Percent Yield Calculations

Percent yield calculations are one of the most commonly used calculations in organic chemistry lab. Unfortunately the calculations are also one of the most common areas where students make mistakes. Understanding how to routinely and accurately carry out percent yield calculations will bolster understanding of the chemistry behind the calculation and simultaneously help improve grades.

Percent Yield calculations can be broken down into 4 simple steps.

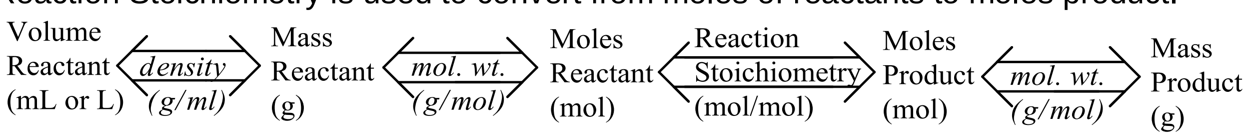
1. Determine the moles (not grams, not mLs) of each of the reactants.
2. Calculate how many moles of product can form based on the moles of each reactant. The stoichiometry of the equation must be used for this calculation. The reactant which will produce the smallest amount of the product is the limiting reagent. The limiting reagent is the starting material which will be depleted first. The amount of product formed from the limiting reagent is the theoretical maximum amount of product which can form.
3. Convert the theoretical maximum amount of product which can form in moles (from #2) into grams.
4. Determine the percent yield of the reaction by using knowledge of the actual grams of product formed and #3 above.

Many times steps one, two and three are done together in a single step using dimensional analysis. At the beginning it may be easier to do each step individually, but with experience conducting all three steps in tandem will become more efficient and simple.

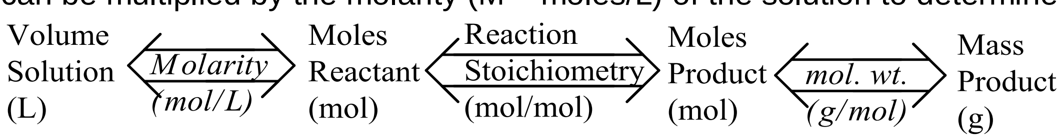
Three practice problems will be shown using both individual steps and tandem steps.

Reminders

* Density is used to convert from volume to mass.
* Molecular weight is used to convert from mass to moles.
* Reaction Stoichiometry is used to convert from moles of reactants to moles product.



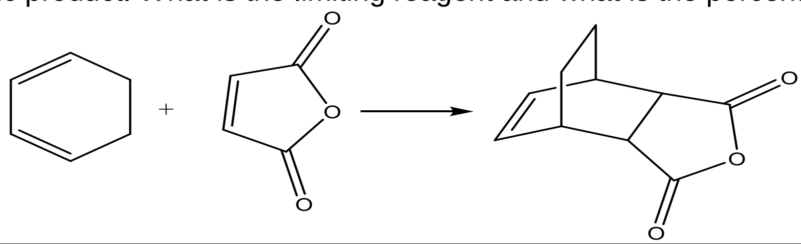
* If a solution as opposed to a neat liquid is used, then the volume (in liters) of solution used can be multiplied by the molarity (M = moles/L) of the solution to determine moles.



* The theoretical amount of product formed must be calculated using **moles** of limiting reagent (not grams, not mLs).
* Keep track of all units. Often when a student is unsure how to proceed, a close examination of the units will direct the correct next multiplication or division.
* Be very aware of the stoichiometry of the reaction.
* All data provided may not have to be used to determine answer.

Revised January 2011

Practice problem 1. One material measured as a solid (g) one material as a neat liquid (mL).
2.897 g of maleic anhydride (MA) is reacted with 2.56 mL of cyclohexadiene (CHD) to produce 3.979 grams of the bicyclic product. What is the limiting reagent and what is the percent yield?



name	cyclohexadiene (CHD)	maleic anhydride (MA)	5,6-anhydride [2.2.2]bicyclo-2-octene
density (g/ml)	0.8405	1.314	
mol. Wt. (g/mol)	80.15	98.06	178.20
volume (mL)	2.56	-	-
mass(g)	-	2.897	3.979

