Moles of Reaction and Limiting Reactant

Consider the gaseous reaction: $N_2(g) + 3\,H_2(g) \longrightarrow 2\,NH_3(g)$

The smallest amount of reaction possible is that one (1) molecule of N_2 combines with three (3) molecules of H_2 to produce two (2) molecules of NH_3. When this simple reaction involving individual molecules occurs $6.022\text{x}10^{23}$ times, it is said that **one mole of reaction** has occurred. In this case (according to the equation above) one mole of reaction is the combination of 1 mole of N_2 with 3 moles of H_2 to produce 2 moles of NH_3. If 2 moles of N_2 combine with 6 moles of H_2 to produce 4 moles NH_3, that would be two moles of reaction.

The moles of reaction depend upon how the equation is written. If the equation is written as:

$$\tfrac{1}{2}\,N_2(g) + \tfrac{3}{2}\,H_2(g) \longrightarrow NH_3(g)$$

Then one mole of reaction would produce 1 mole of NH_3 from one-half mole of N_2 and one and one-half moles of H_2. Essentially one mole of reaction means the equation as written occurs <u>on the molecular level</u> $6.022\text{x}10^{23}$ (1 mole) times.

Consider again the equation: $N_2(g) + 3\,H_2(g) \longrightarrow 2\,NH_3(g)$

To react 2 moles of N_2 with 6 moles of H_2 would produce 2 moles of reaction. Or 3 moles of N_2 reacted with 9 moles of H_2 will produce 3 moles of reaction. And so on. In each case **the moles of reaction can be calculated by dividing the amount of reactant by its coefficient in the equation**. For example,

$$9 \text{ moles } H_2 = \text{? mol reaction}$$

$$9 \text{ mol } H_2 = 9 \text{ mol } H_2 \times \frac{1 \text{ mol reaction}}{3 \text{ mol } H_2} = 3 \text{ mol reaction}$$

Then the amount of product is determined by multiplying the coefficient of the product times the mole of reaction.

$$3 \text{ mol reaction} = \text{? mol } NH_3$$

$$3 \text{ mol reaction} = 3 \text{ mol reaction} \times \frac{2 \text{ mol } NH_3}{1 \text{ mol reaction}} = 6 \text{ mol } NH_3$$

Start the reaction with just 3 molecules of N_2 and 3 molecules of H_2.

NN + NN + NN + HH + HH + HH $\longrightarrow$?

One can see that 1 molecule of N_2 will combine with 3 molecules of H_2 to produce 2 molecules of NH_3.

NN + NN left over and $\overset{\text{H}}{\text{HNH}}$ + $\overset{\text{H}}{\text{HNH}}$ produced

The H_2 will be all used up and there will be 2 molecules of N_2 left over. N_2 is said to be **in excess** and H_2 is said to be **the limiting reactant**, because when one reactant runs out the reaction must stop. The extent of the reaction is limited by the reactant that disappears first.

Still using the equation: $N_2(g) + 3\,H_2(g) \longrightarrow 2\,NH_3(g)$

We need to be able to determine the limiting reactant when the reaction is scaled up to moles of reactants.

Problem 1. Starting with 3 moles of N_2 ($3\times6.022\text{x}10^{23}$ molecules) and 3 moles of H_2, determine which is the limiting reactant, and determine the maximum moles of NH_3 that can be produced. Calculate the moles of reaction for each reactant:

$$3 \text{ mole } N_2 \times \frac{1 \text{ mol rxn}}{1 \text{ mol } N_2} = 3 \text{ mol rxn} \qquad \textit{and} \qquad 3 \text{ mole } H_2 \times \frac{1 \text{ mol rxn}}{3 \text{ mol } H_2} = 1 \text{ mol rxn}$$

The reactant that provides the least moles of reaction is the limiting reactant. All reactants that provide more moles of reaction than the limiting reactant are in excess. When the limiting reactant is used up, there will be no more reaction. So **moles of reaction is determined by the limiting reactant.** In this case 1mol rxn (from H_2) < 3 mol rxn (from N_2), so the H_2 limits the reaction to 1 mole of reaction. The amount of product depends upon the (limiting) moles of reaction.

$$1 \text{ mol rxn} = ? \text{ mol } NH_3 \qquad 1 \text{ mol rxn} = 1 \text{ mol rxn} \times \frac{2 \text{ mol } NH_3}{1 \text{ mol rxn}} = 2 \text{ mol } NH_3$$

It is a little more complicated if reactant masses are given (instead of moles).

