PERFORMANCE ENHANCEMENT FOR MINIATURE QMS THROUGH APPLICATION OF A MAGNETIC FIELD

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INTRODUCTION

One of the challenges of deploying miniature mass spectrometers (MS) in harsh environments is that of reducing the size (to render the MS system portable), whilst at the same maintaining instrument performance in terms of MS resolution, sensitivity and mass range. Previous work has identified that application of a static magnetic (B) field can improve the resolution of a miniature quadrupole mass spectrometer (QMS) and this simple method of performance enhancement offers advantages for field deployment [1-3]. The B field may be applied transversely (radially) to the quadrupole mass filter (QMF) or axially and performance improvements have been observed experimentally in both cases. The experimental results have been successfully simulated on the basis of our QMS model, which computes the individual trajectories of large numbers of ions (typically 10^6) injected randomly into the QMF. Mass spectra may be obtained for a range of applied voltages (U/V), electrode length and inscribed radius (r_0), RF frequency and ion energy.

Hitherto the modelling has been for the ideal case of hyperbolic electrodes. However it is well known that many important effects are observed for circular electrode QMF's which are still the most widely used. Accordingly we have recently adapted our QMS model [4] to allow simulation of any electrode geometry (circular, square or hyperbolic) and configuration. The program now allows instrument simulation not only for the range of conditions above but also allows r/r_0 ratio to be specified. The program allows electrodes to be misaligned or displaced so as to examine the effect of manufacturing tolerances on QMS performance. Our findings continue to show benefit with B field application. We present here the results of recent instrument simulations for two HEMS application areas: (i) detection of low mass isotopes (1<m/z<6 Da) at high resolution and (ii) detection of ^{12}C/^{13}C isotope ratios for point of care diagnosis of medical disorders.

METHOD

Custom software (QMS_2D) was used to simulate the performance of a circular electrode QMF. Our approach has been described previously in [4] and the model has been adapted to include the additional B field. The program calculates ion trajectories by solving the modified Mathieu equation using a fourth order Runge-Kutta algorithm. The addition of a B field couples the three equations of motion:

$$\frac{d^2x}{d\xi^2} = -x(a - 2q\cos(2\xi)) + \left(\frac{dy}{d\xi}b_3 - \frac{dz}{d\xi}b_2\right)$$

$$\frac{d^2y}{d\xi^2} = y(a - 2q\cos(2\xi)) + \left(\frac{dz}{d\xi}b_1 - \frac{dx}{d\xi}b_3\right)$$

$$\frac{d^2z}{d\xi^2} = \left(\frac{dx}{d\xi}b_2 - \frac{dy}{d\xi}b_1\right)$$

These equations are written in a dimensionless form where the only dimension that appears is that of length displacement.
Time, $t = 2\xi\omega$; angular frequency, $\omega = 2\pi f$. U is the direct potential; V is the alternating potential amplitude; $a = \frac{4eU}{m\omega^2 r_0^2}$ & $q = \frac{2eV}{m\omega^2 r_0^2}$
m is the mass of the ion; r_0 is the inscribed radius of QMS.
The components of the magnetic field, **B**, are: $(b_1, b_2, b_3) = \left(\frac{2eB_x}{m\omega}, \frac{2eB_y}{m\omega}, \frac{2eB_z}{m\omega}\right)$

EFFECT OF B FIELD ON QMF WITH CIRCULAR RODS

Hyperbolic electrodes produce an optimal electric field. This can be approximated by using circular electrodes with a specific ratio of rod radius-to-inscribed QMF radius (r/r_0) providing an easier-to-manufacture ample approximation to the ideal hyperbolic case.