<u>Tandem steps 1,2&3.</u>
Steps one, two and three can be carried out at the same time.
This calculation must be carried out for all reactants.
For maleic anhydride

$$\underbrace{\frac{2.897\_g\_MA(g)}{} x \frac{1\_mole\_MA(mol)}{98.06grams\_MA(g)}}_{\text{Step 1}} x \underbrace{\frac{1\_mol\_Product}{1\_mol\_MA}}_{\text{Step 2}} x \underbrace{\frac{178.20\_grams\_product}{1\_mol\_Product}}_{\text{Step 3}} = 5.265\_grams\_Product$$

For cyclohexadiene

$$\underbrace{2.45\_mL\_CHD x \frac{0.845gCHD}{1\_mL\_CHD} x \frac{1\_moles\_CHD}{80.15\_g\_CHD}}_{\text{Step 1}} x \underbrace{\frac{1\_moles\_product}{1\_mole\_CHD}}_{\text{Step 2}} x \underbrace{\frac{178.20grams\_product}{1\_mole\_product}}_{\text{Step 3}} = 4.78\_g\_Product$$

Since 4.78 is smaller than 5.265, cyclohexadiene is the limiting reagent and 4.78 g is the theoretical maximum amount of product which can form.

<u>Individual steps</u>
<u>Step 1</u>. Alternatively steps one, two and three may be done individually. Determine the moles of all reagents.
-If the reagent is in grams then just use the molecular weight to convert to moles.
-If the reagent is in volume, then use density, then molecular weight to convert to moles.
-Keep track of all units to ensure the correct multiplication is taking place.

$$\frac{2.897\_g\_MA}{} x \frac{1\_mole\_MA}{98.06\_grams\_MA} = 2.954x10^{-2} moles\_MaleicAnhydride$$

$$\frac{2.56\_ml\_CHD}{} x \frac{0.8405\_g\_CHD}{1\_ml\_CHD} x \frac{1\_mole\_CHD}{80.15\_g\_CHD} = 2.68x10^{-2} moles\_Cyclohexadiene$$

<u>Step 2</u>. Calculate how many moles of a product can be formed based on the moles of each reactant. The reaction stoichiometry must be used. This reaction has a 1:1 stoichiometry. Determine the

limiting reagent.

$$\frac{2.954x10^{-2} moles\_MA}{} x \frac{1\_moles\_product}{1\_mole\_MA} = 2.954x10^{-2}\_moles\_Product(fromMA)$$

$$\frac{2.68x10^{-2} moles\_CHD}{} x \frac{1\_moles\_product}{1\_mole\_CHD} = 2.68x10^{-2}\_moles\_Product(fromCHD)$$

The reactant which will product the smallest amount of product is the limiting reagent.
Since 2.68x10^{-2} is smaller than 2.954x10^{-2}, cyclohexadiene is the limiting reagent in this problem.

Step 3. Using the moles of product which form from the limiting reagent , determine the grams of product that can form. This amount is the theoretical maximum of product.

$$\frac{2.68x10^{-2} moles\_Product}{} x \frac{178.20\_grams\_product}{1\_mole\_product} = 4.78\_grams\_Product$$

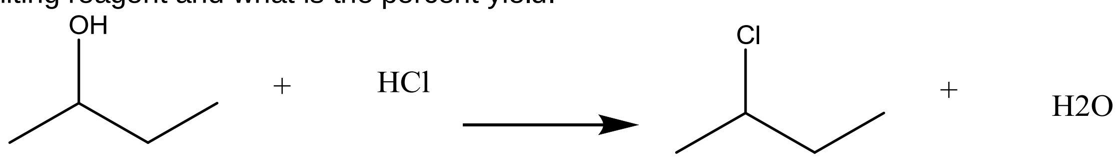
Both methods give the same answer. Initially students may want to carry out the steps individually, but the tandem method is more efficient.

