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# Prediction of the effects of imperfect construction of a QMS filter

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**Modelling techniques have previously predicted the observed behaviour of perfectly manufactured QMS mass filters. These methods are extended to examination of the behaviour of imperfect QMS filters; this examination considers the behaviour of QMS filters with one rod displaced radially inward as this is a simple manufacturing defect that arises when a rod does not fit correctly into the mounting.**

**The results demonstrate the well known, but poorly documented property, that exchanging the connections of a poorly performing QMS device sometimes improves performance. This is shown to arise because only a displacement of a *y*-rod produces a large effect. The results also show that displacement of a *y*-rod may produce a spurious additional peak known as a precursor. More detailed investigation suggests that precursors are not separate peaks but are formed because a section of the main peak is removed causing an apparent double peak.**

**Finally results confirm that adjustment of the voltage applied to a displaced rod can be used to significantly improve the QMS behaviour. A small change by a fraction $\alpha$ in the position of a single rod may be compensated by a change of $2\times\alpha$ in the voltage applied to that rod. Copyright © 2007 John Wiley & Sons, Ltd.**

**KEYWORDS:** QMS filter; imperfect; prediction; effects; construction

## INTRODUCTION

Since its introduction[1] in 1953 there have been many analytical predictions of the behaviour of the quadrupole mass filter when used as a mass spectrometer [quadrupole mass spectroscopy (QMS)]. Early predictions were for systems with hyperbolic cross-section electrodes, as this is the ideal form. However, instruments are usually constructed with circular cross-section electrodes to simplify manufacture. As it is very difficult to dismantle and re-assemble a QMS filter in a consistent manner, there is only one report[2] of experimental observations of the effects of changing from hyperbolic rods to round ones using the same instrument.

A number of publications predict the behaviour of QMS filters using circular electrodes; early ones are reviewed by Dawson.[3] More recent predictions[4–8] produced results that show good agreement between analysis and experimental behaviour. In particular, these predict that performance with circular section electrodes is poorer than with hyperbolic electrodes and also suggest an optimum value for the dimensionless parameter $r/r_0$ that agrees with the experimental value found by trial and error.

Even for circular section electrodes, published analytical investigations assume that construction is perfect. There is only one, difficult to obtain, publication by Story[9] describing measurements of the effects of imperfect manufacture; fortunately the largely qualitative results are reproduced by Dawson.[3] Reviews such as Dawson's and comments by experimentalists indicate that imperfect construction usually results in severely degraded QMS performance. A later review by Dawson[10] includes consideration of early computations of the effects of manufacturing imperfections. This shows how the fine structure often observed in mass peaks arises and indicates the effects of manufacturing imperfections with estimates of the limit they place on maximum resolution.

A further well-known, but apparently unpublished, feature is that if a QMS instrument has poor performance it is sometimes possible to obtain significant improvement by re-connecting the electrical supplies so that the *x*-rods and the *y*-rods, Fig. 1, are interchanged. This is similar to the effect noted by Ding *et al.*,[8] who exchanged the connections on a QMS constructed with *x*- and *y*-rods with different diameters. The effect is also shown by Konenkov *et al.*,[11] who show the effects of the addition of a hexapole field, for example caused by changing the positions of *y*-rods. They show that effects of such additional fields can be reduced by interchanging the *x*- and *y*-rods.

A cross-section of a QMS filter is shown in Fig. 1 with the axes labelled in the conventional manner. It is usual to refer to the rods intersected by the *x*-axis as the *x*-rods and those intersected by the *y*-axis as the *y*-rods. Both *x*-rods have the same voltage $U - V\cos\omega t$ applied to them while both *y*-rods have a voltage $-U + V\cos\omega t$ applied (minor

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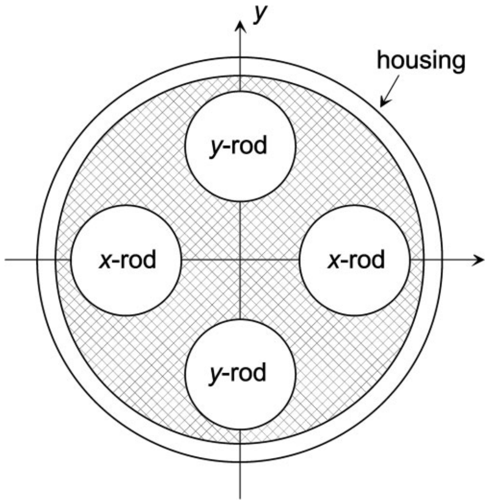


**Figure 1.** Cross-section of a QMS filter.

variations of these expressions may be used, for example $U$ and $V$ may be doubled and a factor 0.5 included). Ions travel through the QMS in the direction of the $z$-axis. In the diagram, the shaded area is free space; the rods and housing are conducting material. For a perfectly constructed device all rods have the same radius, $r$, and the distance between the rods and the axis is denoted by $r_0$, the radius of the inscribed circle that just touches all four rods.

