Stoichiometry:

Calculations with Chemical Equations

Objectives

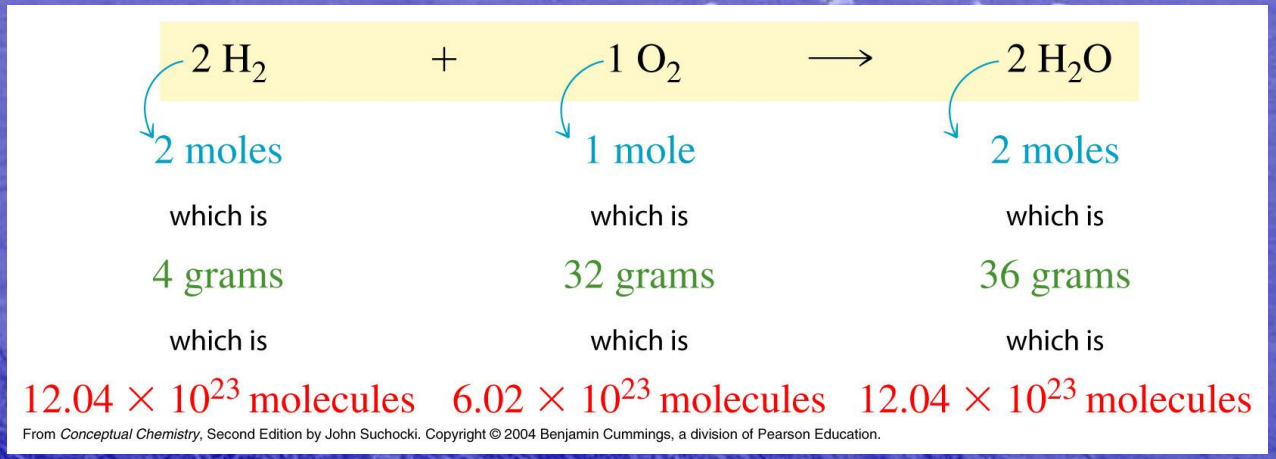
- Use chemical equations to predict amount of product from given reactants
- Determine percentage yield
- Determine limiting reactant

Working with equations: STOICHIOMETRY

- Predict how much product is obtained from given amount of reactant
- Predict how much reactant is needed to give required amount of product
- Predict how much of one reactant is required to give optimum result with given amount of another reactant

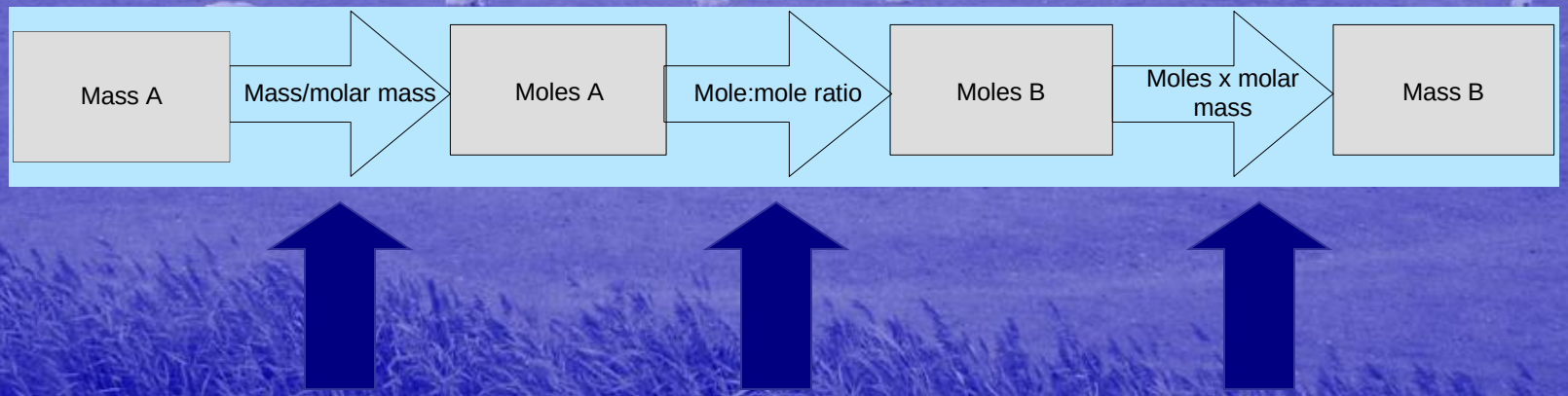
Relating moles, masses and molecules

- Note:
- Conservation of mass (4 g + 32 g = 36 g)
- But not necessarily conservation of moles (2 moles + 1 mole = 2 moles)