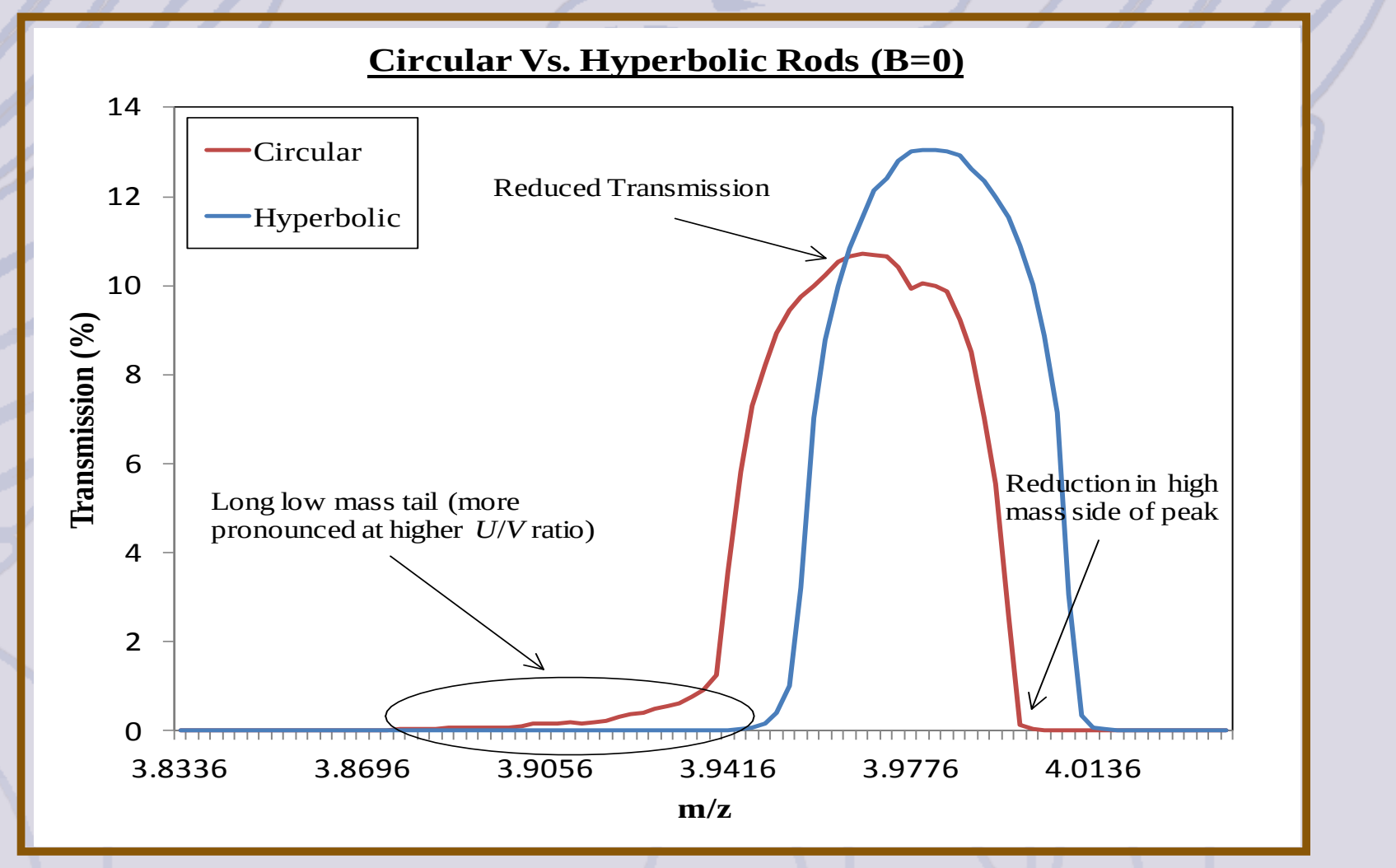

Fig.1 Simulated mass spectra for He^+ single ion species for hyperbolic and circular (r/r_0 = 1.127) rods