Problem 2. Starting with 100.0 g N_2 and 30.0 g H_2 determine the theoretical yield of NH_3 (maximum grams that can be produced) by the reaction: $\mathbf{N_2(g) + 3\ H_2(g) \longrightarrow 2\ NH_3(g)}$

Solution: First determine the limiting reactant. **To determine the limiting reactant, calculate moles of reaction for each reactant.** The reactant with smallest moles of reaction is limiting.

$$? \text{ mol rxn} = 100.\text{ g } N_2 \times \frac{1 \text{ mol } N_2}{28.01 \text{ g } N_2} \times \frac{1 \text{ mol rxn}}{1 \text{ mol } N_2} = 3.57 \text{ mol rxn}$$

$$? \text{ mol rxn} = 30.0 \text{ g } H_2 \times \frac{1 \text{ mol } H_2}{2.016 \text{ g } H_2} \times \frac{1 \text{ mol rxn}}{3 \text{ mol } H_2} = 4.96 \text{ mol rxn} > 3.57 \text{ mol so } N_2 \text{ limiting}$$

$$? \text{ g } NH_3 = 3.57 \text{ mol rxn} \times \frac{2 \text{ mol } NH_3}{1 \text{ mol rxn}} \times \frac{17.03 \text{ g } NH_3}{1 \text{ mol } NH_3} = 121.6 \text{ g } NH_3 \text{ produced (= theoretical yield)}$$

The amount of H_2 in excess (or left over) can be determined by subtracting the amount of H_2 used up from the initial amount of H_2. The amount used up depends upon the moles of reaction.

$$? \text{ g } H_2 \text{ used} = 3.57 \text{ mol rxn} \times \frac{3 \text{ mol } H_2}{1 \text{ mol rxn}} \times \frac{2.016 \text{ g } H_2}{1 \text{ mol } H_2} = 21.6 \text{ g } H_2 \text{ used}$$

so 30.0 g H_2 starting – 21.6 g H_2 used = 8.4 g H_2 remaining

Problem 3. 120.0 g Br_2 are mixed with 120.0 g F_2 and reacted according to the equation, $Br_2(g) + 5\ F_2(g) \longrightarrow 2\ BrF_5(g)$, until one of the reactants is used up. Calculate the maximum grams of BrF_5 that can be produced and which reactant and how any grams will be left over.

Problem 4. 200.0 g Cl_2 react with 300.0 g Fe_2O_3 according to the equation: $6\ Cl_2(g) + 2\ Fe_2O_3(s) \longrightarrow 4\ FeCl_3(s) + 3\ O_2(g)$, until one react is used up. Determine the theoretical yield of $FeCl_3(s)$, and which reactant and how grams will remain.

Problem 5. 94.0 g CaO is reacted with 94.0 g C(s) according to the equation: $2\ CaO(s) + 5\ C(s) \longrightarrow 2\ CaC_2(s) + 5\ CO_2(g)$, until one of the reactants is used up. Determine the theoretical yield of CaC_2 , and which reactant and how many grams will remain.

Answers:

3. (Br_2) mol rxn 0.751> **0.632 mol rxn** (F_2) $\Rightarrow$ 221. g BrF_5 ; 101.0 g Br_2 used $\Rightarrow$ 19.0 g remain

4. (Cl_2) **mol rxn 0.470**<0.939 mol rxn (Fe_2O_3) $\Rightarrow$ 304.9 g $FeCl_3$; 150.1 g Fe_2O_3 used $\Rightarrow$ 149.9 g left

5. (CaO) **mol rxn 0.838**<1.567 mol rxn (C) $\Rightarrow$ 107.4 g CaC_2 ; 50.3 g C used $\Rightarrow$ 43.7 g C left

Solutions.

3. $120.0\text{ g }Br_2 \times \frac{1\text{ mol }Br_2}{159.8\text{ g }Br_2} = 0.7509\text{ mol }Br_2 \times \frac{1\text{ mol rxn}}{1\text{ mol }Br_2} = 0.7509\text{ mol rxn}$

$120.0\text{ g }F_2 \times \frac{1\text{ mol }F_2}{38.00\text{ g }F_2} = 3.158\text{ mol }F_2 \times \frac{1\text{ mol rxn}}{5\text{ mol }F_2} = 0.6316\text{ mol rxn}$

$0.6316\text{ mol rxn} \times \frac{2\text{ mol }BrF_5}{1\text{ mol rxn}} \times \frac{174.9\text{ g }BrF_5}{1\text{ mol }BrF_5} = 220.9\text{ g }BrF_5$