## ELECTRIC FIELD COMPUTATION

Our previous papers[4,5,7] described computations of QMS performance for systems with circular section rods. The method requires that the electric field is known to high accuracy at all positions $x,y$ with $-r_0 \leq x \leq r_0$ and $-r_0 \leq y \leq r_0$. The model uses the field values to determine the motion of ions as they travel through the filter in the $z$-direction. The fields may be determined using any method of computation provided the values are of sufficiently high accuracy. If the rods are long enough, it is sufficient to determine the electric field in the instrument ignoring the effect of rod length; this reduces the field computation from a three-dimensional problem to a two-dimensional one.

Our computation of the field[4] to the necessary high degree of accuracy was completed in a long, but acceptable time, by using the many symmetrical features of the QMS. The technique is not applicable to investigations of QMS filters with manufacturing errors that remove the symmetry, as the computation time becomes excessive. Attempts to use commercial field calculation packages were unsuccessful, as agreement with experimental observations was poor when the fields produced were used to model QMS behaviour. However, we have now used Poisson Superfish;[12] a program produced for particle accelerator design by Los Alamos National Laboratory (LANL). This produces fields that meet the requirements of our QMS model; fields computed with Superfish for correctly positioned round rods gave results with our model that were almost the same as those using our own field values. The LANL package does not rely on any symmetrical features of the QMS and the over-relaxation method results in a computation time about two orders of magnitude less than our method.

Computation of the two-dimensional field values is apparently a simple problem. Figure 1 is the cross-section of a QMS filter; all that is required to compute the fields in infinitely long QMS is the determination of the potential throughout the free space region: that is the area inside the housing not occupied by the rods. The housing has no significant effect[5] provided that it has a radius of at least $3.6 \times r_0$. The computation requires solution of Laplace's equation in two dimensions with boundary conditions of 0 V at the housing surface, +1 V at the surface of the $x$-rods and −1 V at the surface of the $y$-rods with a scale such that $r_0 = 1$ unit. The field at any point is the gradient of the potential and, as it is a conservative field, the values required by the QMS model are obtained by scaling the computed values to match the actual QMS dimensions and voltages.

Most field evaluation methods require a grid, a mesh, of points in the solution region and use one of several standard numerical techniques to determine the potential at every mesh point. The accuracy to which the field must be computed depends on the geometrical form of the grid, the mesh size and the numeric precision of the computer; these quantities tend to interact so that modifying one changes the requirements for the others. Our previous computations[5,7] used a simple relaxation method with a uniform square grid throughout the shaded area except where it intersects the electrodes. At the intersections an interpolation technique was used and significantly improved the field values compared with those when the rod surface was approximated to fit exactly to points on the grid. We determined the necessary mesh size and the degree of accuracy for the potential by repeatedly decreasing the grid interval and increasing the number of iterations until no significant change was observed in the behaviour of the QMS model. The model predictions matched the measured behaviour of real filters as far as it is possible to perform comparisons.

Our final selection of grid interval was $r_0/800$, and such a large number of iterations were required that we let the iteration process continue to the limit of the computer accuracy rather than include elaborate tests to end the iteration process. Without the interpolation technique, a much smaller grid interval is required; this greatly increases the field computation time. Attempts to convert the computation process to use over-relaxation methods were not successful.

The Superfish program is also a relaxation method but uses triangular mesh elements rather than square ones and has a number of sophisticated techniques that enable it to apply over relaxation methods. Our first test with Superfish was to determine the field for an ideal circular electrode QMS with $r/r_0$ at the near optimum value of 1.127. This field and our own field values were both used to simulate the behaviour of identical filters. Figure 2 shows one particular simulated QMS peak created using the parameters in Table 1; the resolutions, $\Delta m/m$, at half height for these settings are $1/335$ (simple relaxation) and $1/320$ (Superfish). In general, the peaks are almost identical in shape but the



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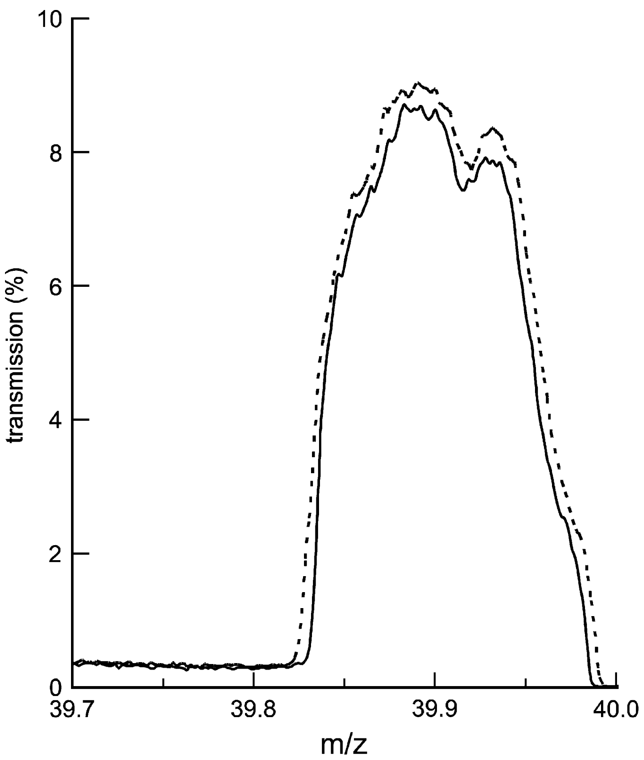


**Figure 2.** Computed peaks for settings in Table 1; fields determined with our relaxation method (solid line) and Poisson Superfish (broken line).

