Quantitative skills

Problem Solving is a skill that you will need to develop for all aspects of your degree in Chemistry. It applies equally to solving problems with a **numerical** answer (**quantitative** result) or with a **conceptual** answer (**qualitative** result).

What are the key steps to solving a problem?

- **Understand the question:** What am I being asked to work out?
- **Consider the context**: What information and/or restrictions have I been given?
- **Choose a method**: What formula or approach can I use to answer the question? Is this method appropriate to the context of the question?
- **Interpret the result:** Does my answer make sense? Does it answer the question? Does it meet the criteria set out in the question?

This is a **cycle** where steps can/should be repeated until a final result is achieved.

How do you write a quantitative result?

Scientific notation

$$p = 1.00 \text{ x } 10^5 \; Pa$$

Vector or Scalar?

- A **scalar** quantity only has a magnitude (size)
    - *Examples*: Energy, wavelength, work
    - Variables in *italics* are scalars: E, λ, W
- A **vector** is a quantity that has both magnitude (size) and direction.
    - *Examples*: Force, momentum, electric field
    - Variables in **bold** are vectors: **F**, **p**, **E**
    - We often define vectors in term of components within a given coordinate system.

      Example: the position vector which describes a location in 3D space can be expressed in Cartesian coordinates: $\mathbf{r} = \{x, y, z\}$

How do you know if the result makes sense?

Units

- **All** quantitative answers have **two** parts: the **numerical** part and the **units**.
- **All** quantitative answers **must** be reported with the appropriate **units**.
- The **absence of units** means that the quantity is **dimensionless.** That means that the physical quantity being reported <u>has no units</u>.
    - *Examples:* quantum number, order of a reaction, absorbance
- Sometimes experimentally measured quantities have **arbitrary units**. In this case, quantitative results are obtained through calibration or an internal reference.
    - *Example*: intensity in an NMR spectrum

Order of magnitude

- How big do you expect the answer to be?
- Do not forget to consider the unit prefix!

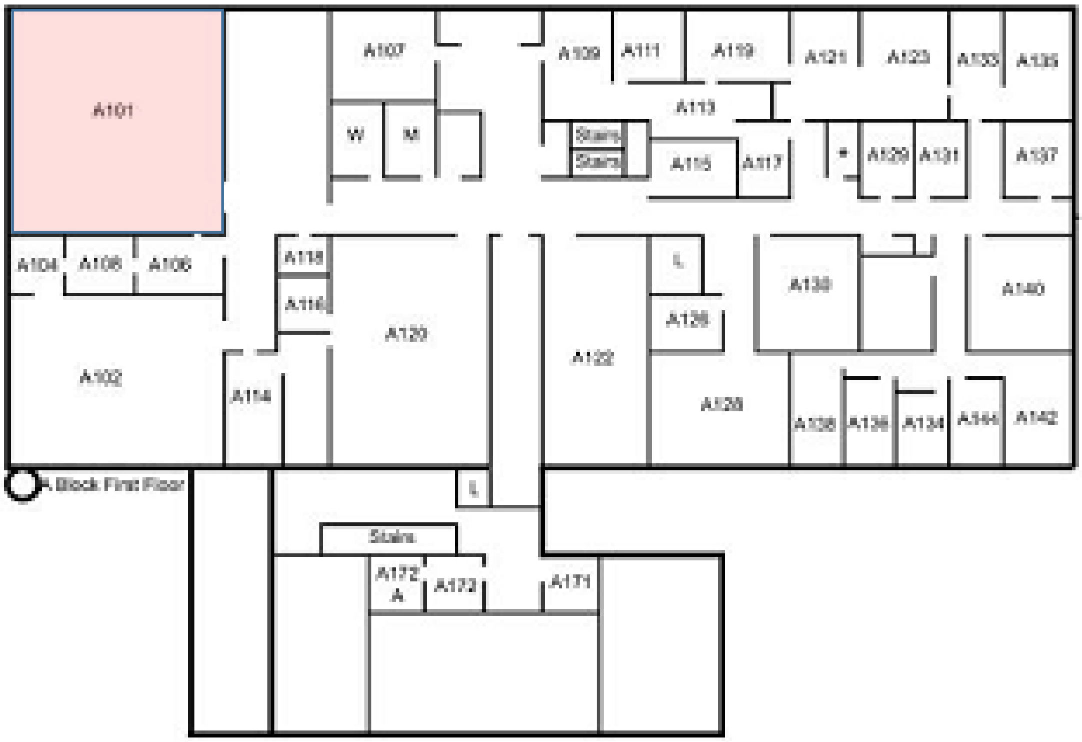
Sign/Direction

- Should my answer be positive or negative?
- For vector quantities, does the direction make sense?