$0.6316\text{ mol rxn} \times \frac{1\text{ mol }Br_2}{1\text{ mol rxn}} \times \frac{159.8\text{ g }Br_2}{1\text{ mol }Br_2} = 100.9\text{ g }Br_2\text{ used}$

so $120.0\text{ g }Br_2 - 100.9\text{ g }Br_2 = 19.1\text{ g }Br_2$ left

4. $200.0\text{ g }Cl_2 \times \frac{1\text{ mol }Cl_2}{70.91\text{ g }Cl_2} = 2.820\text{ mol }Cl_2 \times \frac{1\text{ mol rxn}}{6\text{ mol }Cl_2} = 0.4701\text{ mol rxn}$

$300.0\text{ g }Fe_2O_3 \times \frac{1\text{ mol }Fe_2O_3}{159.6\text{ g }Fe_2O_3} = 1.880\text{ mol }Fe_2O_3 \times \frac{1\text{ mol rxn}}{2\text{ mol }Fe_2O_3} = 0.9398\text{ mol rxn}$

$0.4701\text{ mol rxn} \times \frac{4\text{ mol }FeCl_3}{1\text{ mol rxn}} \times \frac{162.2\text{ g }FeCl_3}{1\text{ mol }FeCl_3} = 305.0\text{ g }FeCl_3$

mol rxn excess for Fe_2O_3 = 0.9398 – 0.4701 =

$0.4697\text{ mol rxn} \times \frac{2\text{ mol FeO}}{1\text{ mol rxn}} \times \frac{159.6\text{ g }Fe_2O_3}{1\text{ mol }Fe_2O_3} = 149.9\text{ g }Fe_2O_3$

Or once **moles** of reactants are calculated one can set up the problem as follows:

	$6\,Cl_2$	$+\ 2\,Fe_2O_3 \longrightarrow$	$4\,FeCl_3$	$+\ 3\,O_2$	
	0.4701	0.9398			moles of rxn = moles / coefficient
starting quantities (in moles)	2.820	1.880	0	0	
change line	–2.820	–0.9402	+1.880	+1.410	= coefficient ×0.4701
Final quantities (in moles)	0	0.9398	1.880	1.410	

$1.880\text{ mol }FeCl_3 \times \frac{162.2\text{ g }FeCl_3}{1\text{ mol }FeCl_3} = 304.9\text{ g }FeCl_3\text{ produced}$

$0.9398\text{ mol }Fe_2O_3 \times \frac{159.6\text{ g }Fe_2O_3}{1\text{ mol }Fe_2O_3} = 150.0\text{ g }Fe_2O_3\text{ remaining}$

5. $94.0\text{ g CaO} \times \frac{1\text{ mol CaO}}{56.08\text{ g CaO}} = 1.676\text{ mol CaO} \times \frac{1\text{ mol rxn}}{2\text{ mol CaO}} = 0.8381\text{ mol rxn}$

$94.0\text{ g Ca} \times \frac{1\text{ mol C}}{12.01\text{ g C}} = 7.827\text{ mol C} \times \frac{1\text{ mol rxn}}{5\text{ mol C}} = 1.565\text{ mol rxn}$

$$0.8381\text{ mol rxn} \times \frac{2\text{ mol CaC}_2}{1\text{ mol rxn}} \times \frac{64.10\text{ g CaC}_2}{1\text{ mol CaC}_2} = 107.4\text{ g CaC}_2$$

$$0.8381\text{ mol rxn} \times \frac{5\text{ mol C}}{1\text{ mol rxn}} \times \frac{12.01\text{ g C}}{1\text{ mol C}} = 50.3\text{ g C used}$$

so 94.0 g C –50.3 g C =43.7 g C left

Or $2\,CaO + 5\,C \longrightarrow 2\,CaC_2 + 5\,CO_2$

0.8381	1.565			= moles / coefficient = mol rxn (0.8381 is limiting)
1.676	7.827	0	0	= moles starting
–1.676	–4.191	+1.676	+4.191	= moles of change = coefficient × limiting mol rxn (0.8381)
0.0	3.636	+ 1.676	+4.191	= final moles

so $1.676\text{ mol CaC}_2 \times \frac{64.10\text{ g CaC}_2}{1\text{ mol CaC}_2} = 107.4\text{ g CaC}_2$ produced

and $3.636\text{ mol C} \times \frac{12.01\text{ g C}}{1\text{ mol C}} = 43.7\text{ g C}$ left