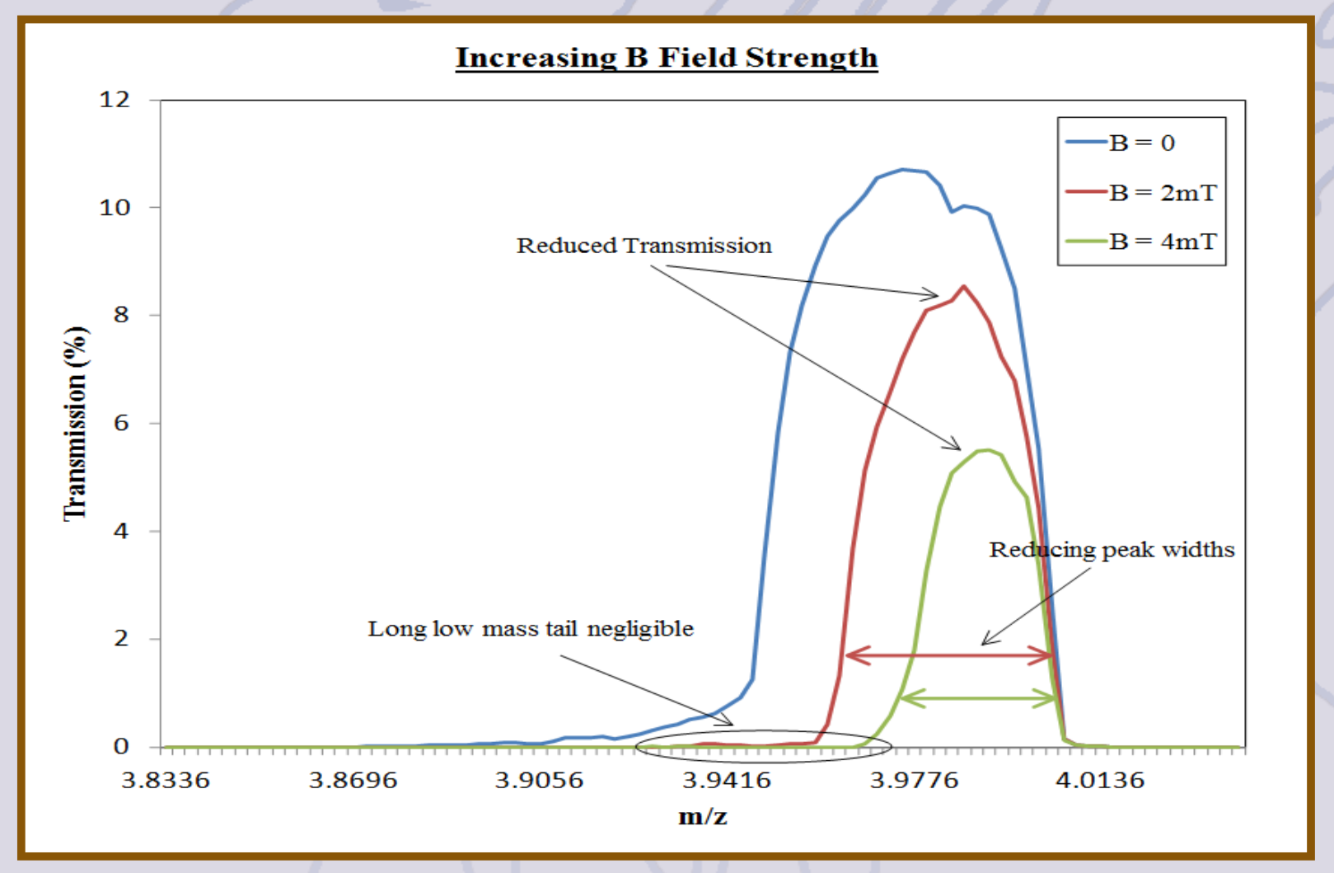

Fig.2 Simulated mass spectra for He^+ single ion species for circular (r/r_0 = 1.127) rods with increasing B field applied from 0 to 4mT

Although circular rods are more cost effective than hyperbolic, they suffer from reduced performance due to: increased peak width, lower transmission, and a long low-mass tail (fig. 1).

