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PERFORMANCE SIMULATION OF A RESIDUAL GAS ANALYSER OPERATING IN THE FIRST AND THIRD STABILITY ZONES

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Quadrupole Mass Filter (QMF) Overview

- One component of a Quadrupole Mass Spectrometer/Residual Gas Analyser.
- Selective mass to charge ratio filtering.
- Ideal electrodes are hyperbolic.
- Circular electrodes more common.
- Rectilinear electrodes more suitable for MEMS fabrication.

POTENTIAL FIELD DISTRIBUTION

HYPERBOLIC ELECTRODES
\[ \Phi(x,y) = \frac{A}{\sqrt{x^2 + y^2}} \]

CIRCULAR ELECTRODES
\[ \Phi(x,y) = \sum_{n=0}^{\infty} \frac{A_n}{r^n} \]

Mass Scan Lines
Zones 1 and Zone 3

Performance simulation Why is it important?

- Quantify effects of electrical and mechanical tolerance on QMF performance.
- Improve product cost performance by targeting design development to key areas.
- Develop new techniques for assessing performance.
- Present understanding may be inadequate when applied to MEMS electrostatic lenses.
- Attempt to apply different technologies to advance instrument design for novel applications.

Stability zones

- Large number of stable operating zones. Only a small number of practical interest.
- Zone 1 most common.
- Excitation amplitudes vary with zone, lowest for zone 1.
- Achievable resolution and sensitivity varies with operating zone.

POTENTIAL FIELD

\[ \omega = \frac{U}{M} \]

\[ \omega = \frac{V}{Q} \]

End view of micro-engineered quadrupole lens with 500 µm electrode radius [1].
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Computer simulation
- Identify optimum r/r0 ratio.
- Characterise performance sensitivities.
- Increase understanding of novel electrode topologies.

Simulation Software
- Public domain and custom software used.
  - Custom software for hyperbolic electrode mass filter.
    - QMS2-Hyperbolic for ion trajectory simulation.
  - Public domain and custom software for circular electrode mass filter.
    - 2D Field Solver Poisson/Superfish.
    - QMS2-Field for ion trajectory simulation.

Simulation software
- Circular rods –
  - Suite of programs [5,6].
    - Automesh.
    - Poisson.
    - SF7.
    - WSFPlot.
    - Third party tools.
    - DLL allow integration into custom software.

Simulation Software
- QMS2 - Field
  - Solves F = ma by numerical integration.
  - Analytically generated field files and comparison with previously published results used validate software.
  - Uses field data generated Poisson/Superfish.

Circular electrodes - Zone 1
Spectral Response
- Confirm previously reported findings [7,8].
- Peak transmission dependant on r/r0.
- Low mass tail varies with r/r0.
- Peak shape and width varies with r/r0.
- Mass peak shifts to lower m/z value as r/r0 increases.

Circular rods – Zone 3
Spectral response
- Peak shape varies with r/r0, more marked for lower resolution setting.
- Secondary peaks more apparent with lower resolution.
- Low mass tail apparent at lower resolution and extremes of r/r0.
- Peak height difference changes with r/r0.
Circular electrodes – Zone 3

Performance characteristics

- Resolution varies with \( r/r_0 \).
- Peak in resolution at \( r/r_0 = 1.117 \).
- Resolution sensitivity to \( r/r_0 \) greater at higher resolution setting.
- Peak width varies with \( r/r_0 \), more pronounced at higher instrument resolution.
- Peak width minimum occurs at \( r/r_0 \approx 1.117 \) @ Res. 10% PH.

Ion trajectory analysis

- Use Discrete Fourier Transform (DFT) to generate power spatial frequency spectra from time sampled spatial ion trajectory for x and y axis.
- Script written in MatLab to produce ion trajectory spatial power spectra from time sampled ion trajectories generated by QMS2-Hyperbolic and QMS2-Field.
- Good correlation with analytical calculation.
- Spatial power spectra provides an alternative method of assessing the field quality of circular electrodes QMFs.

Hyperbolic Electrodes

Ion Trajectories (Zone 1 & 3)

- Ion trajectories vary with stability zone and operating point.
- Ion trajectories vary with ion entry conditions.
- Greater number of spatial frequencies in Zone3.
- Well defined spatial frequency power peaks.

Circular Electrodes

Ion Trajectories - Zone 1

- Similar ion trajectories to hyperbolic rod.
- Ion trajectory dependent on \( r/r_0 \).
- Increased spatial peaks associated with non ideal fields.
- Increased base power level.

Ion Trajectories - Zone 3

- Ion trajectories similar to hyperbolic rod.
- Ion trajectory dependent on operating point \((a, q)\).
- Ion trajectories dependent on \( r/r_0 \).
- Increased spatial peaks associated with non ideal field.

Alternative Geometries

Square Electrodes

- Approximate circular rod fields with other geometries.
- Ion trajectories similar to hyperbolic and circular rod filters.
- Requires further investigation to identify suitable geometry.
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Alternative Geometries
Square Electrodes 2
- Geometry results in noisy spatial frequency spectrum.
- Multipole coefficients far from ideal. Quadrupole term not close to unity.
- Correlation between spatial frequency plot and multipole coefficients.
- Incorrect peak shape.

Misaligned Y axis electrode
Zone 1
- Mass peak shifts with increasing mass positional error [13].
- Shift direction different for inward and outward displacements.
- Pre cursor evident for both inward and outward displacement.

Misaligned X and Y electrodes
Zone 1
- X electrode displacement results in shift to lower mass position with minor change to peak shape and amplitude.
- Y electrode displacement results in slightly smaller shift accompanied by significant changes to peak shape and structure.

COMPENSATION METHOD - 1
\[-(U-V_o \cos \omega t)/2\]
\[(U-V_o \cos \omega t)/2\]
X \quad Y
\(r_0\)
\(+\) \quad \(-\)

COMPENSATION METHOD - 2
YGAIN = 1 + 2\(\alpha\)
\(-\(U-V_o \cos \omega t)/2\)
\((U-V_o \cos \omega t)/2\)
XGAIN = 1

Where \(\alpha\) = displacement of electrode as a fraction of \(r_0\)
This technique is the subject of a number of patents [14].

Conclusions
- Combination of custom and standard software packages produce powerful and flexible simulation toolset.
- Effects of \(r/r_0\) different for Zone 1 and Zone 3 operation.
- Multipole coefficients give a measure of field quality.
  - Not obvious how to select optimum.
- Power spatial frequencies provide a fast method of identifying an area of interest.
- Methods exist to compensate for mechanical tolerance.
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References and Bibliography


THANK YOU
THE END