Quadrupole Size Comparison

APPLICATION NOTE

How Quadrupole Size Affects Research

Mass Spectrometry is one of the most widely used analytical techniques and the most common mass analyzer is the quadrupole. Quadrupole technology has been used for more than 50 years to separate masses in a variety of applications. However, when it comes to quadruple mass spectrometry, QMS, there are a lot of options for researchers to consider. Most of the options rely on one main factor, quadrupole size. The most common quadrupole is the 6 mm or ¼", which can be found in residual gas analyzers (RGA), analytical tandem gas chromatograph / mass spectrometers (GC/MS), and even process gas analyzers. However, while 6 mm may be the most common it is not necessarily the best option for all applications. Because of this, Extrel manufactures three different sizes of quadruples including the 6 mm, 9.5 mm and Extrel's most popular quad size, the 19 mm (¾"). Whether to pick a different sized quadrupole can be a confusing prospect for researchers new to QMS.

Looking at the advantages of each quad will help a researcher choose the correct direction to take. Transmission, Sensitivity, Mass Range and Resolution are all factors that can vary based on the quadrupole size.

One advantage of Extrel systems is that the RF/DC power supply has a set power output, which means that there are no additional power requirements when going between quad sizes. The same power supply can be used for all sizes.

Figure 1. 19 mm quadrupole (left) versus a 9.5 mm quadrupole (right).

Experimental

Sensitivity (mA/Torr)

Sensitivity tests were conducted using a spherical vacuum chamber housing three separate mass spectrometer probes. The sampling method utilized a metering valve to provide a room air leak of approximately 5 x 10^{-6} Torr and measuring the nitrogen signal on m/z 28. This signal was resolved to nominal mass of a 1 amu width and tuned for maximum intensity. The baseline (with the ion source powered off) was subtracted from the signal, and the background chamber pressure subtracted from the sample pressure. Data was collected for approximately 30 seconds with the ion source powered on, followed by approximately 30 seconds with the ion source powered off. The following equation was used to calculate the sensitivity of each mass spec in mA/Torr:

$$Sensitivity\left(\frac{mA}{Torr}\right) = \frac{\frac{(I_{signal} - I_{background})}{Preamplifier\ Gain}}{(P_{sample} - P_{background}) \times \%N_2}$$

Where:

I_{signal} = Signal intensity (in mV) of m/z 28 with the ion source powered on

$I_{background}$ = Signal intensity (in mV) of m/z 28 with the ion source powered off

Preamplifier Gain = Gain resistor of the preamplifier (in Ω)

P_{sample} = Sample pressure (in Torr)

$P_{background}$ = Background chamber pressure (in Torr)

$\%N_2$ = Partial pressure of nitrogen (in %) in the sample (78.08%)

Mass Spec #1 ***(19 mm quad – MAX-QMS)*** collected data scanning from m/z 27 – m/z 29 using a requested scan rate of 0.5 seconds, combined with a 190 sample prescan. This led to 20 "microscans" of 50 samples/mass and a 0.481 actual scan time. All data was collected using the Faraday plate detector tied to the conversion dynode.

Mass Spec #2 ***(9.5 mm quad – MAX-LT)*** collected data scanning from m/z 26 – m/z 30 using a requested scan rate of 0.5 seconds, combined with a 100 sample prescan. This led to 20 "microscans" of 50 samples/mass and a 0.497 actual scan time. All data was collected using the Faraday plate.

Mass Spec #3 ***(6 mm quad – Extrel RGA)*** collected data scanning from m/z 23 – m/z 34 using a scan speed of 500 samples/second, combined with 20 samples/amu. The probe's auto zero function was set to "every sample". This led to approximately two second scan times. All data was collected using the Faraday plate.

