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The Application of Dual Channel High Speed Oscilloscope Analog-to Digital Converters to Time-of-Flight Mass Spectrometry

August Hidalgo, Jennifer Sanderson, Kai Chen
Agilent Technologies, Inc., Santa Clara, California

Introduction

Summary Statement: An improved sample rate TOF data acquisition system that has enhanced resolution and dynamic range modes, which run simultaneously.

In TOFMS, the digitization rate of the detector signal has a direct effect on the resolution of the system. Commercially available ADCs have a sample rate which limits resolution and/or a bit depth, which limits dynamic range. Having access to high sample rate ADCs developed for oscilloscopes, a Dual Channel 20GSa/s TOF data system has been developed, resulting in an increase in resolution and in dynamic range. The architecture allows for numerous novel signal processing techniques, thereby allowing optimization to different detector speeds, accommodating decreases in detector pulse width and greatly reducing the detector's pulse width as a contribution to degrading resolution. These resolution enhancements can run simultaneously with an extended dynamic range mode.

Experimental

Component Description and Data System Block Diagram

The TOFMS data acquisition system starts with two DC-8GHz bandwidth pre-amps. The pre-amps gain and bandwidth are programmable, which allows for different detector gains and pulse widths, and to accommodate multiple operating modes. A dual channel 20 GSa/s, 8-bit ADC (analog to digital converter) is configurable to run one channel at 20GSa/s or 2 channels at 10GSa/s, this speed and flexibility will accommodate future decreases in detector pulse width. The digitized signal(s) are read into an FPGA (field programmable gate array). The FPGA's parallel processing power allows for real time signal processing at the full sample rate.

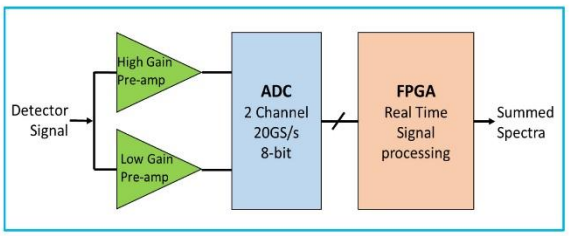

Figure 1. Block Diagram

Experimental

Extended Dynamic Range Mode

The analog signal from the detector is split and routed to two pre-amps, each with different gains. These two signals are digitized at 10GSa/s. This data can be down sampled and filtered in real time. The high gain signal and the low gain signal are combined, which also increases the bit depth to 11bits and greater.

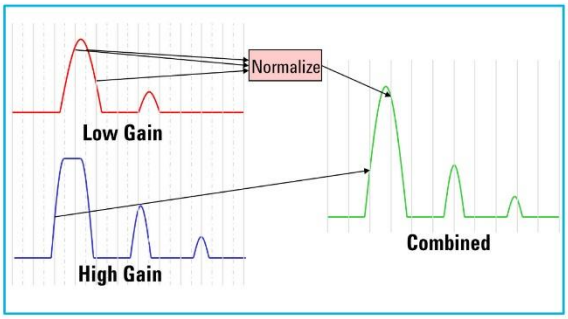

Figure 2. Extended Dynamic Range Mode

High Resolution Mode

In standard operation all digitized points are passed to the summing function. The width of the resultant peak is a combination of the pulse width of the detector and the transient to transient variation in arrival time. In resolution enhancement mode only the digitized data points associated with a peak apex are significant. This data containing both signal response and accurate arrival time is passed to the summing function.

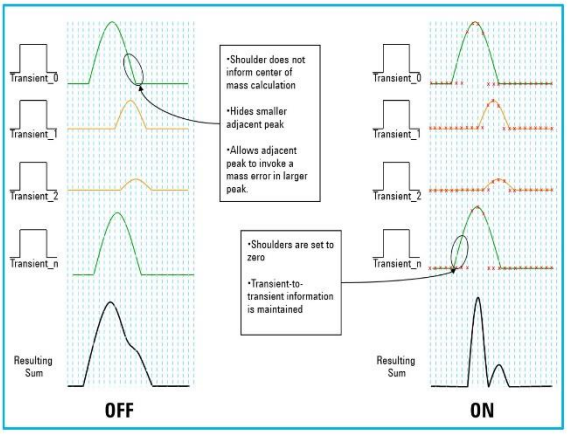

Figure 3. High Resolution Mode

Results and Discussion

System Configuration

The data was taken with the Agilent 7250A GC/Q-TOF. The data system was configured for simultaneous "Extended Dynamic Range Mode" and "High Resolution Mode". These two signals are digitized at 10GSa/s, processed and down sampled to 5GSa/s, increasing the bit depth.