Significant figures

- How precise is my answer? How many decimal places should I use?

Example 1: Estimate the volume of room C/A 101



Step 1. Understand the question

Volume

Step 2. Consider the context

Estimate (no dimensions given)

Step 3. Choose a method

Assume a simple rectangular box

V = length x width x height

Step 4. Interpret the result

Consider the potential solutions to this problem listed below. Which answers can immediately be eliminated? Why?

a) $V = 1.5$ km wrong unit (distance!)

b) $V = 120$ L too small!

c) $V = 250\ cm^3$ too small!

d) $V = 500$ no units

e) $V = 100\ m^2$ wrong units (area)

f) $V = 20\ km^3$ too large!

g) $V = -250\ m^3$ cannot be negative

h) $V = 2 \times 10^5\ nm^3$ too small!

i) $V = 1000\ dm^3$ too small!

j) $V = 8.5 \times 10^5$ L reasonable ($850\ m^3$)

k) $V = 1000\ m^3$ reasonable

l) $V = 1.2 \times 10^4\ m^3$ too large

Unit Conversion

Table 1. SI base units

quantity	unit	symbol
mass	kilogram	kg
time	second	s
distance	meter	m
temperature	kelvin	K
electric current	ampere	A
amount of a substance	mole	mol
luminous intensity	candela	cd

Table 2. Common units

quantity	unit	Symbol for SI unit	SI base units
frequency	hertz	Hz	s^{-1}
force	newton	N	$kg\ m\ s^{-2}$
pressure	pascal	Pa	$kg\ m^{-1}\ s^{-2}$ (= $N\ m^{-2}$)
energy	joule	J	$kg\ m^{2}\ s^{-2}$ (= N m)
temperature	kelvin	K	K
electric charge	coulomb	C	A s
electric potential	volt	V	$kg\ m^{2}\ s^{-3}\ A^{-1}$ (= $J\ C^{-1}$)
capacitance	farad	F	$kg^{-1}\ m^{-2}\ s^{4}\ A^{2}$ (= $C\ V^{-1}$)
resistance	ohm	Ω	$kg\ m^{2}\ s^{-3}\ A^{-2}$ (= $V\ A^{-1}$)
power	watt	W	$kg\ m^{2}\ s^{-3}$ (= $J\ s^{-1}$)

Table 3. Metric System Prefix Table

Prefix	Symbol	Multiplier	Exponential
tera	T	1,000,000,000,000	10^{12}
giga	G	1,000,000,000	10^{9}
mega	M	1,000,000	10^{6}
kilo	k	1,000	10^{3}
hecto	h	100	10^{2}
deca	da	10	10^{1}
-	-	1	10^{0}
deci	d	0.1	10^{-1}
centi	c	0.01	10^{-2}
milli	m	0.001	10^{-3}
micro	µ	0.000001	10^{-6}
nano	n	0.000000001	10^{-9}
pico	p	0.000000000001	10^{-12}
femto	f	0.000000000000001	10^{-15}

Table 4. Some common non-SI units

Name	Symbol	Quantity	Definition
calorie	cal	energy	4.184 J
angstrom	Å	distance	10^{-10} m
mile	mi	Distance	1609 m
Celsius	°C	temperature	$T\ (°\mathrm{C}) = T(\mathrm{K}) - 273.15$
minute	min	time	60 s
hour	h or hr	time	3600 s
day	d	time	86 400 s
litre	L	volume	1 dm^3 = 10^{-3} m^3
tonne	t	mass	1 t = 10^3 kg
atmosphere	atm	pressure	1.013 x 10^5 Pa

Unit conversion guide

Step 1: Determine the relationship between the current unit and the desired unit. Refer to Tables 1 - 4 for useful unit relationships.

e.g. 1000 mL = 1 L; 10^3 mg = 1 g = 10^{-3} kg; 1 hr = 60 min; 1 mL = 1 cm^3

Step 2: Convert the relationship from (step 1) to a fraction with the desired unit on top and the current unit on the bottom.

Conversion from L to mL:

$$\frac{1000\ \text{mL}}{1\ \text{L}}$$

Conversion from kg to mg:

$$\frac{1\ \text{g}}{1\ \text{g}} = \frac{10^3\ \text{mg}}{10^{-3}\ \text{kg}} = \frac{10^6\ \text{mg}}{1\ \text{kg}}$$

Conversion from minutes to hours:

$$\frac{1\ \text{hr}}{60\ \text{min}}$$

Conversion from cm^3 to mL

$$\frac{1\ \text{mL}}{1\ \text{cm}^3}$$

Step 3: To change multiple units at once, or to change a single unit in multiple steps, generate a conversion fraction for each desired change in unit and multiply together. If the unit is expressed with a power > 1, apply the same power to the entire fraction.