Stoichiometry with equations: The roadmap

- Equations are in moles, but we measure in *grams*
- Three conversions required:
- A is given substance; B is target substance
  1. Must convert grams A to moles A using molar mass
  2. Use coefficients in equation to get moles B from moles A
  3. Convert moles B to grams B using molar mass

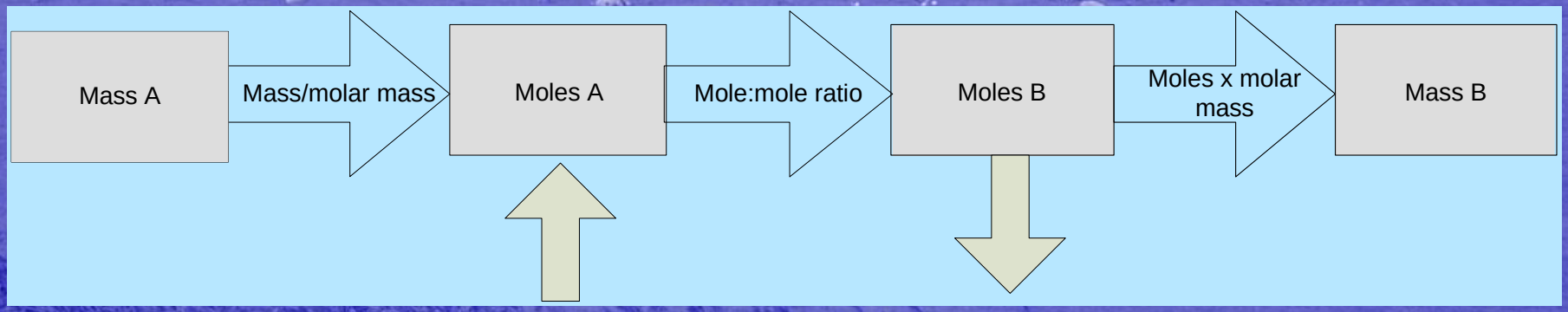


Types of problems: Moles A → moles B

$$aA + bB = cC + dD$$

- Single step
- Mole:mole ratio:
- *a* mol A ≡ *b* mol B
- Target/given

$$\frac{moles\ B}{moles\ A} = \frac{b}{a}\ mol\ B / mol\ A$$



Mole:mole ratio problems

- $CH_4 + 2O_2 = CO_2 + 2H_2O$
- How many moles of H_2O are produced from 5 moles of CH_4?

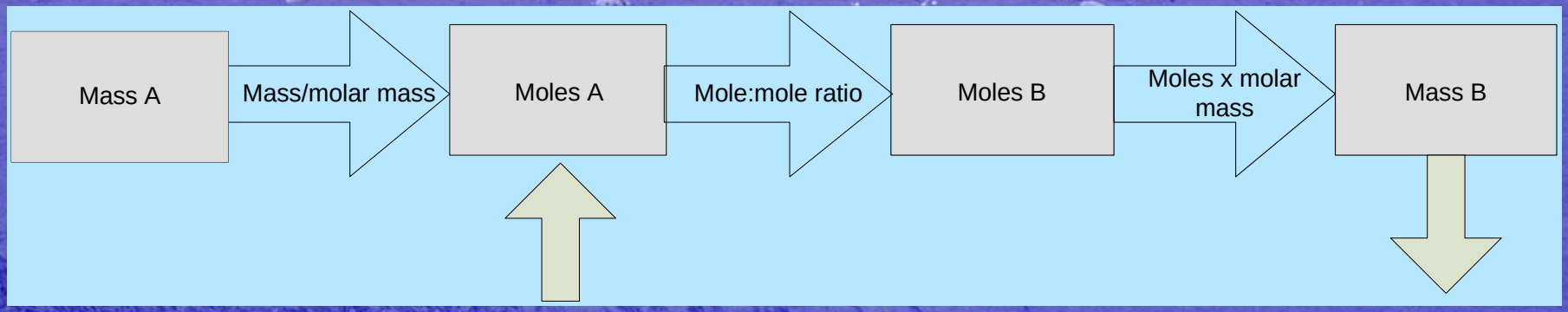
Moles A → mass B

1. Convert moles A → moles B:

   Mole:mole ratio (target/given):