Transverse application of a B field along the x-axis eliminates the long low-mass tail and reduces peak width (fig. 2). As the B field is increased, the resolution increases but the transmission decreases (fig. 3).

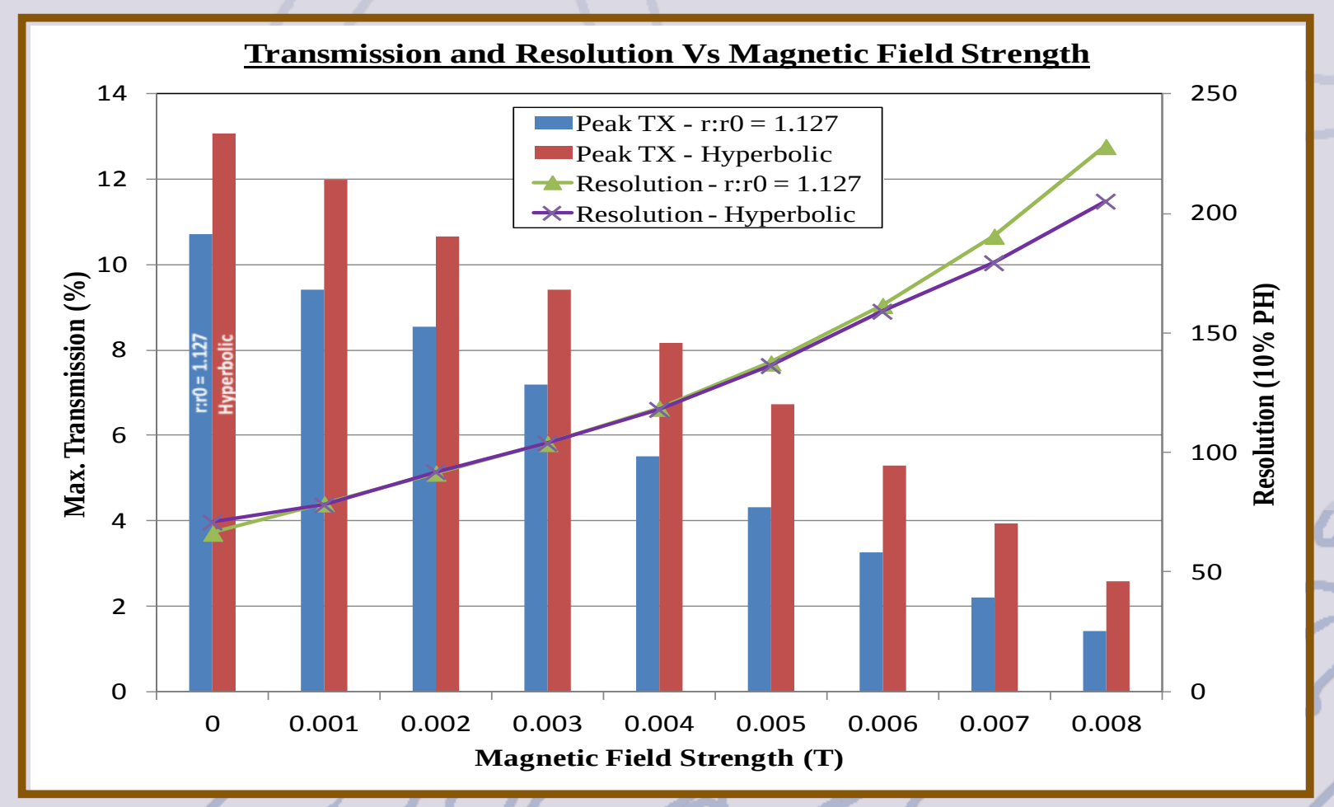

Fig.3 Simulated He^+ single ion species. Effect on transmission and resolution as B field is increased for both circular and hyperbolic rods

EFFECT OF B FIELD ON r/r_0 RATIO

Minor changes to the r/r_0 ratio can have significant effects on the resolution, transmission and peak shape. Previous work has shown that for a conventional QMF (without B field) the optimum ratio is ~1.120-1.130 [5] for U/V > 99.7% (operating in zone 1).