Step 4. Using knowledge of actual amount of product formed, calculate the % yield.

$$\frac{Actual\_Mass\_Product\_Formed(g)}{Theoretical\_Maximum\_Mass\_Product(g)} x100\% = \%yield\_Product$$

$$\frac{3.979\_g\_Product}{4.78\_g\_product} x100\% = 83.2\_\%\_yield\_Product$$

Practice Problem 2. One material measured as a solution (M) one as a mass (g).
4.24 mL of 2-butanol is reacted with 10.2 mL of 6.0 M HCl to form 2.8798 grams of 2-chlorobutane. What is the limiting reagent and what is the percent yield.



name	2-butanol (BuOH)	Hydrochloric Acid (6.0 M)	2-chlorobutane	Water
density (g/ml)	0.81	1.314		1.00
mol. Wt. (g/mol)	74.1	36.5	92.6	18.00
volume (mL)	4.24	10.2	-	
mass(g)	-	-	2.8798	

Tandem steps 1,2 and 3

$$\frac{4.24\_ml\_BuOH}{} x \frac{0.810\_g\_BuOH}{1\_ml\_BuOH} x \frac{1\_mole\_BuOH}{74.1\_g\_BuOH} x \frac{1\_mol\_product}{1\_mol\_BuOH} x \frac{92.6\_g\_Prod}{1\_mol\_Prod} = 4.28grams\ Product$$

$$\frac{10.2\_ml\_HCl}{} x \frac{1L\_HCl}{1000\_ml\_HCl} x \frac{6.0\_mol\_HCl}{1\_L\_HCl} x \frac{1\_mol\_product}{1\_mol\_HCl} x \frac{92.6\_g\_Prod}{1\_mol\_Prod} = 5.7\_grams\ Product$$

Since 4.28 is less than 5.7, 2-butanol is the limiting reagent and the maximum theoretical amount of product which can form is 4.28 g.

Individual steps Step 1. Determine the moles of all reagents.
-If the reagent is in grams then just use the molecular weight to convert to moles.
-If the reagent is in volume, then use density, then molecular weight to convert to moles.
- If the reagent is in volume with a set molartiy, then use volume and molarity to determine moles. Remember Molarity has units of mole/Liter

Moles of 2-butanol

$$\frac{4.24\_ml\_2-BuOH}{} x \frac{0.810\_g\_BuOH}{1\_ml\_BuOH} x \frac{1\_mole\_BuOH}{74.1\_g\_BuOH} = 4.63x10^{-2} moles\_2-Bu\tan ol$$

Moles of HCl

$$\frac{10.2\_ml\_HCl}{} x \frac{1\_L\_HCl}{1000\_mL\_\_HCl} x \frac{6.0\_mole\_HCl}{1\_L\_HCl} x = 6.1x10^{-2} moles\_HCl$$

Step 2. Calculate how many moles of a product can be formed based on the moles of each reactant. The reaction stoichiometry must be used. This reaction has a 1:1 stoichiometry. Determine the limiting reagent.

$$\frac{4.63x10^{-2} moles\_BuOH}{} x \frac{1\_moles\_product}{1\_mole\_BuOH} = 4.63x10^{-2}\ \_moles\_\Pr oduct$$

$$\frac{6.1x10^{-2} moles\_HCl}{} x \frac{1\_moles\_product}{1\_mole\_HCl} = 6.1x10^{-2}\ \_moles\_\Pr oduct$$

The reactant which will product the smallest amount of product is the limiting reagent.
Since 4.63x10^{-2} is smaller than 6.1x10^{-2}, 2-butanol is the limiting reagent.

Step 3. Using the moles of the limiting reagent ,determine the theoretical maximum grams of product that can form. Keep track of units to avoid errors.

$$\frac{4.63x10^{-2} moles\_\Pr oduct}{} x \frac{92.6\_grams\_product}{1\_mole\_product} = 4.28\_grams\_product$$

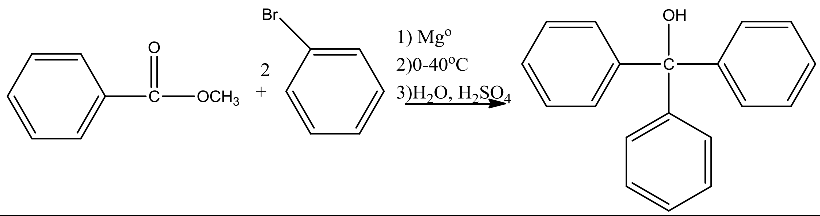
This same answer was obtained when the steps were carried out sequentially.