Transmission (%)

Transmission tests were conducted using a spherical vacuum chamber (Extrel Serial No.: 01876) housing three separate mass spectrometer probes. The sampling method utilized a metering valve to provide a room air leak of approximately 5 x 10^{-6} Torr and measured the maximum ion signal while scanning from ions m/z 23 to 34. This signal was resolved to a nominal mass of a 1 amu width and tuned for maximum intensity. The resolution was decreased, uniformly over the scan range, until a minimum resolution was achieved without any peak overlap between nitrogen and oxygen signals. Data was collected for approximately 30 seconds using the low (open) resolution, followed by approximately 30 seconds with the high (closed), nominal resolution. The following equation was used to calculate the transmission of each mass spec in percent:

$$Transmission\ (\%) = \frac{Intensity_A}{Intensity_B} \times 100\%$$

Where:

$Intensity_A$ = Signal intensity (in mV) of the scan using nominal resolution (1-amu wide peaks)

$Intensity_B$ = Signal intensity (in mV) of the scan using low resolution (maximum peak width prior to interference due to overlapping)

Mass Spec #1 ***(MAX-QMS)*** collected data scanning from m/z 23 – m/z 34 using a requested scan rate of 0.5 seconds, combined with a 190 sample prescan. This led to 8 “microscans” of 50 samples/mass and a 0.481 actual scan time. All data was collected using the Faraday plate detector tied to the conversion dynode.

Mass Spec #2 ***(MAX-LT)*** collected data scanning from m/z 23 – m/z 34 using a requested scan rate of 0.5 seconds, combined with a 100 sample prescan. This led to a 9 “microscans” of 50 samples/mass and a 0.476 actual scan time. All data was collected using the Faraday plate.

Mass Spec #3 ***(Extrel RGA)*** collected data scanning from m/z 23 – m/z 34 using a scan speed of 500 samples/second, combined with 20 samples/amu. The probe’s auto zero function was set to “every sample”. This lead to approximately two second scan times. All data was collected using the Faraday plate.

Maximum Resolution (M/ΔM)

High resolution testing was conducted using a spherical vacuum chamber (Extrel Serial No.: 01876) housing two mass spectrometer probes, Mass Spec #1 and Mass Spec #2, and a metering valve to bleed UHP Argon into the chamber. The testing was conducted on Mass Spec #3 using a cylindrical vacuum chamber and a 0.05”, restrictive tubing, differentially pumped, inlet to bleed UHP Argon into the chamber. The pressure of argon was increased to achieve a chamber pressure of approximately 5 x 10^{-6} Torr. Argon was scanned at m/z 40, then the tune for each mass spec was optimized to achieve the highest resolution on the peak. The resolution is calculated by using the following equation:

$$Resolution = {}^{M}/_{\Delta M}$$

Where:

M = Mass of the ion measured in amu

ΔM = Full width of the ion measured at half of the maximum intensity, in amu (Full Width Half Max)

Mass Spec #1 ***(MAX-QMS)*** collected data scanning from m/z 39.7 – 40.3 amu using a requested scan rate of 1 second, combined with a 100 sample prescan. This led to 30 “microscans” of 500 samples/mass and 0.982 actual scan time. All data was collected using the electron multiplier detector.

Mass Spec #2 ***(MAX-LT)*** collected data scanning from m/z 39.7 – m/z 40.3 using a requested scan rate of 1 second, combined with a 100 sample prescan. This led to 16 “microscans” of 1000 samples/mass and a 0.976 actual scan time. All data was collected using the electron multiplier detector.

Mass Spec #3 ***(Extrel RGA)*** collected data scanning from m/z 39 – m/z 41 using a scan speed of 500 samples/second, combined with 20 samples/amu. The probe’s auto zero function was set to “every sample”. This led to approximately two second scan times. All data was collected using the Faraday plate.

Results

Sensitivity (mA/Torr)

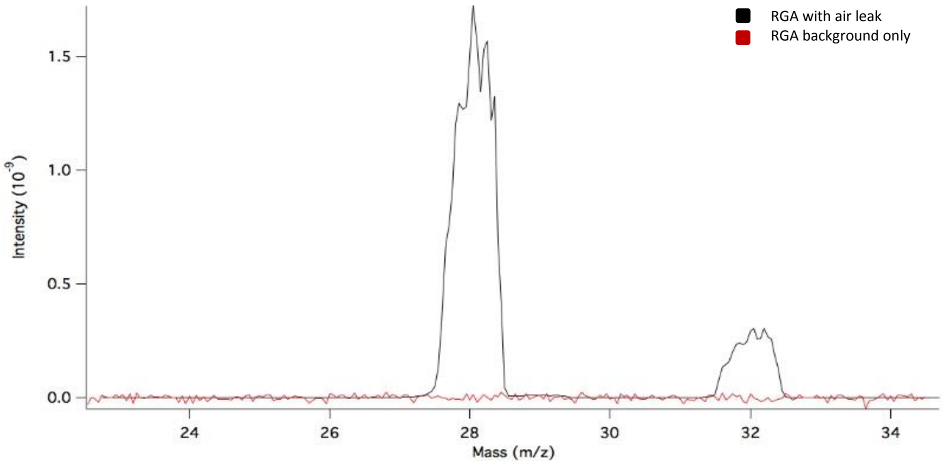

Figure 2. Example of the milliamp per Torr test that is performed to quantify the general sensitivity of a gas analyzer. This example shows the background spectra taken versus the 1 x 10^{-6} Torr spectra taken once an air leak was added to the system.

