# Mass Spectrometry for Fusion Applications

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## Nuclear Fusion

In a rapidly developing world where demand for energy is ever increasing, the importance of the discovery of a sustainable source of energy is becoming ever more imperative. Nuclear fusion allows a near inexhaustible supply of energy from widely available fuels. Waste produced is non-toxic and doesn't contain $CO_2$ or harmful greenhouse gases. The main by-product of the process is inert helium gas which is non-radioactive and useful for many industrial uses such as cryogenics and the production of some metals.

Nuclear fusion produces energy by controlling the fusion of atoms to produce around four million times the energy of chemical reactions, such as burning fossil fuels and over four times the energy of nuclear fission. Fuels used in nuclear fusion reactors are easily obtainable and plentiful, for example, tritium is produced during the fusion process from lithium, which is in turn common enough to supply fusion reactors for over a thousand years from mineral supplies alone, ocean supplies will enable millions of years of operation. Deuterium, another fuel is present in all natural water supplies, and can be distilled from these.

The supply of energy from nuclear fusion reactions is predicted to be analogous to current nuclear fission reactors, around 1 to 1.7 gigawatts, with a similar initial cost. As technology develops it is predicted that as outputs increase, costs will decrease significantly.  will increase and costs decrease.

To obtain perfect conditions for nuclear fusion three parameters need to be optimised.  In typical deuterium-tritium fusion reactions, temperatures in excess of 100 million degrees are needed. Typically, a range of heating systems are used in tandem to deliver the temperature required to sustain the fusion plasma allowing high energy collisions to occur. The plasma density is crucial to allow collisions to occur, this is a challenge in vacuum systems where the mean free path can significantly limit collisions.  In nuclear fusion reactors, electromagnets are employed with field strengths in excess of 10 Tesla. Enabling confinement of the plasma species, allowing collisions as well as preventing plasma ignition loss by keeping it away from the reactor wall. Confinement time is also a crucial parameter, this is the time which the particles are confined within the plasma, in current technology this is in the order of a few seconds.

## Nuclear Fusion Compounds

In nuclear fusion reactions two or more nuclei are combined forming one or more new nuclei along with subatomic particles. Elements smaller than iron generally have a large binding energy per nucleon. The main examples used for nuclear fusion are light elements such as hydrogen and helium isotopes, where the nuclear fusion reaction is highly exothermic.

## Typical nuclear fusion reaction

*$^{2}H + ^{3}H \Rightarrow He$ (3.5 MeV) + neutron (14.1 MeV)*

## Mass Spectrometry for Fusion Applications

### Mass Spectrometry

Quadrupole Mass spectrometry is a well-established analysis technique, routinely used for gas, vapour plasma and surface analysis. The spectrometer's ionisation source is typically an electron impact ion source in which electrons from a heated filament are accelerated to 70 eV before impacting with the gas molecules. The emitted electrons ionise all molecules present, allowing them to be filtered by the integral mass filter and in-turn detected by the sensitive detection electronics. For general vacuum applications such as leak detection, vacuum and precursor quality, this technique offers high sensitivity and fast response. This is particularly useful in reaction monitoring where real time analyses of precursor and reaction products is readily available. For contaminant monitoring and vacuum quality at UHV, the inherent high sensitivity employed, where detection limits can be as low as $10^{-16}$ mbar. Improvements in ion source technology have allowed extremely low outgassing from ion source components, further improving detection capabilities.

## Threshold Ionisation Mass Spectrometry (TIMS)

Hydrogen isotope separation is one of the most critical technological problems in nuclear fusion research, and, in order to assess accurately the performance of hydrogen isotope separation, quantitative analysis of hydrogen isotopes takes priority and becomes the first essential problem to be addressed. However, since hydrogen isotopes have almost identical shape, size, and chemical properties, separation and analysis of hydrogen isotopes has historically have proved to be difficult, and in some cases intractable, using the conventional mass resolved mode of mass spectrometry. One method that has been employed successfully is the Threshold Ionisation Mass spectrometry (TIMS) technique. In conventional mass spectrometry, the ionisation energy of an electron impact ionisation source is set to a value of 70 eV to allow all species to be ionised by electron bombardment. The ability of some systems to control the electron energy allows another dimension of analysis to be carried out. The ability to use lower electron energies is advantageous to modify the ionisation of species. Controlling the electron energy allows improvements in species selectivity. The TIMS technique takes advantage of this technique in nuclear fusion research where it can selectively ionise deuterium from a mixed stream of helium and deuterium.

