# A Design and Simulation Tool for Miniature Mass Spectrometers

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## 1. INTRODUCTION

The ongoing trend towards miniaturisation in mass spectrometry has resulted in the realisation of miniature and microengineered forms of all of the main MS instruments (e.g. QMS, Ion Trap, magnetic sector) some of which are now commercially available. One of the driving forces behind the trend towards miniaturisation is the application of MS techniques in harsh or hitherto inaccessible environments. We present here a mass spectrometer computer simulation tool that accurately simulates the mass spectra experimentally obtained from a miniature QMS operated under a wide range of conditions. Instrument behaviour is described by determining the individual trajectories of a large numbers of ions ($10^8$) as they are injected from the ion source into the mass spectrometer. From the computer simulated mass spectra, instrument resolution and sensitivity may be calculated and overall instrument performance determined for a user selected mass (analyte) range. The simulation tool also allows the user to see the effect of instrument design changes and importantly the effect of manufacturing tolerances on the resulting mass spectra. Future work includes the provision of a retention time parameter to control the injection times of ion mixtures into the QMF, enabling the simulation GC/MS systems.

## 2. QMF PERFORMANCE SENSITIVITY - PEAK SHAPE

❖ Mass spectra peak shape and peak position vary with $r/r0$ ratio.

❖ Zone 1 exhibits increasing low mass tails as $r/r0$ increases above the ideal [1]. Zone 3 operation much improved, exhibits minimal low mass tails even at extremes of $r/r0$.

❖ Low mass tails for zone 3 operation are of insufficient magnitude to affect peak width, even at 10% PH.

❖ Mass peaks shift to lower mass position with increasing $r/r0$, reflecting the increasing quadrupole coefficient of the multipole field [2].
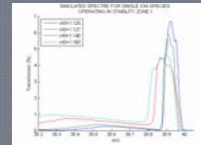


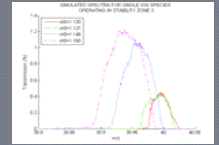Fig. 1 Simulated spectra for Ar+ (m/z=40) for a range of r/r0 operating in stability zone 1.



Fig. 2 Simulated spectra for Ar+ (m/z=40) for a range of $r/r0$ operating in stability zone 3.

## 3. QMF PERFORMANCE SENSITIVITY- RESOLUTION AND TRANSMISSION

❖ Performance characteristics of a QMF vary with $r/r0$ ratio.

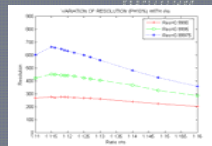❖ Performance characteristics exhibit a minimum or maximum for $r/r0$ = 1.15 - 1.25.

❖ Performance sensitivity to $r/r0$ dependent on the instrument resolution setting. Decreasing with decreasing instrument resolution.

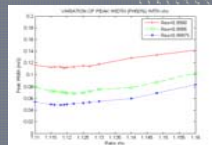❖ Ion transmission through the QMF exhibits a minimum at the optimum $r/r0$ ratio for high instrument resolution settings.
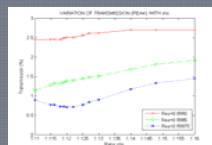
❖ Either side of the optimum $r/r0$ performance sensitivity is approximately constant for a given instrument resolution setting.

❖ Defocusing of the stability boundaries increases as $r/r0$ moves further from the ideal.

❖Defocusing effects more pronounced closer to the stability tip.



Fig. 3 Variation of resolution (10% PH) as a function of the ratio $r/r0$ for operation in stability zone 3.



Fig. 4 Variation of peak width (PH 50%) as a function of $r/r0$ for operation in stability zone 3.



Fig. 5 Variation of transmission as a function of the $r/r0$ for operation in stability zone 3.

## 4. QMF - PEAK SPLITTING

❖ Low mass tails increase as $r/r0$ moves further from the ideal. This effect much reduced on zone 1 operation.

❖ Peak splitting characteristics are due to non-linear resonances, maximum for $r/r0$ = 1,140.

❖ Peak splitting is more pronounced at lower ion energies. Ions experience an increasing number of rf cycles as ion energy decreases.

❖ Non-linear resonances require time to build up.
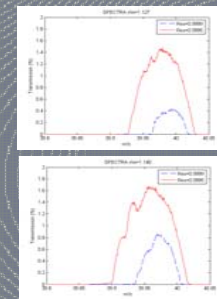
❖ Peak structure in evidence across the mass peak.



Fig 6 Simulated mass spectra for Ar+ single ion species operating in stability zone 3 for two values of $r/r0$.

## 5. SPATIAL POWER FREQUENCY SPECTRA

❖ An ideal quadrupole field produces deterministic spatial power frequency peaks.

❖ The multipole components of a non ideal field, introduce additional spatial power frequency peaks [3].

❖ The "idealness" of the generated field can be quantified by the magnitude and quantity of the additional peaks, providing a figure of merit for the field.

❖ Spatial power frequency spectra (SPFS) provide a quicker and more accurate method of assessing field quality than examination of multipole coefficients.

❖ SPFS provides the basis for an iterative process to assess the suitability of novel microengineered structures for use as QMFs.



Fig. 7 Ion trajectory power frequency spectra for two values of $r/r0$ for operation in zone 1.

## 6. MAGNETIC SECTOR

Recently the method has been applied to miniature magnetic sector mass spectrometers with uniform magnetic fields. For a perfect system the resolution depends on: (i) magnetic field (B), (ii) ratio of slit width to separation and (iii) ion mass (m). Ions move in circular paths with radii given by:

$$r \approx 1.4397 \times 10^{-4} \sqrt{(V/B^2 m)}$$

where V is the ion energy (eV). Typical spectra are shown in Fig. 8 with the detail peak shapes shown in the inset.

As for the QMS model the ion source conditions may be varied to Include distributions (Gaussian) in (a) intensity (b) exit angle and (c) energy.
The effect of (a) is to produce rounded peaks, (b) increases peak width and produces a tail on the high mass side of the peak, (c) reduces resolution and peak height but the peak remains symmetrical
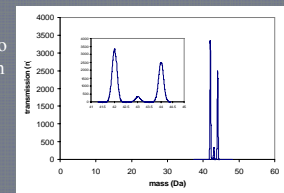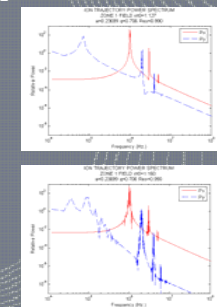


Fig.8 Simulated mass spectra for magnetic sector instrument (multiple ion species) inset shows peak shapes

## 7. REFERENCES

[1] J. R. Gibson and S. Taylor, "Prediction of quadrupole mass filter performance for hyperbolic and circular cross section electrodes," Rapid Commun. Mass Spectrom., 14, pp. 1669-1673, 2000.
[2] D. J. Douglas and N. V. Konenkov, "Influence of the 6th and 10th spatial harmonic on the peak shape of a quadrupole mass filter with round rods," Rapid Commun. Mass Spectrom., 16, pp. 1425-1431, 2002.
[3] T.J.Hogan, S.Taylor "Performance Simulation of a Quadrupole Mass Filter Operating in the First and Third Stability Zones," IEEE Trans. on Instr. & Meas. (in press)