When a magnetic field is applied the optimum r/r_0 ratio remains moderately constant across the range ~1.120-1.160 (fig. 4). However, as the r/r_0 ratio is increased the transmission reduces and is more profound at larger B field magnitudes (fig. 5).

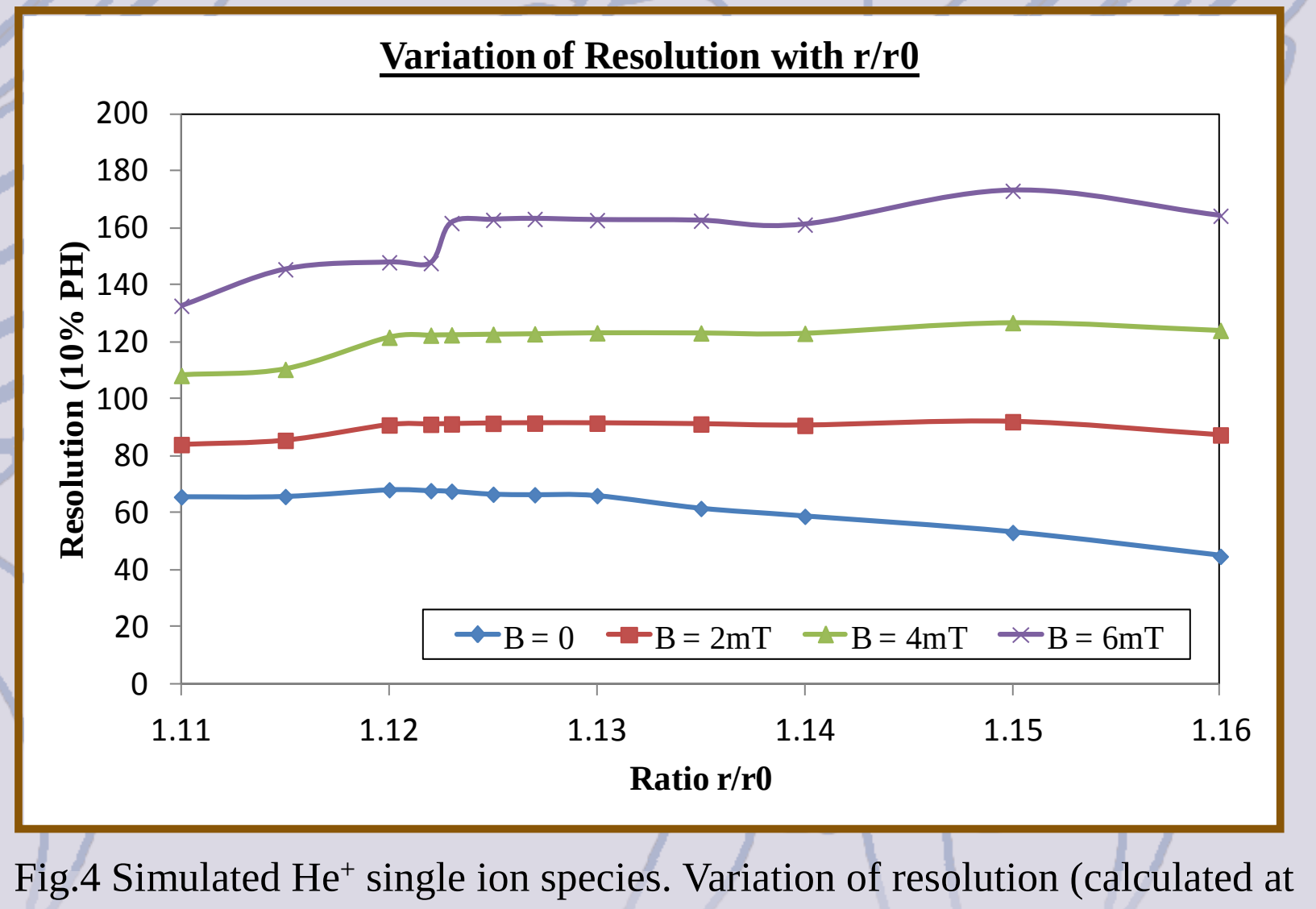

Fig.4 Simulated He^+ single ion species. Variation of resolution (calculated at 10% of peak height) for various r/r_0 with increasing B field. U/V = 99%