**Table 1.** QMS parameters used to compute Figs 2–8

| Parameter | Value |
|---|---|
| Rod length | 254 mm |
| $r_0$ | 2.76 mm |
| $r/r_0$ | 1.127 |
| Housing radius ($3.6 \times r_0$) | 9.936 mm |
| Frequency | 2 MHz |
| Resolution setting $\eta$ | 0.998 |
| Ion $m/z$ | 40.0 |
| Number of ions injected at each mass point | $10^5$ |
| Ion source radius (uniformly illuminated) | 0.5 mm |
| Ion energy | 2.0 eV |
| Ion beam divergence | 0 (ions parallel to $z$-axis) |

peak using the Superfish field for the selected conditions is very slightly larger, is slightly broader and its mass centre is at a marginally higher position. The differences are small and repetition of many of our previous computations using fields for different $r/r_0$ values gave similar results for high values of $r/r_0$, but for lower values the peaks were the same size or the one using our fields was the larger. This suggests that Superfish generates fields corresponding to a very slightly larger value of $r/r_0$ than the one using our computation method.

It is probable that the reason Superfish produces acceptable results for the QMS field whereas other packages, most of which use the finite element technique, do not is a feature of the mesh. Using relaxation or finite element methods, the mesh is usually generated automatically. Our own method of a uniform mesh is simple and does not require automatic generation; elements are the same size at all positions except where the mesh intersects conductors where interpolation corresponds to mesh elements that closely fit the electrode shape. Superfish mesh generation is similar; the elements are triangular and, although not identical, do not vary in size by large amounts in different regions of the QMS system.

Nearly all commercial field determination packages were developed to solve problems in fluid mechanics or material stress analysis then adapted for electric field problems. Their automatic mesh generators produce mesh elements, usually triangular, of significantly different shapes and sizes. This is because the type of problem for which they were developed is usually concerned with effects in regions of rapid change. The mesh generator identifies regions in which geometrical conditions change rapidly and produces a much finer mesh in these regions than elsewhere. For a QMS, such a mesh generator creates many small elements close to the rods and only a few large ones near the central axis. Thus high resolution is obtained near the rods and poor resolution closer to the centre. However, in a QMS filter, and in particle accelerators for which Superfish was developed, most charged particles that pass through the system do not travel close to the electrodes and the most accurate field values are required in the region near the axis rather than close to the rods.

Another feature that affects accuracy is that our method and Superfish are able to use many more mesh elements, typically 10 to a 100 times more, than most commercial finite element packages.

The differences apparent in Fig. 2 are probably another feature of the mesh generation. Our interpolation technique should accurately fit the grid to the rod at all points of intersection; it approximates the rods to a large number of chords internal to the rod surfaces. The Superfish mesh is a set of triangles external to the rods and the result is that the rods are modelled as many sided polygons external to the rods; this corresponds to a slightly larger effective value of $r$ and smaller value of $r_0$ and hence increases $r/r_0$.

Because Superfish is able to produce electrical field values for a QMS instrument without relying on symmetrical features, it was possible to use the package to determine fields for systems with simulated manufacturing defects. In general, complex combinations of such defects may occur, but to determine the effects of imperfections it is convenient to model each type of defect separately. The most common defects are those of wrongly positioned rods and rods that do not have identical diameters. A feature of these defects is that they produce poorer peak shape and lower transmission and sometimes result in spurious additional peaks. Spurious peaks on the low mass side of the main peak are precursors and those on the high mass side are post-cursors; precursors are the more commonly observed form of spurious peak.

## QUADRUPOLE LENGTH AND MASS SCAN

The theoretical consideration of a QMS instrument assumes that it is operated by setting the ratio of the magnitude of the d.c. voltage, $U$, and amplitude of the a.c. voltage, $V$, to a fixed

