POSTER ABSTRACT

A Design and Simulation Tool for Miniature Mass Spectrometers

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The ongoing trend towards miniaturization in mass spectrometry has resulted in the realization 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 miniaturization 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 behavior is described by determining the individual trajectories of large numbers of ions (108) 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 (analtye) 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.. In the case of the QMS the effects of the ratio of circular electrode radius r to electric field radius r0 on the performance characteristics have been investigated for Mathieu stability zone 1 ($a \approx 0.237$, $q \approx 0.706$) and zone 3 ($a \approx 3.16$, $q \approx 3.23$) operation. We demonstrate that the performance sensitivity to r/r0 ratio is different for zone 3 than those previously reported for zone 1. The magnitude and variation of the 'tail' in the mass spectral peak shapes apparent for zone 1 is much decreased for zone 3 and does not influence instrument resolution. Variation in ion trajectories and associated power spatial frequency spectra when operated in zone 1 and zone 3 with varying r/r0 geometrical ratios are also presented. We demonstrate that these provide and alternative method for determining an ideal value for r/r0 in QMS instruments. The effect of instrument size and operating conditions (voltages and frequencies) may also be readily simulated using the program and by this means the choice of an MS instrument for a given application may be determined.

Our simulation methodology is generic and our approach is therefore applicable to other types of MS instruments (e.g. magnetic sector and GC-MS) and we also present preliminary results simulating these systems.