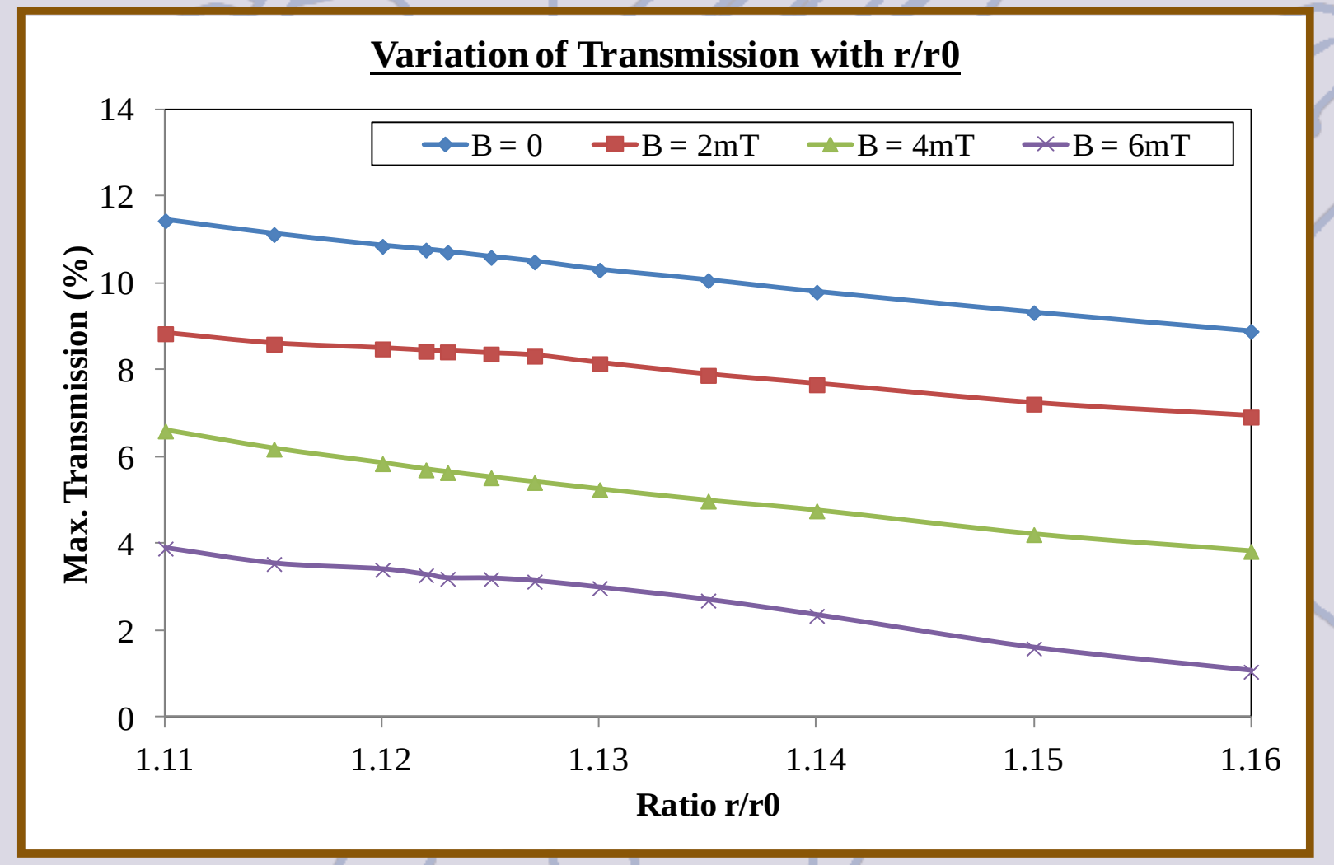

Fig.5 Simulated He^+ single ion species. Variation of transmission (at peak maxima) for various ratios of r/r_0 with increasing B field. U/V = 99%

UREA BREATH TEST

The non-invasive ^{13}C urea breath test (UBT) is a well established clinical procedure for detecting Helicobacter Pylori (H. Pylori) in exhaled breath. The test requires a baseline breath sample before the patient ingests urea labelled with ^{13}C. A comparison of the relative abundance of ^{12}C/^{13}C in the exhaled CO_2 of the patient pre- and post-urea indicates the presence or absence of H. Pylori.

The UBT is typically carried out using large, bulky and expensive magnetic sector MS equipment. More recently portable QMS have been used but struggle to achieve the required resolution. However, using a modified portable QMS with an applied B field can provide improved resolution, enhanced peak shape, and reduce peak overlap allowing for more accurate diagnosis.