*A typical quadrupole mass spectrometer.*

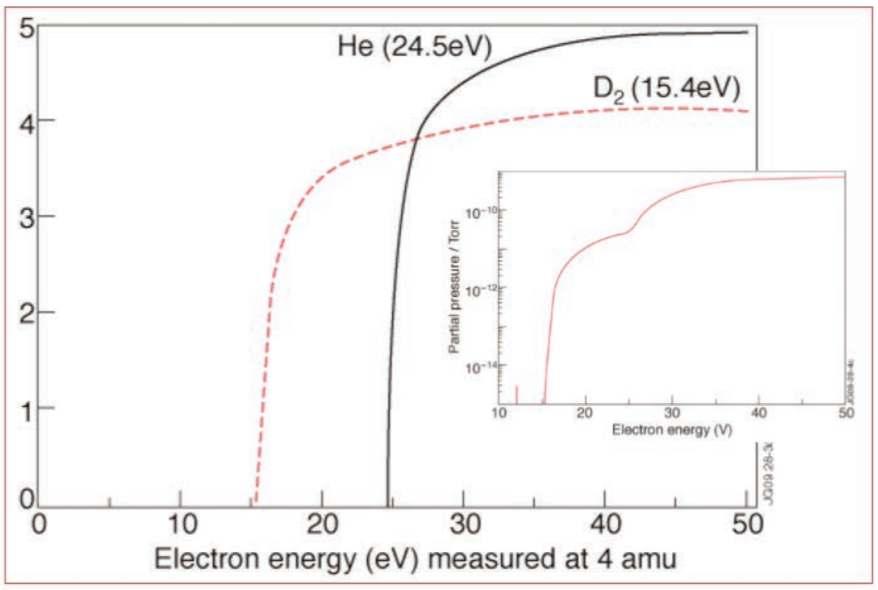
## Threshold Ionisation in Nuclear Fusion

In nuclear fusion, where helium is a by-product of the fusion reaction, the accurate determination of the helium/deuterium ratios is an essential requirement for process characterisation. Quantification is not possible within the limitations of mass resolution of a conventional quadrupole mass spectrometer due to the unresolvable mass overlap of both $D_2$ and He at m/z 4. The mass separation is 0.025 amu. In conventional quadrupole mass spectrometry, unit mass resolution is used.

When the two gases are present simultaneously, a typical electron energy spectrum for m/z 4 is as shown for an example 1:1 mixture of $D_2$:He. The onset of an ion signal at around 15.4 eV is due to production of deuterium ions and the sharp increase in the signal at around 24.5 eV is due to the onset of ionisation of the helium in the mixture. The ionisation threshold energies for $D_2^+$ from $D_2$ and $He^+$. from He are consistent with published data [NIST Standard Reference Database 107, Kim Y-K, Irikura KK, Rudd ME, Ali MA,].

The TIMS spectrum shows a deconvolution of these two species. Applying rudimentary calculations to TIMS spectra such as that shown below, allows the presence of $D_2$ in Helium to be quantified to levels of <10 ppm.

The TIMS technique is not confined only to the separation of He/$D_2$ and has seen further use to 3 amu using the same methodology. For any conventional type of mass spectrometry this proves even more challenging due to the mass separation (0.0058 amu) of the helium 3 isotope ($^3He$) and any hydrogenated deuterium (HD). However, this has been proven to be a routine measurement using TIMS.