Figure 4. Agilent 7250A GC/Q-TOF

Extended Dynamic Range with High Resolution

Polycyclic Aromatic Sulfur Heterocycles (PASH) compounds were spiked into gasoil matrix and a calibration curve from 100fg/µL to 1,000pg/µL was performed to determine the linear dynamic range in high resolution mode. 4 orders of magnitude were achieved with analytes 2-Methylthiophene, Dibenzothiophene and 4,6-Dimethyl Dibenzothiophene

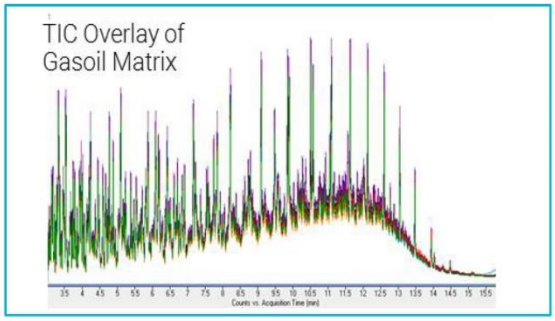

Figure 5. Total Ion Chromatogram (TIC) of gasoil matrix spiked with PASHs.

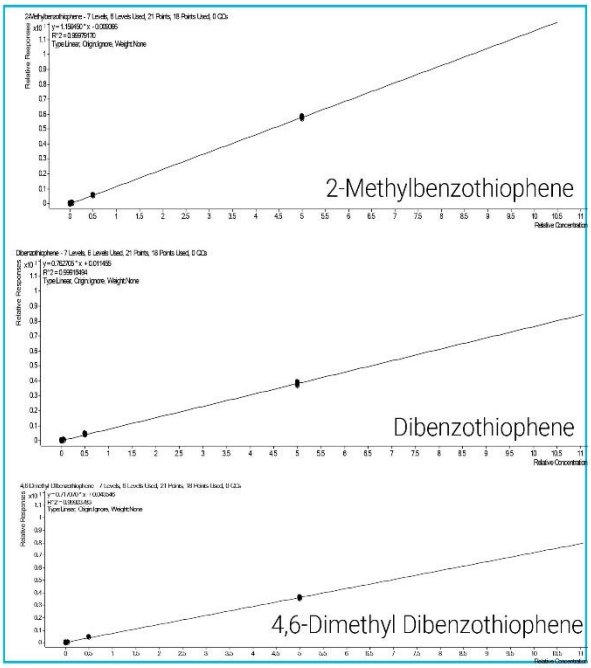

Figure 6. Calibration curves of PASH analytes

At the lowest concentration of the calibration curve, high resolution is maintained for the quantitation ion. Concentrations at or near the saturation point have excellent resolution as well, as can be seen below in Figure 7 and 8.

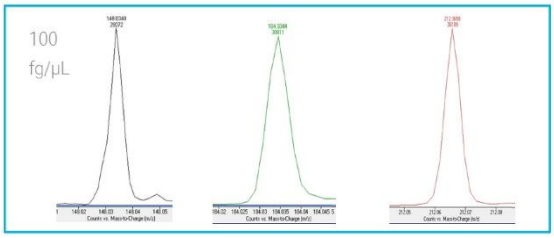

Figure 7. Quantitation ion 100fg/µL: PASH analytes

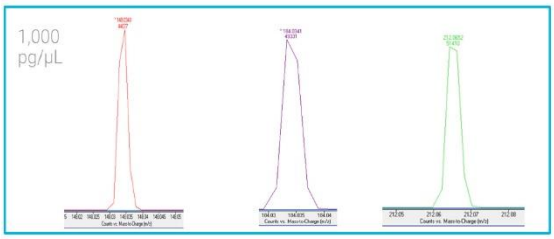

Figure 8. Quantitation ions 1000pg/µL: PASH analytes

Results and Discussion

Detectability Comparison Example

Thiamethoxam, spiked at 5ppb in avocado matrix, have two qualifier ions that are not well resolved and have mass errors of more than 20ppm when measured on prior instrument platforms. The new data system resolves the ions from the matrix interference, resulting in sub-ppm mass error.