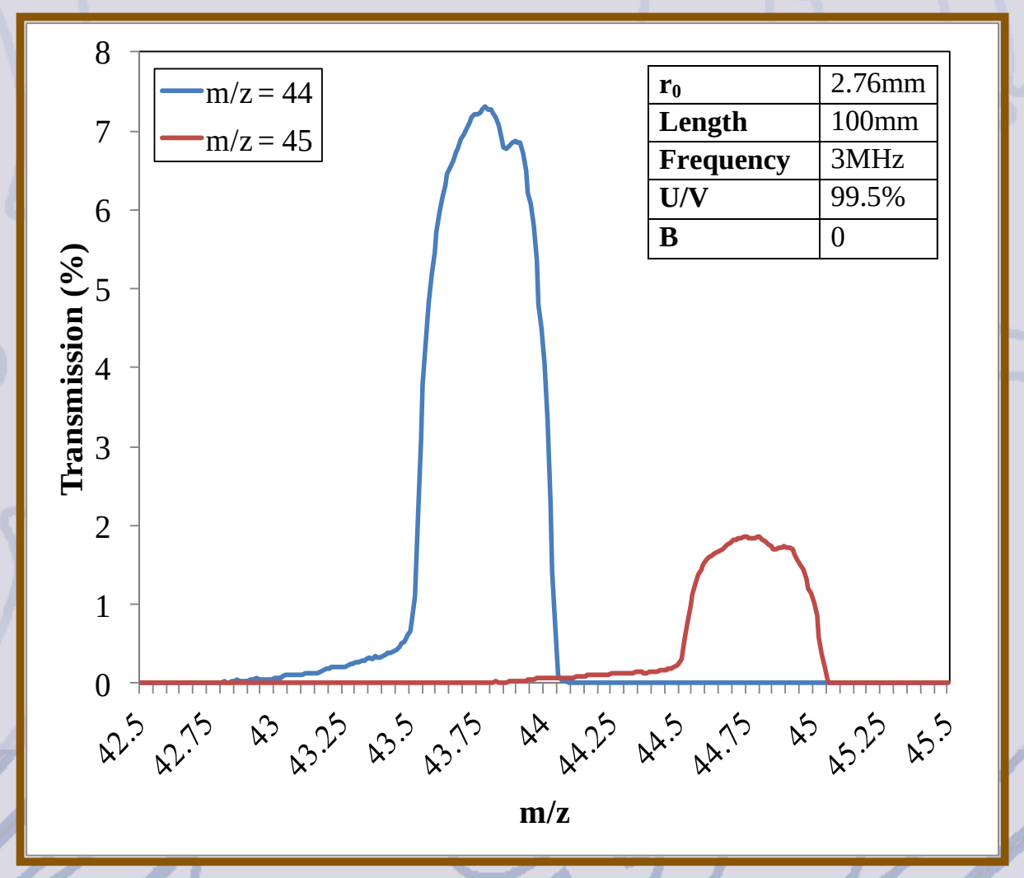

Fig.6 Simulated mass spectra for $^{12}CO_2^+$ and $^{13}CO_2^+$ using circular rods (r/r_0 = 1.127). No magnetic field applied (B = 0). U/V = 99.5%

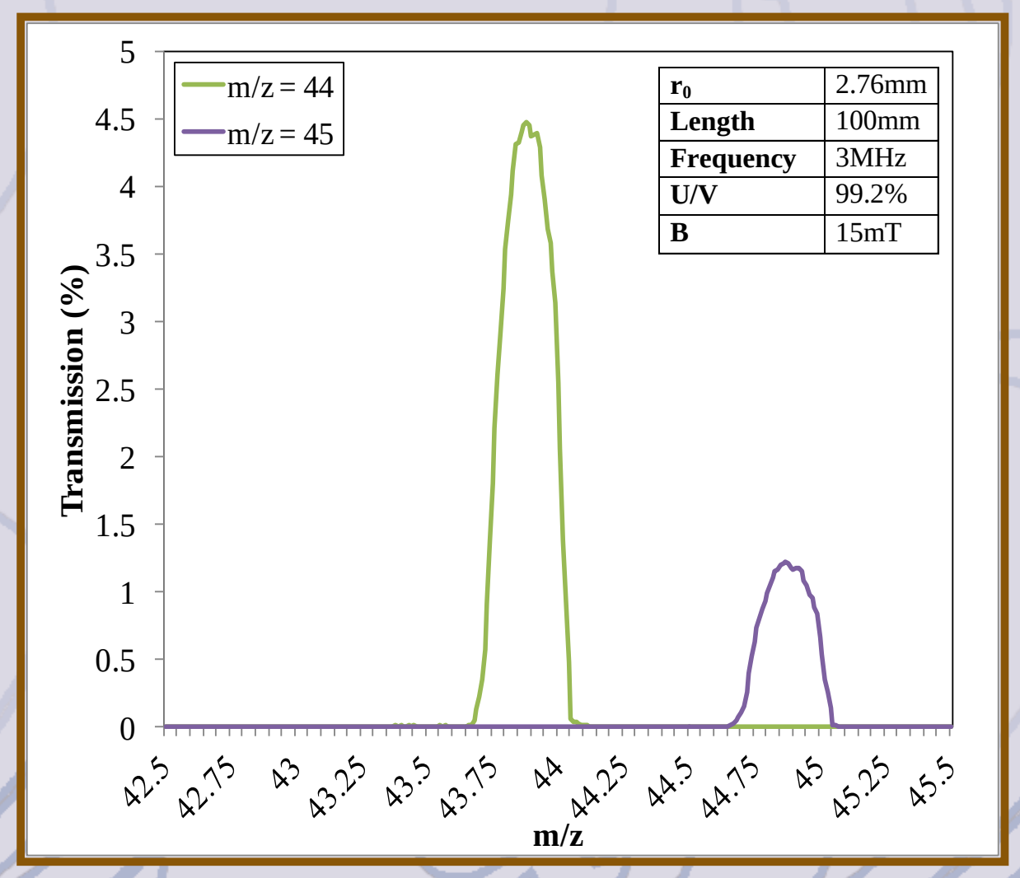

Fig.7 Simulated mass spectra for $^{12}CO_2^+$ and $^{13}CO_2^+$ using circular rods (r/r_0 = 1.127). B = 15mT. U/V = 99.2%

FURTHER INFORMATION

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We gratefully acknowledge EPSRC Engineering and Physical Sciences Research Council