*Showing threshold ionisation energies of He and $D_2$ at 4 amu.*

## Ultra-High Resolution Mass Spectrometry

As discussed earlier, the resolution offered by conventional mass spectrometry techniques is not adequate to resolve the mass overlaps found in typical techniques.

In conventional mass spectrometry, the quadrupole mass filter allows the ions produced at the ionisation source to be selected by mass and transported to the detector. A quadrupole mass filter consists of two pairs of parallel, equidistant poles which are biased at equal and opposite potentials. The twin potentials contain fixed DC and alternating RF components. The resulting electric field allows ions of a single m/z ratio onto the detector.

The equations below show the relationship between the applied voltages on pairs of poles on both the x and y planes:

*Y plane* $-(V_{dc} + V_{rf} \cos \omega t)$
*X Plane* $+(V_{dc} + V_{rf} \cos \omega t)$

*Showing a series of mass spectrometer filter assemblies (from L-R 20 mm, 9 mm, 6 mm triple filter, 6 mm single filter, 6 mm shortened for high pressure).*

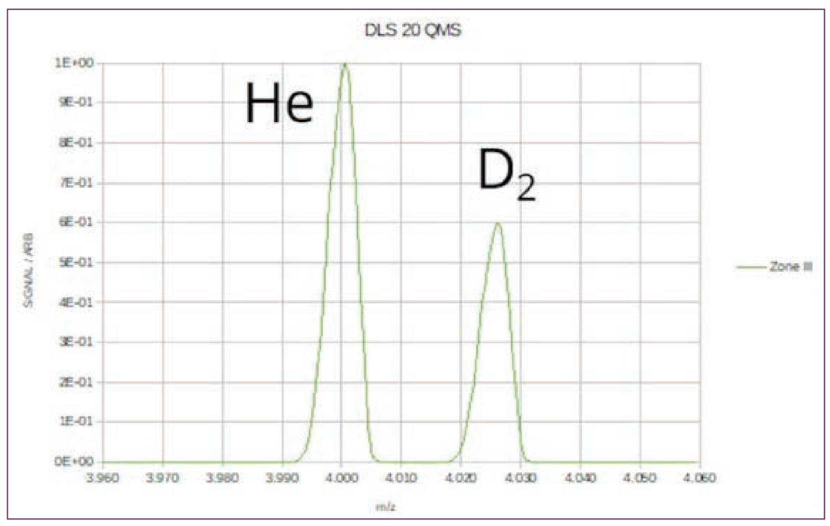
Improvements in performance can be gained by increasing the quadrupole pole diameter, allowing enhancements in stability, sensitivity and mass resolution. Commercial quadrupole mass spectrometers are available with diameters ranging from 6 mm to 20 mm.

However, with increasing pole diameter, power requirements to maintain the RF and DC components increase exponentially, meaning that conventional power supply electronics cannot be used. For many typical applications and where unit mass resolution is required, such as leak detection and precursor analysis, a pole diameter of 6 mm the most efficient solution. Where power requirements are modest and performance is high.

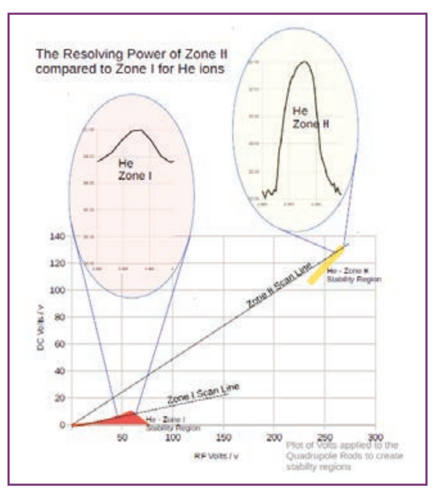
For more demanding applications, such as nuclear fusion fuel species characterisation, overlapping species require enhanced mass resolution to resolve these overlaps. A mass overlap is defined by an unresolvable peak at adjacent masses, where the unit mass remains the same. The below table shows typical nominal and exact masses for common nuclear fusion species.