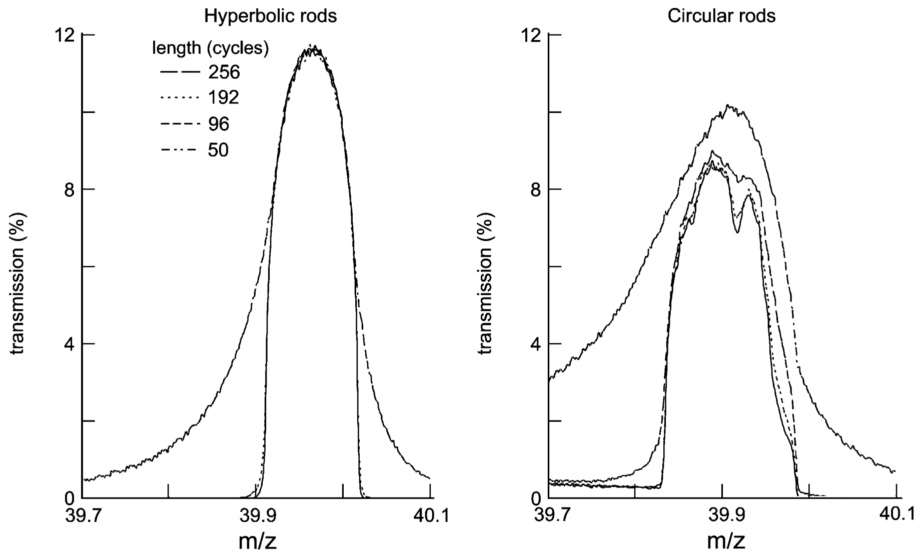


**Figure 3.** Variation of QMS filter performance with QMS length.

value and varying both voltages to perform a mass scan. This results in constant resolution $\Delta m/m$ throughout the scan. Many commercial instruments apply an offset to the d.c. voltage such that $U = kV + c$ instead of $U = kV$. With careful choice of $k$ and $c$, this results in $\Delta m$ remaining almost constant throughout the scan which users prefer. However, this method corresponds to the instrument resolution changing at every point on the mass scale, whereas examination of the effects of varying construction on QMS behaviour requires consistent behaviour. Therefore all our model predictions are with $U = kV$, that is constant resolution. As in previous papers we define the resolution setting by $\eta$ so that $U = \eta kV$ where $k \approx 2.979$ and corresponds to the peak of lower stability zone;[3] hence $\eta = 1$ corresponds to the limiting value of resolution. Although some results are presented for a range of values of $\eta$, most comparisons are illustrated for the case $\eta = 0.998$.

Behaviour of a QMS depends on the number of cycles of the radiofrequency field experienced by an ion as it travels through the instrument. Therefore, the best method of defining QMS length is by the number of radiofrequency cycles seen by ions rather than by the physical length. We define QMS length as this number of radiofrequency cycles which depends on the ion velocity, the actual QMS length and the radiofrequency $\omega$. Because ions are injected into a QMS so that all have the same kinetic energy, their velocities are a function of mass. Thus low mass ions travel faster and experience fewer cycles of the radiofrequency field than high mass ions and the QMS length varies with ion mass. As we showed previously for circular electrodes,[4] once the number of cycles experienced by an ion exceeds some value, the behaviour of the QMS filter does not change significantly if the number of cycles is further increased. However, if the length is below this optimum value for low mass ions, a QMS filter will exhibit a mass-dependent behaviour. Figure 3 illustrates how the predicted peak shape varies with number of cycles for an ideal hyperbolic electrode system and for a system with correctly positioned round rods. For hyperbolic rods a QMS length corresponding to the lowest mass ions experiencing about 150 cycles of the field is generally adequate; for a perfect round rod system a similar length is adequate although some further changes in peak structure are observed if the system length is increased up to about 250 cycles. Resolutions for the maximum length cases in Fig. 3 are $1/405$ for hyperbolic rods and $1/350$ for circular section rods. As we will show, if one of the rods is displaced, variation of behaviour with length is more complicated.

## INITIAL PREDICTIONS OF THE BEHAVIOUR OF AN IMPERFECT QMS

The range of possible imperfections and the manner in which they interact with the various QMS parameters are extremely large and as a result it is impossible to present all possible cases. We have modelled a very common imperfection and the results show features that have been observed in real instruments.

Radial inward displacement of one rod is a common fault, as it corresponds to a rod not fitting correctly into the supports. Our first investigation was to examine the same peak as that used for Fig. 2 with one rod displaced so that it was closer to the axis than it should be by $0.005 \times r_0$. For a large QMS, $r_0$ is typically 10 mm and this displacement is 50 μm, smaller systems have $r_0$ about 2.5 mm with $0.005 \times r_0 = 12.5$ μm, while microquads[13] have $r_0$ of 1 mm or less and this displacement is $\leq$5 μm. Figure 4 compares the original peak with correctly positioned rods, the peak when the $x$-rod is moved and the peak when the $y$-rod is moved.

The first observation is that when the $x$-rod is moved the peak position moves but there is only a small change in the peak size and shape. When the $y$-rod is moved large effects are observed. This behaviour matches the feature that exchanging the connections to the $x$ and $y$-rods sometimes improves performance of a QMS. It is only displacement of the $y$-rod that seriously affects behaviour so if poor performance is caused by a displaced $y$-rod, the exchange converts it into an $x$-rod and it has a much smaller effect.

