in terms of their **volumes at a given set of conditions**, rather than the **mass in grams** of the gas. Let's look at an example.

Explosives: A sample stoichiometric calculation

You might have wondered what makes an explosive ... explosive. Why do explosives do so much damage to things when they're set off? The short answer is that many explosives are chemicals that can undergo rapid **decomposition** from a dense form to many small gas molecules. Ammonium nitrate, NH_4NO_3, is such a substance, and it will be the subject of our stoichiometry example.

When heated to approximately 300 ^oC, ammonium nitrate decomposes violently:

$$2\ NH_4NO_3(s) \rightarrow 2\ N_2(g) + O_2(g) + 4\ H_2O(g)$$

How many liters of each gas (at 25 ^oC and 1.00 atm) could be produced from the detonation of a 500. g bottle of NH_4NO_3? What is the total volume of gas (at the same conditions) produced?

This is a stoichiometry problem, and we solve it just like we'd solve any other stoichiometry problem. The **only** wrinkle here is that they've asked us about the **volume of gases** produced instead of the grams of a product. In this problem, we'll follow these steps:

1. **Convert** mass NH_4NO_3 to moles using the formula weight,
2. **Relate** moles NH_4NO_3 to moles of one of the gaseous products using the chemical equation.
3. **Convert** moles of gas to liters using the ideal gas equation. *This is the only step that is different from the types of problems you've already worked!*

First, **convert** the 500. grams of NH_4NO_3 to moles using the formula weight (80.05 g/mol).

$$500.\ g\ NH_4NO_3 \times \frac{1\ mol\ NH_4NO_3}{80.05\ g\ NH_4NO_3} = 6.25\ mol\ NH_4NO_3$$

We can now **find the number of moles of each gas** (N_2, O_2, H_2O) produced using the balanced chemical equation.

$$6.25\ mol\ NH_4NO_3 \times \frac{2\ mol\ N_2}{2\ mol\ NH_4NO_3} = 6.25\ mol\ N_2$$

$$6.25\ mol\ NH_4NO_3 \times \frac{1\ mol\ O_2}{2\ mol\ NH_4NO_3} = 3.13\ mol\ O_2$$

$$6.25\ mol\ NH_4NO_3 \times \frac{4\ mol\ H_2O}{2\ mol\ NH_4NO_3} = 12.5\ mol\ H_2O$$

Now we **convert** the number of moles of gas to volumes using the ideal gas equation. The conditions will be the same for each gas - the only thing that changes is the number of moles.

$$PV = nRT,\ \text{or} \quad V = \frac{n \times R \times T}{P}$$

P = 1.00 atm
V = ??? (trying to find this)
n = 6.25 mol N_2, 3.13 mol O_2, 12.5 mol H_2O

R = 0.08206 L·atm/mol·K (constant)
T = 25 °C = 298 K

Nitrogen:

$$V = \frac{(6.25\ mol\ N_2) \times (0.08206\ L \cdot atm/mol \cdot K) \times (298\ K)}{(1.00\ atm)} = \mathbf{153\ L\ N_2\ gas}$$

- V = **153 L N_2 gas**

Oxygen:

$$V = \frac{(3.13\ mol\ O_2) \times (0.08206\ L \cdot atm/mol \cdot K) \times (298\ K)}{(1.00\ atm)} = \mathbf{76.5\ L\ O_2\ gas}$$

- V = **76.5 L O_2 gas**

Water vapor:

$$V = \frac{(12.5\ \text{mol}\ H_2O) \times (0.08206\ \text{L} \cdot \text{atm} / \text{mol} \cdot \text{K}) \times (298\ \text{K})}{(1.00\ \text{atm})} = \mathbf{306\ L\ H_2O\ gas}$$

- V = **306 L H_2O vapor**

The problem also asks us for the **total volume of gas**. Gas volumes are additive, so this is the sum of all the individual volumes of gas: **536 L gas produced from the decomposition**.

If you'd been asked to calculate only the total gas volume and not each of the individual volumes, you could have added the moles of nitrogen gas, oxygen gas, and water vapor together and used the ideal gas law once.

<u>Explosions: Why are they damaging?</u>

This isn't part of the sample problem, but you might still be wondering why this reaction would be dangerous. The products are nitrogen, oxygen, and water vapor - all seemingly harmless substances.

To explain the hazard, let's look at volumes and pressures. Solid ammonium nitrate has a density of about 1.73 grams per mL at room conditions. So, 500 grams of ammonium nitrate solid takes up about 289 mL of space (0.289 L). The products of the decomposition take up 536 L of space - more than **1800 times the space**!

Assume our five hundred grams of ammonium nitrate was sealed in a pipe with an internal volume of 1.00 L - large enough for the solid with room to spare. After the decomposition, there are **21.9 moles of gas** total in the pipe (verify this). Assuming a temperature of 300 ºC in the pipe, let's find the pressure against the walls of the pipe. We can approximate this with the ideal gas equation.

$$PV = nRT, \quad P = \frac{n \times R \times T}{V}$$

P = ??? (trying to find this)
V = 1.00 L
n = 21.9 mol gas

R = 0.08206 L·atm/mol·K (constant)
T = 300. °C = 573 K

$$P = \frac{(21.9\ \text{mol}\ N_2) \times (0.08206\ \text{L} \cdot \text{atm} / \text{mol} \cdot \text{K}) \times (573\ \text{K})}{(1.00\ \text{L})} = \mathbf{1030\ atm}$$

- P = **1030 atm inside the pipe**

1030 atm is equal to about 15100 psi – well above the bursting pressure of common metal pipes.

Summary

This note pack deals with the stoichiometry of gases using an explosive as an example problem. Since we are often concerned with other properties of a gas rather than its mass, we can couple the ideal gas law to a stoichiometric calculation to determine amounts of gas in liters at a certain set of conditions. We can conceivably calculate the pressure, volume, or temperature of the gaseous product of a reaction if given the other two and the amount of starting material.