| Mass | Component | Exact Mass Value (u) | Mass | Component | Exact Mass Value (u) |
|---|---|---|---|---|---|
| 1 | $H^+$ | 1.0078252 | 4 | $^4He^+$<br>$HT^4$<br>$D_2^+$<br>$H_2D^+$ | 4.002600<br>4.023875<br>4.028204<br>4.029650 |
| 2 | $D^+$ | 2.014102 | 5 | $DT^+$<br>$H_2T^+$<br>$D_2H^+$<br>$HeH^+$ | 5.03005<br>5.03170<br>5.035825<br>5.01045 |
| 3 | $^3He^+$<br>$T^+$<br>$HD^+$<br>$H_3^+$ | 3.016030<br>3.016050<br>3.021825<br>3.023475 | 6 | $T^+$<br>$D_2^+$<br>$^{12}C^{++}$<br>$HeD^+$ | 6.032<br>6.042<br>5.999<br>6.0168 |

An example of a typical mass interference in nuclear fusion is $^4He^+$ and $D_2^+$, which have a mass separation of 0.026 amu. This is unresolvable in conventional mass spectrometry. The developments of larger quadrupole diameter mass filters, up to 20 mm, more stable and powerful power supplies and operation in the second stability region 'Zone-H' have all contributed to improvements in ultra-high resolution quadrupole MS systems. An example spectrum of a 20 mm road diameter quadrupole, operating in zone-H can be seen below. The system was able to resolve the adjacent peaks, with the ability to quantify both $^4He^+$ and $D_2^+$ mixtures to 1 ppm for all components by mass.




*Data showing the separation of $^4He^+$ and $D_2^+$ by mass.*




*Showing the improvements in resolution using the first and second stability regions of RF/DC quadruple mass spectrometers.*

Further examples include the quantification of $^3He^+$ in HD, where the mass separation is even lower, 0.0058 amu.

Recent improvements in RF technology have allowed the introduction of ultra-high resolution quadrupole mass spectrometers, these have the capability to resolve the low mass species found in nuclear fusion reactions by mass.

Commercial quadrupole mass spectrometers are normally operated in what is termed 'Stability Zone 1' where the pole voltages are relatively low, this is shown in the red shaded region in the figure (left).

At higher probe voltages, there is a second stability zone, termed 'Zone H', shown in the yellow shaded region, when operated in Zone H, the quadrupole mass spectrometer has much greater mass resolution. For a mass spectrometer to operate in Zone H, high power and ultra-stable RF control electronics are necessitated, recent improvements in RF control technology have allowed this innovation.


*Advanced multi-zone high power RF control electronics.*

Due to the high-power demands of Zone H, the current mass limit of mass spectrometers of this type is 20 amu, ideal for nuclear fusion applications. The addition of a switchable RF supply between zone 1 and zone H, allows conventional operation to 200 amu.

## Conclusions

This article describes the challenges researchers face when quantifying species and compounds used in nuclear fusion reactions. Recent improvements in ion source and quadrupole technology have given researchers the tools required to deal with mass interferences, and quantify common nuclear fusion species. Threshold ionisation mass spectrometry (TIMS) allows enhanced mass selectivity when analysing gas mixtures in which the dominant ions produced are at the same mass number. Many low mass species have very low first ionisation potentials, typically less than 20 eV, allowing selective ionisation of these species in the presence of air gases and water vapour. In particular, the TIMS technique simplifies the identification of the onset ionisation energies for the components of a gas mixture which in turn improves the reliability of conclusions to be drawn from the measurements.

The development of 20 mm pole diameter, ultra-high resolution, quadrupole mass spectrometers, operating in the second stability zone, termed Zone-H, has further improved the analysis and quantification of species less than 20 amu. For common nuclear fusion mass interferences such as $^4He$ and $D_2$, quantification is possible to 1 ppm of each of the species, this is an improvement of a factor of 100 over the TIMS method.

With the imminent proliferation of nuclear fusion energy, researchers and engineers have a number of analysis techniques at their disposal, which allow the quantification of the major components for nuclear fusion.