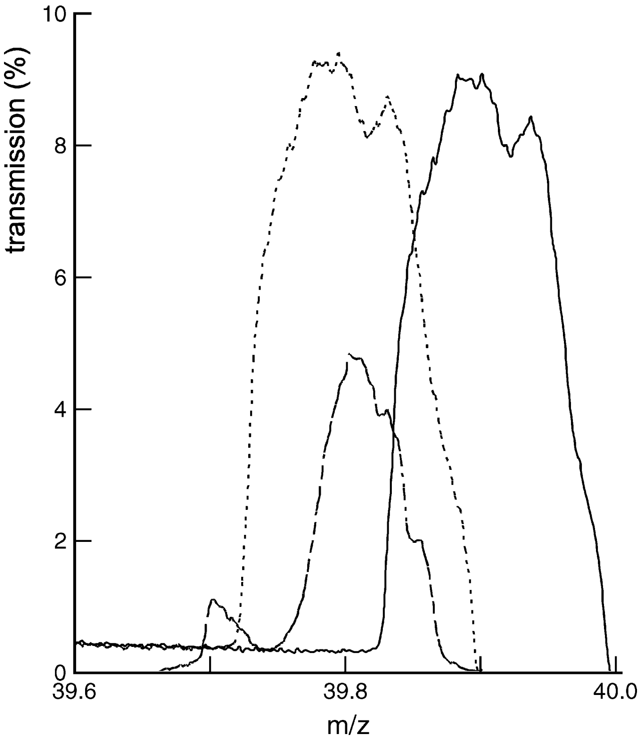


**Figure 4.** Effect of inward radial movement of one rod; solid line no movement, dotted line $x$-rod moved, chain line $y$-rod moved.

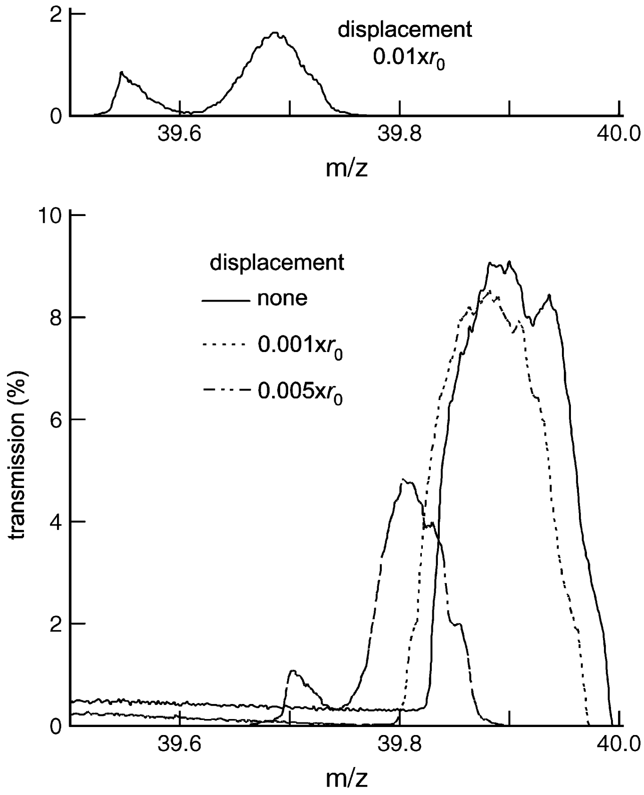


**Figure 5.** Variation of QMS filter behaviour with radial inward $y$-rod displacement.

The second obvious effect is that for this particular QMS at the selected operating conditions movement of the $y$-rod causes the peak to split into two parts; that is a precursor is observed. The height and position of the main peak are not the same as those when the rod is not moved. The change in position with movement of an $x$-rod or a $y$-rod may in part be attributed to a change in $r/r_0$. If one rod is moved, it is difficult to define $r_0$, but it might be considered to be some average of the rod positions. In our previous paper[5] we did not comment on the fact that when $r/r_0$ is changed the position of the mass peaks changes, although this can be deduced from Fig. 1 in that paper. It was not discussed because the effect cannot be easily measured in real instruments as, although the voltages set the mass scale, the mass scale used in practice is obtained by calibrating the system using a sample of known composition rather than by using computed voltage values.

Other effects are that the low mass tail we described previously[7] which is present when the ion source diameter is relatively large is missing when the $y$-rod is displaced. There is some evidence of structure on the high mass side of the displaced rod peak, although this may just correspond to the structure observed on peaks when the resolution is not set to a very high value. An improvement is that the main peak width is reduced; however, although this is desirable, as is removal of the low mass tail, the precursor makes the system unusable.

## INVESTIGATIONS OF ROD DISPLACEMENT

An obvious investigation is to observe the effect of changing the radial $y$-rod displacement; Fig. 5 shows the behaviour corresponding to the settings of Table 1 as the radial displacement of the rod is changed.