19 mm Quad - MAX-QMS	9.5 mm Quad – MAX-LT	6 mm Quad – Extrel RGA
I_{signal} = 2084.25 mV $I_{background}$= 0.15 mV $Preamplifier\ Gain$= 10^8 Ω P_{sample}= 7.75×10^{-6} Torr $P_{background}$= 6.5×10^{-7} Torr $\%N_2$= 78.08 %	I_{signal} = 4054.86 mV $I_{background}$= 14.75 mV $Preamplifier\ Gain$= 10^9 Ω P_{sample}= 6.01×10^{-6} Torr $P_{background}$= 1.4×10^{-7} Torr $\%N_2$= 78.08 %	I_{signal} = 1.721×10^{-9} A $I_{background}$= 2.364×10^{-13} A P_{sample}= 6.31×10^{-6} Torr $P_{background}$= 1.0×10^{-7} Torr $\%N_2$= 78.08 %
Sensitivity: 3.76 mA/Torr	**Sensitivity: 0.88 mA/Torr**	**Sensitivity: 0.35 mA/Torr**

Table 1. Sensitivity values.

Transmission (%)

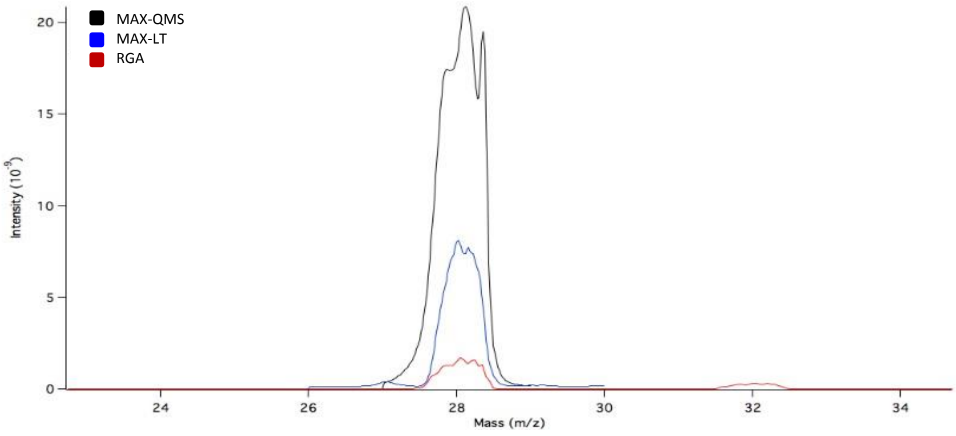

Figure 3. Representative spectra for the three quadrupole sizes used in the testing of total transmission of the systems. The signal is first optimized, then switched to RF only mode to measure the amount of signal lost compared to the amount of signal generated by the ionizer.

19 mm Quad – MAX-QMS	9.5 mm Quad – MAX-LT	6 mm Quad – Extrel RGA
$Intensity_A$ = 2144.78 mV $Intensity_B$= 2959.80 mV	$Intensity_A$ = 2761.03 mV $Intensity_B$= 8192.02 mV	$Intensity_A$ = 1.24×10^{-9} A $Intensity_B$= 4.30×10^{-9} A
Transmission = 72.5%	**Transmission = 33.7%**	**Transmission = 28.8%**

Table 2. Transmission (%) values.