Step 4. Using knowledge of actual amount of product formed, calculate the % yield.

$$\frac{Actual\_Mass\_\Pr oduct\_Formed(g)}{Theoretical\_Maximum\_Mass\_\Pr oduct(g)} x100\% = \% yield\_\Pr oduct$$

$$\frac{2.8798\_g\_\Pr oduct}{4.28\_g\_product} x100\% = 67.3\_\%\_yield\_2-ChloroBu\tan e$$

Practice Problem 3. Non 1 :1 stoichiometry. Both materials measured as a neat liquid (mL).
7.3 mL of methylbenzoate is reacted with 10.0 mL of bromobenzene in an excess of magnesium shavings and an acid work-up to produce triphenylmethanol. What is the limiting reagent, the theoretical maximum amount of product which can form, and the percent yield? (An excess of magnesium is used.)



name	methyl benzoate (MB)	Bromobenzene (BrB)	triphenylmethanol
density (g/ml)	1.09	1.50	
mol. Wt. (g/mol)	136.1	157.02	260.3
volume (mL)	7.3	10.0	-
mass(g)	-	-	10.655

Tandem steps 1,2 and 3

$$\frac{7.3\_ml\_MB}{} x \frac{1.09\_g\_MB}{1\_ml\_MB} x \frac{1\_mole\_MB}{136.1\_g\_MB} x \frac{1\_mol\_Prod}{1\_mol\_MB} x \frac{260.5\_g\_Prod}{1\_mol\_prod} = 15\_g\_Product$$

$$\frac{10.0\_ml\_BrB}{} x \frac{1.50\_g\_BrB}{1.00\_mL\_BrB} x \frac{1\_mol\_BrBe}{157.02\_g\_BrB} x \frac{1\_mol\_Prod}{2\_mol\_BrB} x \frac{260.5\_g\_Prod}{1\_mol\_Prod} = 12.5\_g\_Product$$

Because 12.5 is smaller than 15, bromobenzene is the limiting reagent and the theoretical maximum amount of product which can form is 12.5 grams.

IndividuallyStep 1. Determine the moles of all reagents.
-If the reagent is in volume, then use density, then molecular weight to convert to moles.
-If the stoichiometry is not 1:1 pay close attention when calculating the limiting reagent.
-Keep vigilant concerning units.
-It is not necessary to calculate this for magnesium since it was used in excess.

$$\frac{7.3\_ml\_MeBenzoate}{} x \frac{1.09\_g\_MeBenzoate}{1\_ml\_MeBenzoate} x \frac{1\_mole\_MeBenzoate}{136.1\_g\_MeBenzoate} = 5.8x10^{-2} moles\_Methyl\_Benzoate$$

$$\frac{10.0\_ml\_Br-Benzene}{} x \frac{1.50\_g\_Br-Benzene}{1.00\_mL\_Br-Benzene} x \frac{1\_mol\_Br-Benzene}{157.02\_g\_BrBenzene} = 9.55x10^{-2} moles\_BromoBenzene$$

Step 2. Calculate how many moles of a product can be formed based on the moles of each reactant. The reaction stoichiometry must be used. Determine Limiting Reagent.
This reaction does NOT have a 1:1 stoichiometry in regard to all reactants. Examine the reaction.

$$\frac{5.8x10^{-2} moles\_MB}{} x \frac{1\_moles\_product}{1\_mole\_MB} = 5.8x10^{-2}\_moles\_Product$$

$$\frac{9.55^{-2} moles\_BrB}{} x \frac{1\_moles\_product}{2\_mole\_BrB} = 4.78x10^{-2}\_moles\_Product$$

4.78 x 10^{-2} is smaller than 5.8 x 10^{-2}, therefore Bromobenzene is the limiting reagent. Note that the limiting reagent in this case is the reagent which is present in the larger volume.

Step 3. Using the moles of the limiting reagent , determine the theoretical maximum grams of product that can form. Keep track of units to avoid errors.

$$\frac{4.78x10^{-2} moles\_MethylBenzoate}{} x \frac{1\_moles\_Triphenylmethanol}{1\_mole\_MethylBenzoate} x \frac{260.5\_g\_Triphenylmethanol}{1\_mole\_Triphenylmethanol} = 12.5\_grams\_produc$$

Step 4. Using knowledge of actual amount of product formed, calculate the % yield.

$$\frac{Actual\_Mass\_Product\_Formed(g)}{Theoretical\_Maximum\_Mass\_Product(g)} x100\% = \frac{10.655\_g\_Product}{12.5\_g\_product} x100\% = 85.2\_\%\_yield$$