Very small $y$-rod displacements, up to about $0.001 \times r_0$, have only a small effect; they cause a small movement of the peak position but there is no significant change in the peak shape. As the displacement is increased a precursor appears, and both precursor and main peak move towards a lower mass position with increasing displacement. The main peak height decreases with displacement, but once there is a distinct precursor its height is almost constant until the displacement is over $0.01 \times r_0$. Precursor and main peak separation increases as displacement increases; alternatively this can be stated as the main and precursor positions change at different rates with displacement. Both changes in position are approximately linear functions of the rod displacement.

We also moved the rod radially outward, although this fault is less likely to occur with most rod mounting mechanisms. The form of the peak for an outward displacement was almost the same as that for an inward displacement by the same amount; the only significant difference was that outward movement caused the peak to move to a higher mass position instead of to a lower mass position.

## QMS LENGTH

The effect of changing QMS length on peak shape is simple and easily described for hyperbolic and perfect round rod QMS systems; variations of peak shape with QMS length is more complex when one rod is displaced. Figure 6 is produced in the same manner as Fig. 3 but is for the case of a rod displaced radially inward by $0.005 \times r_0$. The behaviour

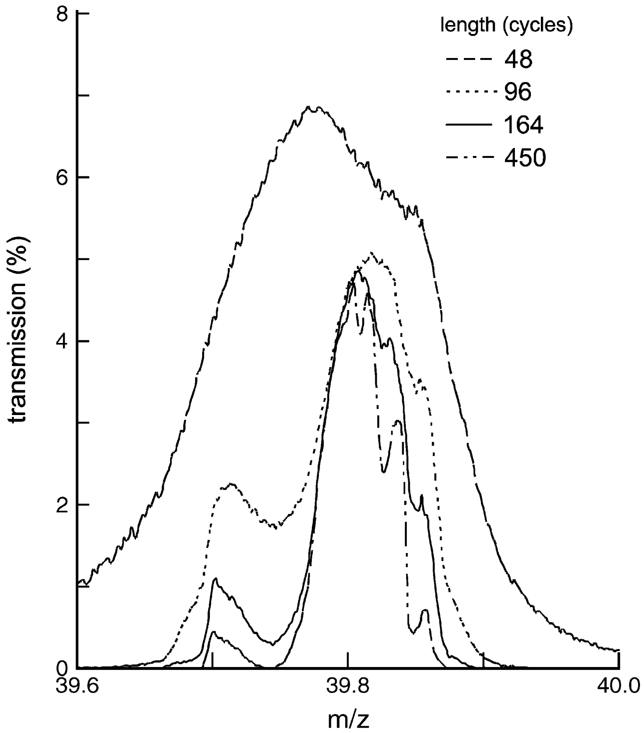


**Figure 6.** Variation of QMS filter performance with QMS length when one $y$-rod is displaced radial inward by $0.005 \times r_0$.

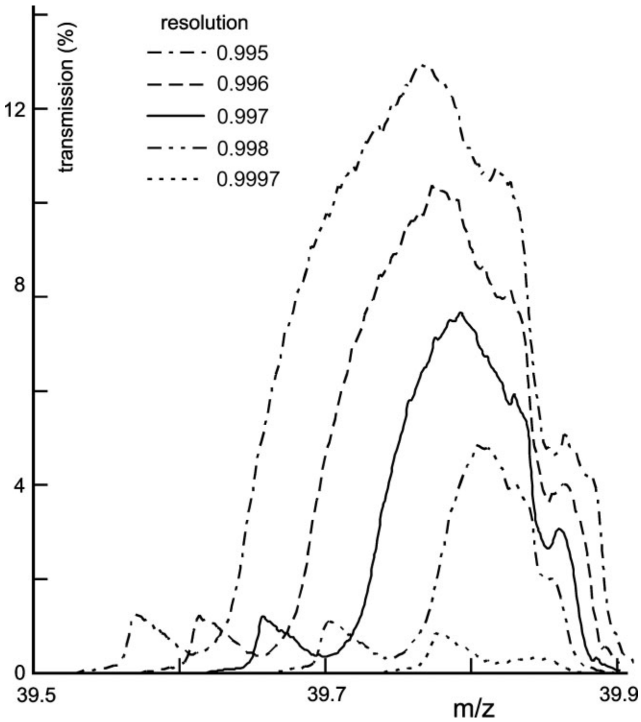


**Figure 7.** Effect of resolution setting on a QMS filter with a single $y$-rod displaced.

is quite complicated, although the main peak and precursor are fully formed by 150 cycles: about the same length as appears adequate for perfect filters. However, as for the perfect round rod, the detailed shape continues to change as the length increases. The shape is complex and continues changing significantly for much longer; the filter must be over 400 cycles long before further changes are insignificant.

To summarise, a very short QMS with a displaced rod shows no precursor or other structure in the peak; the only apparent effect is a reduced peak height. As the length is increased, the precursor and, eventually, a small post-cursor appear. Increasing the length further results in the structure becoming more complex. It should be noted that while this behaviour is typical, the details vary with resolution setting.