$$\frac{moles\ B}{moles\ A} = \frac{b}{a}\ mol\ B / mol\ A$$

2. Convert moles B → mass B using molar mass B

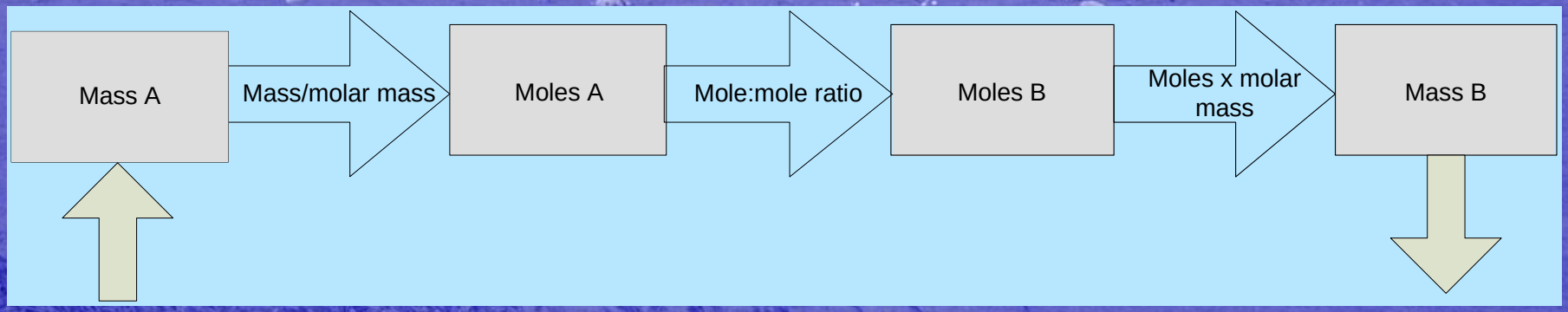


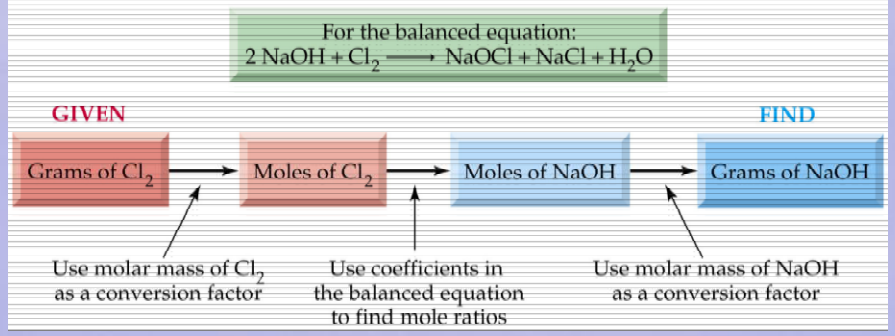
Mole:mass/mass:mole problems

- $CH_4 + 2O_2 = CO_2 + 2H_2O$
- What mass of H_2O is produced from burning 5 moles CH_4?

Mass A → mass B

1. Mass A → moles A using molar mass A
2. Moles A → moles B using mole:mole ratio
3. Moles B → mass B using molar mass B





- Molar mass Cl_2 = 35.5 x 2 = 71.0 g/mol
- Molar mass NaOH = 23.00 + 16.00 + 1.01 = 40.01 g/mol

Summary of stoichiometry problems

- Maximum of three conversions required
  1. Must convert grams A to moles A using molar mass
  2. Use coefficients in equation to get moles B from moles A
  3. Convert moles B to grams B using molar mass
- Maximum of three pieces of information required
  1. Molar mass of given substance (maybe)
  2. Molar mass of target substance (maybe)
  3. Balanced chemical equation (always)

Work this example

- $CH_4 + 2O_2 = CO_2 + 2H_2O$

- What mass of CO_2 is produced by the complete combustion of 16 g of CH_4
  - Atomic weight H = 1, C = 12, O = 16

44 g

- Do stoichiometry exercises

Reaction Yield

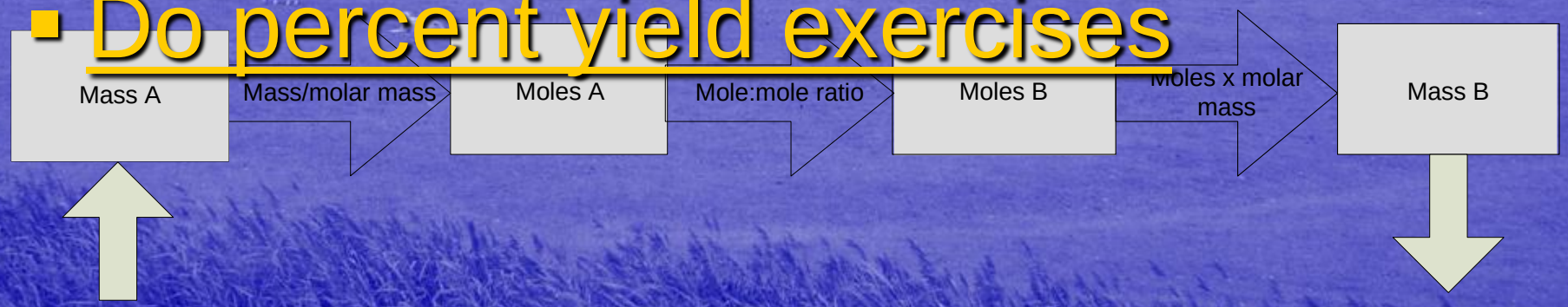
- Actual yield from chemical reaction is normally less than predicted by stoichiometry.
  - Incomplete reaction
  - Product lost in recovery
  - Competing side reactions
- Percent yield is:

Actual yield/Theoretical yield x 100 %

Worked example

- *Actual* yield of product is 32.8 g after reaction of 26.3 g of C_4H_8 with excess CH_3OH to give $C_5H_{12}O$.
- What is theoretical yield? Use stoichiometry to get mass of product:

  convert mass (26.3 g) ⇨ moles ⇨ moles ⇨ mass
- *Theoretical* yield = 41.4 g
- Percent yield = 32.8/41.4 x 100 %
- **Do percent yield exercises**



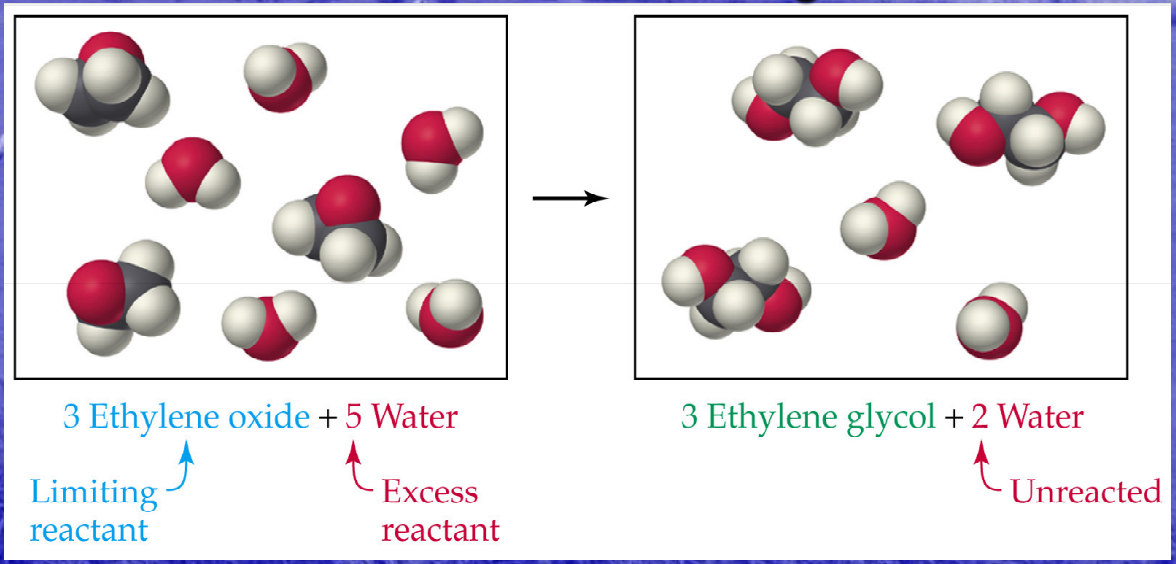
Percent yield practice

Limiting Reactant

- Exact quantities of reactants dictated by the reaction stoichiometry are not the norm
- Usually one reactant is reacted with an excess of the other(s)
  - Burning natural gas in furnace
- This reactant is the *limiting reactant* – amount of products limited by this reactant

Limiting reactant at molecular level

- In the reaction to produce ethylene glycol:
  - 1 mole of ethylene oxide + 1 mole of water → 1 mole glycol
- Here, 2 moles of water remain after conversion of all ethylene oxide into glycol
  - Ethylene oxide is limiting
- More product would be obtained by increasing the ethylene oxide until the water became limiting



Determination of limiting reactant

- Two methods:
- Brute Force
  - Calculate quantity of product from each reactant in turn
- Elegant
  - Compare reaction stoichiometry with actual reactant mole ratios

The Brute Force method

- 30 g CH_4 and 30 g O_2 are reacted. Which is the limiting reactant? How much CO_2 is produced?

$$CH_4 + 2\ O_2 = CO_2 + 2\ H_2O$$

- You could calculate mass of CO_2 *or* H_2O – it doesn't matter

The elegant approach

- Reaction aA + bB = products
  - Stoichiometric mole ratio reactants = a/b
- Actual ratio of reactants = a'/b'
    - If a'/b' > a/b, B is limiting
    - If a'/b' < a/b, A is limiting
- <u>Do limiting reagent exercises</u>

Case of three (or more) reactants

- Determine theoretical molar ratios for each pair based on reaction stoichiometry

  a/b a/c b/c…

- Calculate actual molar ratios for all reactant pairs:

  a’/b’ a’/c’ b’/c’…

- The smallest ratio compared to the theoretical will identify limiting reactant

Practice limiting reactant with three or more reactants