Time-of-flight calculations: exam style questions

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This style of exam question on TOF calculations requires students to use the equation $KE = \frac{1}{2}mv^2$, substitute in $v = \frac{d}{t}$ and rearrange to calculate unknown variables. In addition, students will need to be confident calculating the mass of an ion *in kilograms* given atomic number (A_r) and Avogadro's constant (L).

TOF calculations for a single ion

The key equations will be:

$$m = \frac{A_r}{1000 \times L}$$

And one of the following rearrangements of $KE = \frac{1}{2}m\frac{d^2}{t^2} = \frac{md^2}{2t^2}$:

$$d = t\sqrt{\frac{2KE}{m}}$$

$$t = d\sqrt{\frac{m}{2KE}}$$

$$m = 2KE\frac{t^2}{d^2}$$

A worked example

A $^{35}Cl^{+}$ ion travels through the flight tube of a TOF mass spectrometer with a kinetic energy of 3.65×10^{-16} J. This ion takes 1.04×10^{-5} s to reach the detector.

Avogadro's constant (L) = 6.022×10^{23} mol^{-1}. Calculate the length of the flight tube in metres.

Give your answer to the appropriate number of significant figures.

Stepwise approach

This question requires the student to calculate the mass of the ion *in kilograms*, which is often presented as a separate precursor question to the final TOF calculation.

This first approach involves significant algebraic rearrangement but only a single calculation at the end of the process.

$$m_{35} = \frac{35.0}{1000 \times L} = 5.81 \times 10^{-26} \text{ kg}$$

The first step is to work out the velocity of the ion by rearranging $KE = \frac{1}{2}mv^2$:

$v = \sqrt{\frac{2KE}{m}} = \sqrt{\frac{2 \times 3.65 \times 10^{-16}}{5.81 \times 10^{-26}}} = 1.12 \times 10^5$ ms^{-1}

To answer this question, students need to be able to recall the equation for velocity, $v = \frac{d}{t}$.

$d = vt = 1.12 \times 10^5 \times 1.04 \times 10^{-5} = 1.16$ m

It's helpful to point out that a flight path of around 1 m seems a sensible answer for a TOF mass spectrometer in a laboratory.

Algebraic approach

This second approach is perhaps more mathematically demanding in the first instance but is 'cleaner' and involves only a single calculation on the calculator.

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

Substituting $v = \frac{d}{t}$ into the equation gives us:

$$KE = \frac{md^2}{2t^2}$$

This 'substituted' equation is of paramount importance, and it can be arranged to make d, t or m the subject of the equation.

$$m = \frac{2KEt^2}{d^2}$$

Or

$$t = \sqrt{\frac{md^2}{2KE}} = d\sqrt{\frac{m}{2KE}}$$

Or

$$d = \sqrt{\frac{2KEt^2}{m}} = t\sqrt{\frac{2KE}{m}} = 1.16 \text{ m}$$

There are two approaches to this type of question. One involves stepwise calculations and the other involves significant algebraic rearrangement before 'plugging the numbers in' at the end. Both methods work, although the latter reduces the capacity for error through incorrectly writing down mid-step answers or ignoring significant figures.

TOF calculations for two isotope ions with the same kinetic energy travelling down the same flight tube

Consider two isotope ions in the same mass spectrometer that we will label 1 and 2.

$$KE_1 = KE_2$$

$$\frac{1}{2}m_1v_1^2 = \frac{1}{2}m_2v_2^2$$

Substitute for $v = \frac{d}{t}$ where d is the flight tube (a constant) and t_x is the time of flight (dependent on the isotope ion):

$$\frac{1}{2}m_1\frac{d^2}{t_1^2} = \frac{1}{2}m_2\frac{d^2}{t_2^2}$$

The variables on either side of the equation cancel to give:

$$\frac{m_1}{t_1^2} = \frac{m_2}{t_2^2}$$

If we know the time of flight for isotope 1 (t_1) and the masses of both isotope 1 and 2 (m_1 and m_2 respectively), we can rearrange the equation to give the time of flight for isotope 2 (t_2):

$$t_2^2 = \frac{m_2}{m_1}t_1^2$$

$$t_2 = \sqrt{\frac{m_2}{m_1}}t_1$$

The ratio t_2 to t_1 is simply the square root of the ratio of the masses.

A worked example

A sample of chlorine was analysed in a time of flight (TOF) mass spectrometer and found to contain two isotopes, ^{35}Cl and ^{37}Cl. After ionisation, the ions were accelerated to the same kinetic energy (KE) and then travelled through a flight tube that was 0.750 m long.

The $^{35}Cl^{+}$ ions took 4.56×10^{-4} s to travel through the flight tube.
Calculate the time taken for the $^{37}Cl^{+}$ ions to travel through the same flight tube.

Let's work this out:

$$t_{Cl^{37}} = \sqrt{\frac{37}{35}}t_{Cl^{35}}$$

$$t_{Cl^{37}} = \sqrt{\frac{37}{35}} \times 4.56 \times 10^{-4}$$

$$t_{Cl^{37}} = 4.69 \times 10^{-4}s$$

As expected, the $^{37}Cl^{+}$ ion with the larger mass has a longer time of flight.

An alternative approach

Not all students will be comfortable with deriving the equations above, and some may find that it simply adds 'another equation' to remember. If this is the case, some students may prefer to work out the calculations in a multi-step manner:

1. Calculate the mass of the $^{35}Cl^{+}$ ion *in kilograms* using $m_{35} = \frac{35}{1000 \times L}$, where L is Avogadro's constant (this is often calculated in a previous section of the question).
2. Calculate the velocity of the $^{35}Cl^{+}$ ion using $v_{35} = \frac{d}{t_{35}}$.
3. Calculate the kinetic energy of the $^{35}Cl^{+}$ ion, and therefore the $^{37}Cl^{+}$ ion.
4. Calculate the mass of the $^{37}Cl^{+}$ ion using $v_{37} = \frac{d}{t_{37}}$.
5. Calculate the velocity of the $^{37}Cl^{+}$ ion using $v_{37} = \sqrt{\frac{2KE}{m_{37}}}$.
6. Calculate the time of flight using $t_{37} = \frac{d}{v_{37}}$.

Conclusion

This five- (or six-) step approach to solving these questions seems laborious and creates more room for error. Unless absolutely necessary, it seems more sensible to help students become confident with using $\frac{m_1}{t_1^2} = \frac{m_2}{t_2^2}$.