## EFFECT OF RESOLUTION SETTING WHEN A ROD IS DISPLACED

Results described so far have been for QMS operation with moderate resolution, typically having $\Delta m/m$ in the range 1/300–1/400. If the setting of the system is changed for operation at a significantly different resolution, the behaviour with a radially displaced rod also changes although the general trends are similar.

The effect of changing the QMS resolution setting, $\eta$, with all other settings kept constant was investigated for a system with a displaced $y$-rod. Figure 7 illustrates typical results with settings, except $\eta$, as in Table 1 and one $y$-rod displaced by $0.005 \times r_0$.

The features apparent in Fig. 7 are typical, although details vary with QMS parameters and rod displacement.

- The main peak moves slightly with resolution setting changes; the amount is similar to that observed for a perfect system.
- The main peak height, although less, decreases with increased resolution setting in a manner similar to that observed for a perfect system.
- The precursor position moves by a larger amount than the main peak as resolution setting is changed.
- The precursor height is almost independent of resolution setting.
- The precursor peak is steeper on the low mass side than the high mass side, whereas normal peaks of perfect filters are usually steeper on the high mass side.
- At high resolution the precursor height exceeds the height of the main peak and the precursor continues to be observed for $\eta$ slightly above the limiting value of 1.0.
- At very high resolution the peak structure on the high mass side may be considered a post-cursor.

When a precursor is present, the main peak is not as wide as it is for a perfect system with the same settings, and this is apparent in Fig. 4. Figures 4 and 6 suggest that an alternative description of behaviour of a QMS with a displaced $y$-rod is that a section of the peak is removed. Starting on the low mass side of a scan, the peak rises normally to some level that is almost constant for the particular geometry and rod displacement. From this point, transmission starts to be severely reduced with the reduction increasing as the mass position increases; eventually transmission starts to rise again meeting the falling high mass edge of the peak and creating a double peak effect. The normal method of adjusting QMS controls is to adjust the resolution setting until the desired peak width is obtained rather than setting the controls to measured voltages corresponding to computed values. Using this method an instrument with a displaced rod will be set to a lower value of $\eta$ than one which is perfect and the structure will be interpreted as an additional precursor peak.

## ATTEMPTS TO CORRECT IMPERFECTIONS

A patent by Burns *et al.*[14] describes a method of improving the performance of a QMS instrument that appears to have manufacturing defects. The patent indicates that if the poor performance is caused by a radially inward displacement of one rod, then this will increase the electric field generated by this rod. If the voltage on the displaced rod is slightly reduced without changes to voltages on the other rods, it should be possible to compensate for the effects of the manufacturing error.

Superfish is able to determine the fields for systems with different potentials on each rod, and therefore we used our model to confirm that the patent is correct. Figure 8 uses the settings from Table 1 when one $y$-rod is displaced by $0.005 \times r_0$. The voltage on the displaced rod is decreased by small amounts resulting in the changes to peak shape shown. The model confirms that the patented technique does significantly improve the QMS performance; in this case a reduction by $0.01 \times (-U + V \cos \omega t)$ in the voltage applied to the displaced rod is required to correct for the rod displacement. Further decreases in the voltage on the displaced rod cause the performance to deteriorate with a precursor re-appearing. As for other changes, the peak position changes when the voltage on a single rod is changed,

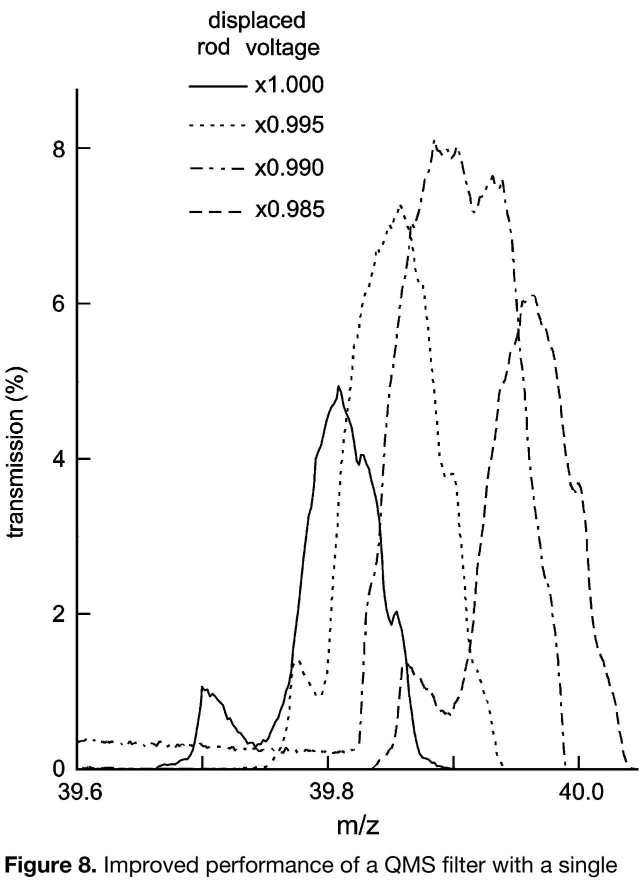


**Figure 8.** Improved performance of a QMS filter with a single $y$-rod displaced by $0.005 \times r_0$. The voltage on the displaced rod is changed by the factors indicated.

the peak moving to higher mass positions as the voltage is decreased. In general, it was found that small changes by a fraction $\alpha$ in a single rod position could be compensated by a change of $2 \times \alpha$ in the voltage applied to that rod.