Conversion from cm^3 to L in two steps

$$\frac{1\ \text{mL}}{1\ \text{cm}^3} \times \frac{1\ \text{L}}{1000\ \text{mL}} = \frac{1\ \text{L}}{1000\ \text{cm}^3}$$

Conversion from m^2 to mm^2

$$\left(\frac{10^3\ \text{mm}}{1\ \text{m}}\right)^2 = \frac{10^6\ \text{mm}^2}{1\ \text{m}^2}$$

Step 4: Multiply the quantity by the conversion fraction(s). The old unit will cancel leaving the new desired unit. This is equivalent to multiplying by 1 because the top and bottom of the conversion factions are (by design) equal.

Conversion from 0.25 L to mL:

$$0.25\ \mathrm{L}\ \times \frac{1000\ \mathrm{mL}}{1\ \mathrm{L}} = 250\ \mathrm{mL}$$

Conversion from 3.45 x 10^{-4} kg to mg:

$$3.45\ \mathrm{x}\ 10^{-4}\ \mathrm{kg} \times \frac{10^{6}\ \mathrm{mg}}{1\ \mathrm{kg}} = 3.45\ \mathrm{x}\ 10^{2}\ \mathrm{mg} = 345\ \mathrm{mg}$$

Conversion from 275 minutes to hours:

$$275\ \mathrm{min}\ \times \frac{1\ \mathrm{hr}}{60\ \mathrm{min}} = 4.58\ \mathrm{hrs}$$

Conversion from 256 cm^3 to L in two steps

$$256\ \mathrm{cm}^3 = \frac{1\ \mathrm{mL}}{1\ \mathrm{cm}^3}\frac{1\ \mathrm{L}}{1000\ \mathrm{mL}} = 0.256\ \mathrm{L}$$

Conversion from 6.43 x 10^{-7} m^2 to mm^2

$$6.43 \times 10^{-7}\mathrm{m}^2 \times \frac{10^{6}\ \mathrm{mm}^2}{1\ \mathrm{m}^2} = 0.643\ \mathrm{mm}^2$$

Step 5: Check the result. Has the value of the quantity increased or decreased? Does this make sense relative to the change in unit? If the new unit is smaller the value should increase. If the new unit is bigger the value should decrease.

Example 1: convert V = 2 x 10^5 nm^3 to m^3

Example 2: convert V = 8.5 x 10^5 L to m^3

Using units to verify an equation

For any equation the units on both sides of the equation must be equivalent. Units of terms added/subtracted in an equation also have to be the same within an equation. Therefore, unit analysis can be used to verify an equation.

Example: Kinetic energy is given by the following relationship. Show that the units of the quantities on the right-hand-side (RHS) of the equation are equal to the unit on the left-hand-side (LHS).

$$KE = \frac{1}{2}mv^2$$

RHS:

Units of *m* mass → kg

Units of *v* velocity → m s^{-1}

Total units = kg (m $s^{-1})^2$ = kg m^2 s^{-2}

LHS:

Units of *KE* energy → J

From Table 2: 1 J = 1 kg m^2 s^{-2}. Therefore, the units on the RHS and the LHS match.

Quantitative Skills: Take Home Messages

Problem solving

It is important to think about what the question is asking, consider what information you have available and to ask the question: does my answer make sense? This will help you in exams but more crucial in ‘real life’ (i.e. research, the lab) where the answer is not necessarily known.

Units

- Memorising equations will only get you so far. It is impossible to remember everything and many quantities have similar or the same variables (e.g. p can be pressure or momentum). Need to understand the context.
- Units can help to provide a solution for how to solve a problem. This is especially true in situations like making up solutions in the lab. Make sure your units cancel out when you calculate volumes, masses, concentrations etc.
- In any equation, the units on each side need to be the same.
- Units of quantities added/subtracted need to be the same. (No adding apples to oranges unless you are counting ‘fruit’!)
- If you have the same unit on the top and bottom of a fraction, they cancel out.
- The ability to work comfortably with units and to convert between different units is a skill that will benefit you throughout your degree and future career.
- Including units in all steps of your calculations will help avoid errors.
- When doing unit conversions, the best way to avoid errors is to write down each step of the conversion. It is very easy to make mistakes when you do these conversions in your head – particularly in a high pressure environment like an exam.