Maximum Resolution (M/ΔM)

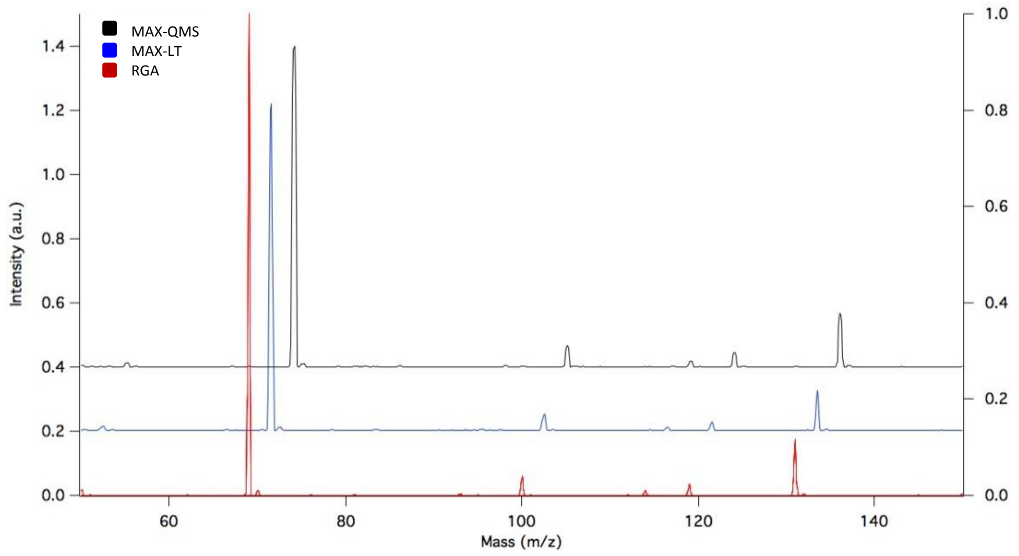

Figure 4. Waterfall plot of the three quad size spectra for the mass range from mass 50 to 150.

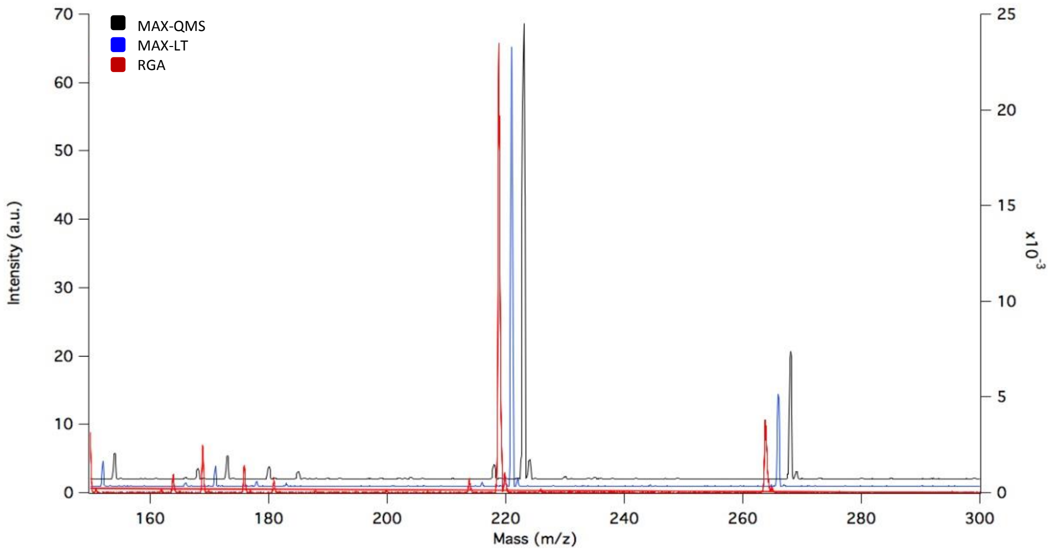

Figure 5. Waterfall plot of the three quad size spectra for the mass range from mass 150 to 300.