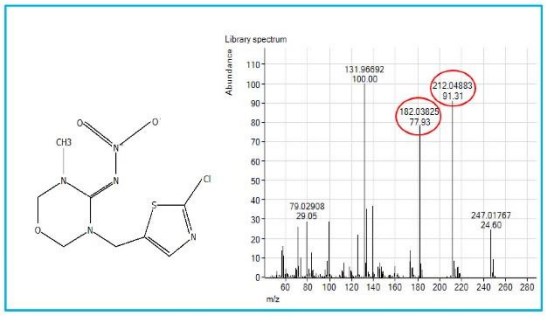

Figure 9. Thiamethoxam in Avocado (5 ppb)

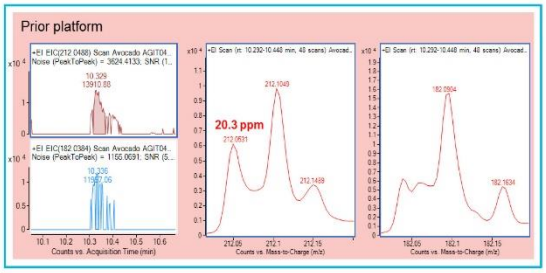

Figure 10. Prior platform result.

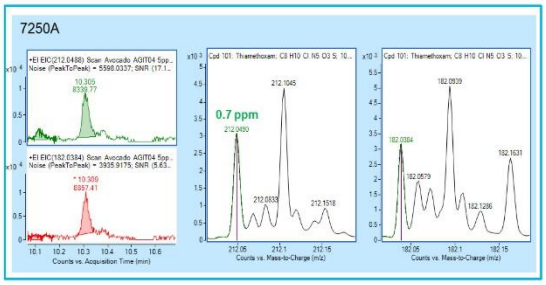

Figure 11. 7250A result.

In-Spectrum Dynamic Range Example

Demonstrated with essential oil an increase from ~3.8 orders of magnitude to ~4.9 with the 7250A

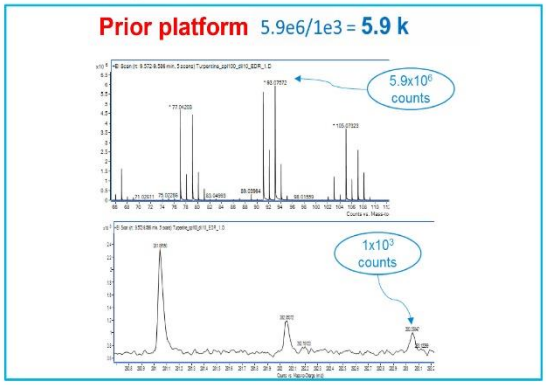

Figure 12. 7200B Ratio of largest to smallest peak with a single spectrum

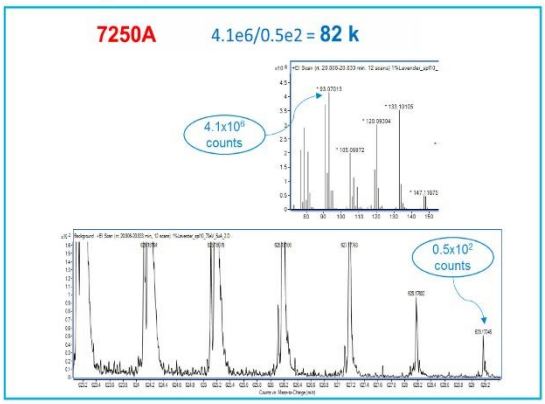

Figure 13. 7250A Ratio of largest to smallest peak with a single spectrum

Conclusions

Highest sample rate and bandwidth TOFMS data acquisition system, allowing for increase in dynamic range without compromising resolution.

Previous limitations to ultimate TOF performance can be significantly eliminated by the use of ultra high speed ADC sampling system combined with real time processing.

Increased resolution improves the detection of trace levels of pesticides in a complex matrix.

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