

**A COMPUTER PROGRAM FOR CALCULATING THE PEAK SHAPE, RESOLUTION AND
SIGNAL TO NOISE RATIO IN TIME-OF-FLIGHT MASS SPECTROMETRY**

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We have developed a computer program (Figure 1) for designing time-of-flight mass spectrometers or understanding their operation. The program calculates a probability density function (PDF)^{1,2} for ion arrival time based on a number of input parameters for the ions' physical properties as well as the instrument configuration. The input parameters modeled as full or partial gaussian distributions are (a) ion initial position, (b) ion initial velocity, (c) detector pulse-width and temporal spread from ion gating. The deflection of ions passing through grids or meshes (d) is also input as either gaussian or hyperbolic functions of velocity spread. The instability of the accelerating voltage (input as ppm peak-to-peak ripple) (e) is also taken into account. Up to two mass/intensity pairs are provided (f). The program convolutes the temporal distributions arising from (c), (d) and (e) into a single temporal spread (g). The distributions (a), (b) and (g) are then processed in a numerical integration with a time-of-flight transform operator to yield the PDF (h). We have found this calculation to be useful to determine the best configuration of the components of TOF instruments and an excellent predictor of resolution.

As well as having the numerical integration mode of operation, the program offers a Monte-Carlo mode that generates a prescribed number of virtual ions with input parameters in accordance with the probabilities determined by the distributions described above. This calculation gives a good indication of how the resolution and sensitivity of TOF instruments are linked.

The program has recently been upgraded with a graphical user interface that takes advantage of fast personal computer technology. The new version allows real-time tuning and auto-optimisation of most parameters. Data can be output in standard text format for presentation and further processing by word processors and spreadsheets.

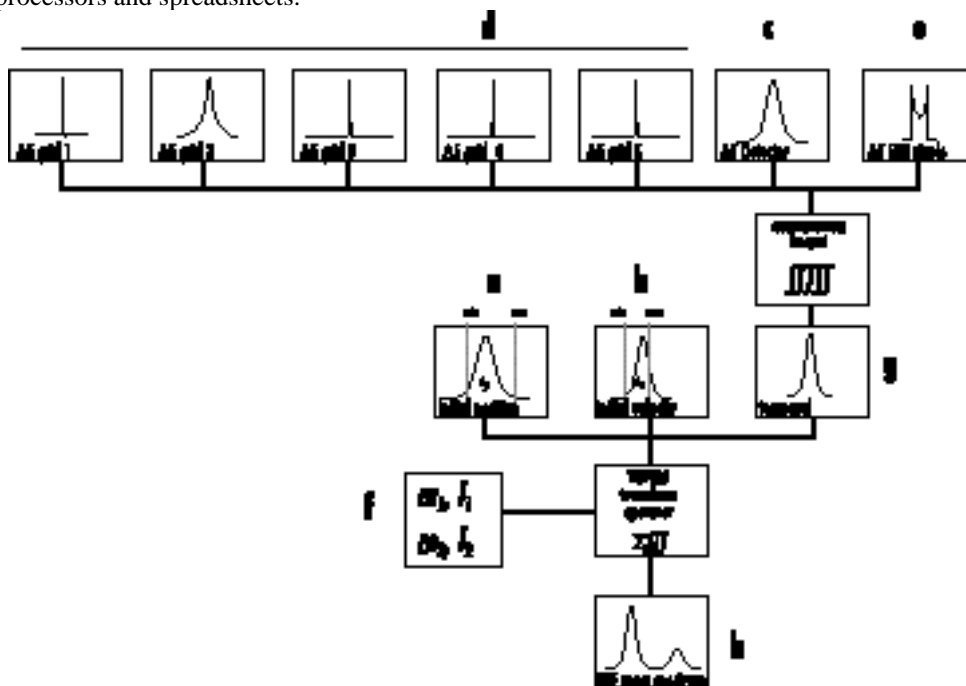


Figure 1

1. R.B. Obsal, K.G. Owens, J.P. Reilly, *Anal. Chem.*, **1985**, 57, 1884
2. J.H.J. Dawson, M. Guilhaus, *Rapid Commun. Mass Spectrom.*, 1989, 3, 155-159

*A copy of this presentation is available at:
<http://www.chem.unsw.edu.au/research/AnalyticalMassSpec>*