## CONCLUSIONS

Our modelling technique combined with electric fields computed using the LANL Poisson Superfish program predicts the behaviour of imperfectly constructed QMS systems. The results confirm the poorly documented feature that a small radial displacement of one $y$-rod in a QMS system results in severely reduced performance. A similar displacement of an $x$-rod changes the peak position but has little effect on the peak shape and will not affect the performance of any real instrument. This is one possible explanation why the performance of a QMS may sometimes be improved by exchanging the electrical connections so that the $x$- and $y$-rods are exchanged.

The behaviour of an imperfect QMS with a displaced $y$-rod will depend on the amount by which the rod is displaced, the number of cycles experienced by an ion, the form of the injected ion beam and the resolution setting. In general, $y$-rod displacement results in a much lower transmission and may result in production of precursors and post-cursors.

The effects of rod displacement combined with variation of all QMS operation conditions were found to be many and complex. However, we suggest that the established description that a precursor is formed might not be strictly correct. It is probable that when a poorly constructed instrument is calibrated, a lower resolution setting is used; the actual effect of rod displacement is an extremely distorted peak shape with a section the peak removed.

The precursor form is not a strong function of resolution setting but is a function of QMS length. Hence, except for very short, very low resolution QMS filters, required manufacturing tolerances are similar for low and high resolution instruments. Our computations suggest that in the absence of other faults a QMS filter should have the $y$-rods positioned to within $0.001 \times r_0$. These suggested limits are for radial displacement assuming identical diameter rods that are parallel and have no tangential displacement.

The difference in peak shape with a precursor having a steep low mass side and less steep high mass side combined with the insensitivity of precursor height to resolution setting suggests that adjusting resolution setting and observing peak shapes may provide additional confirmation that an instrument is poorly constructed and is producing precursors.

Finally, the patented technique of adjusting the voltage of one rod to correct for imperfect manufacture appears to achieve the required objective of compensating for mechanical imperfections by adjusting the applied voltage. At present we have only investigated this over a limited range of QMS settings.

## REFERENCES

1. Paul W, Steinwedel H. Ein neues massenspektrometer ohne magnetfeld. *Zeitschrift für Naturforschung* 1953; **8a**: 448.

2. Brubaker WM. Comparison of quadrupole mass spectrometers with round and hyperbolic rods. *Journal of Vacuum Science and Technology* 1967; **4**: 326.
3. Dawson PH. *Quadrupole Mass Spectrometry and its Applications*. Elsevier: Amsterdam, 1976.
4. Gibson JR, Taylor S. Prediction of quadrupole mass filter performance for hyperbolic and circular cross section electrodes. *Rapid Communications in Mass Spectrometry* 2000; **14**: 1669.
5. Gibson JR, Taylor S. Numerical investigation of the effect of electrode size on the behaviour of quadrupole mass filters. *Rapid Communications in Mass Spectrometry* 2001; **15**: 1960.
6. Douglas DJ, Konenkov NV. Influence of the 6th and 10th spatial harmonics on the peak shape of a quadrupole mass filter with round rods. *Rapid Communications in Mass Spectrometry* 2002; **16**: 1425.
7. Gibson JR, Taylor S. Asymmetrical features of mass spectral peaks produced by quadrupole mass filters. *Rapid Communications in Mass Spectrometry* 2003; **17**: 1051.
8. Ding C, Konenkov NV, Douglas DJ. Quadrupole mass filters with octopole fields. *Rapid Communications in Mass Spectrometry* 2003; **17**: 2495.
9. Story MS. Pacific conference on chemistry and spectroscopy, 1969.
10. Dawson PH. Ion optical properties of quadrupole mass filters. *Advances in Electronics and Electron Physics* 1980; **53**: 153.
11. Konenkov N, Londry F, Ding C, Douglas DJ. Linear quadrupoles with added hexapole fields. *Journal of the American Society for Mass Spectrometry* 2006; **17**: 1063.
12. http://laacg.lanl.gov/laacg/services/download_sf.phtml [accessed 2007].
13. Taylor S, Tindall RF, Syms RRA. Silicon based quadrupole mass spectrometry using micro-electromechanical systems. *Journal of Vacuum Science and Technology* 2001; **B19**: 557.
14. Burns DM, Taylor S, Gibson JR. Quadrupole mass filter, UK Patent GB2390222, 2004; US Patent 6940068 2005; European Patent EP1649488 2006.




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