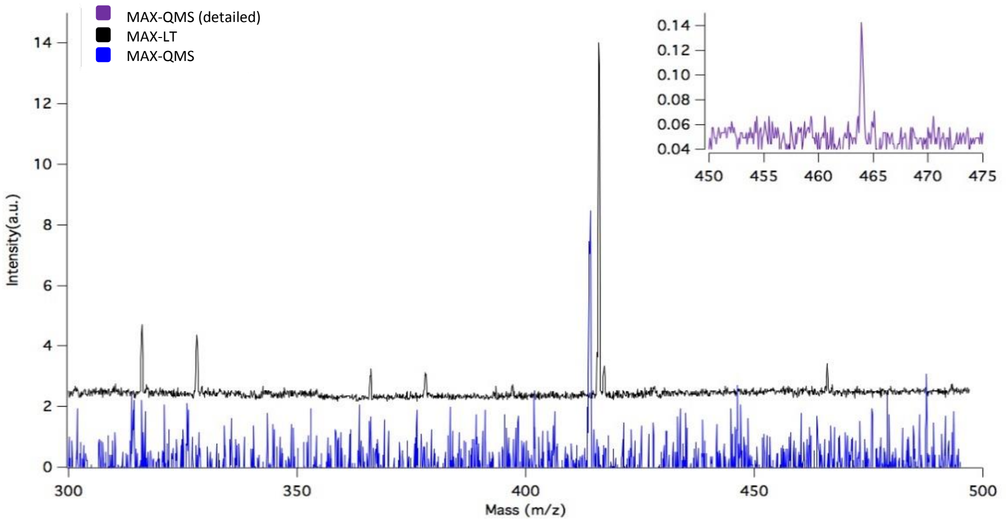

Figure 6. Waterfall plot of the MAX-QMS and MAX-LT for the mass range of 300 to 500 amu. Note that the RGA maxes out at 300 amu. Inset shows the signal and less than 1 amu resolution at 464 m/z for the MAX-QMS.

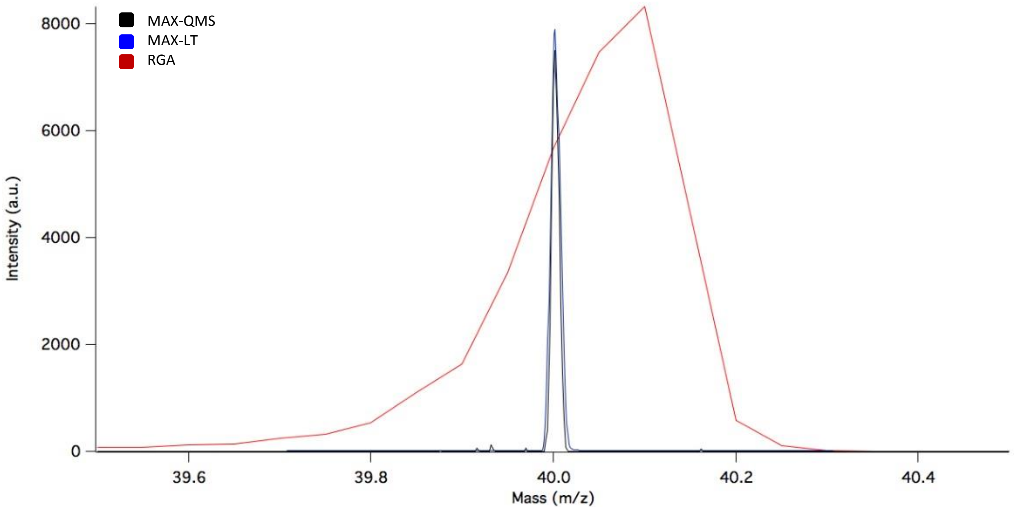

Figure 7. Comparison of resolution at mass 40 for Argon for the three quad sizes.

19 mm Quad – MAX-QMS	9.5 mm Quad – MAX-LT	6 mm Quad – Extrel RGA
0.00838 amu (FWHM)	0.0125 (FWHM)	0.187 amu (FWHM)
Resolution (m/Δm)= 4773	**Resolution (m/Δm) = 3200**	**Resolution (m/Δm) = 214**

Table 3. Resolution values.

Conclusion

Quadrupole size has a direct effect on maximum resolution and transmission. A larger quad size results in better ion transfer and space to separate the ions more efficiently. When choosing a quadrupole size, a researcher should pick the largest quad for the necessary mass range for their research. One advantage to Extrel's systems is that the fixed frequency QPS allows for an incredibly stable signal and when necessary, easy switching between mass ranges on the quadrupoles by just changing one box.

What Pole Size Do I Need?

Total power is fixed for Extrel QPS RF generators.

For a specific mass range, performance and resolution increases with increasing frequency.

Due to the wide loading range of the Extrel QPS, capacitance is no longer an issue for Extrel quads.

Only reduction by going with a larger quad size is a lower mass range for a set frequency.

Conclusion: Go with the biggest quad for the necessary application mass range.

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