The use of Desorption ElectroSpray Ionisation with a novel heated transfer line for the analysis of lubricated surfaces

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INTRODUCTION

Desorption ElectroSpray Ionisation (DESI) is a well-established direct ionisation technique for coupling with mass spectrometry. The ion plume is transferred from the sample region into the front of the mass spectrometer via a narrow, metal transfer line. In this work, we present the deployment of a novel heated transfer line (HTL) for the analysis of metal working fluid (MWF) deposited on machined metal components.

METHODS

Mass spectrometer: Xevo™ G2-XS QTof with a DESI™ XS ion source (Waters, Wilmslow, UK)

Acquisition mode: Sensitivity

Capillary voltage: 0.7 kV (+ve/-ve)

Cone voltage: 40 V (+ve/-ve)

Source temperature: 100 ºC

Gas pressure: 7 psi (~48 kPa)

Acquisition range: 50 – 1200 *m/z*

Solvent: 95:5 MeOH:H_2O + 500 pg/µL Leucine Enkephalin for lock mass, flowing at 2 µL/min.

Acquisition rate: 800 µm/s

Step size: 0.2 mm (between acquisition lines)

Acquisition approach: profiling

Samples: 2 x machined metal aperture plates

Protocol: both aperture plates underwent a standard post-machining, cleaning process. One clean aperture plate was soaked in MWF (Blasocut – Blaser Swisslube, Switzerland) for 5 min., then allowed to drip-dry for 5 min. Both plates, clean (blank) and soaked, were mounted side-by-side on microscope slides and positioned on the DESI XS stage (*Figure 1*). The transfer line was heated step-wise via a heater controlled by an applied voltage (*Table 1*). Data were acquired using MassLynx™ v4.2 and processed using MassLynx v4.2 and UNIFI™ v1.9 (both Waters, UK).

RESULTS & DISCUSSION

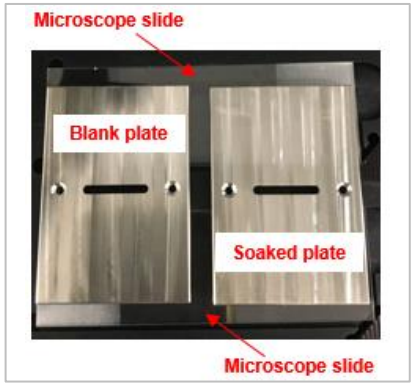

Figure 1. Aperture plates mounted on glass microscope slides and positioned on the DESI XS stage – clean, blank plate on the left and MWF soaked plate on the right.

Table 1. Applied voltages, resulting heater current, and displayed temperature being applied to the HTL – the same values were used for both positive ion and negative ion acquisitions

Voltage (V)	Current (A)	Displayed Temp. (ºC)
0	0.000	26
2	0.682	43
4	1.361	98
6	2.023	191
8	2.676	305
10	3.310	426
12	4.039	563

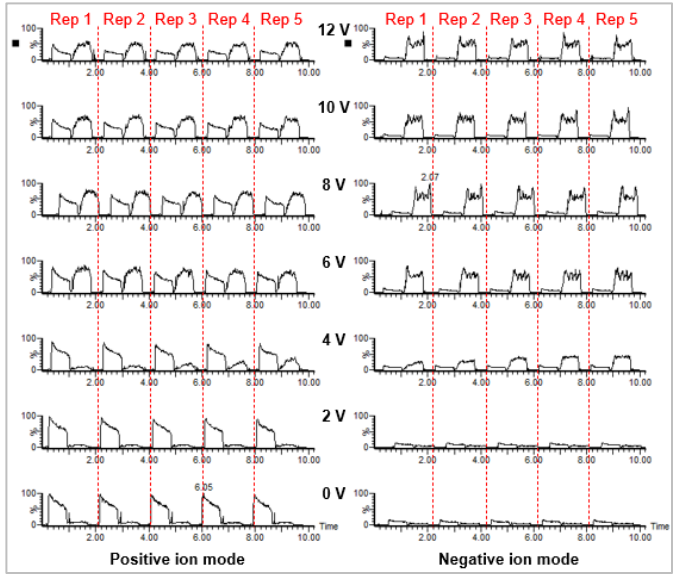

Figure 2. TIC for five replicate lines across the blank and soaked plates at each set voltage from 0 V (ambient temperature) to 12 V (maximum temperature) with the positive ion y-axes (% Intensity) linked, and the negative ion y-axes (% Intensity) linked.

CONCLUSIONS

- A higher temperature applied to the HTL showed clear benefit for analysing the deposited MWF, in both positive ion mode and negative ion mode.
- In positive ion mode, a polymeric component of the MWF was observed at higher temperatures that was not observed at ambient temperature. This polymer was not observed at all on the blank plate.
- The Δ*m/z* of the polymer was 44, suggesting it is poly(ethylene glycol) (PEG).
- In negative ion mode, a similar increase in regularly spaced clusters of ions was observed. These clusters of ions were not observed at all on the blank plate.
- The Δ*m/z* between the ion clusters was 14, suggesting these are different series of hydrocarbons. This is indicative of the base oil used in the MWF.
- The key components of the MWF would not have been observed using a transfer line at ambient temperature – full characterisation of the MWF was only possible using the novel HTL.

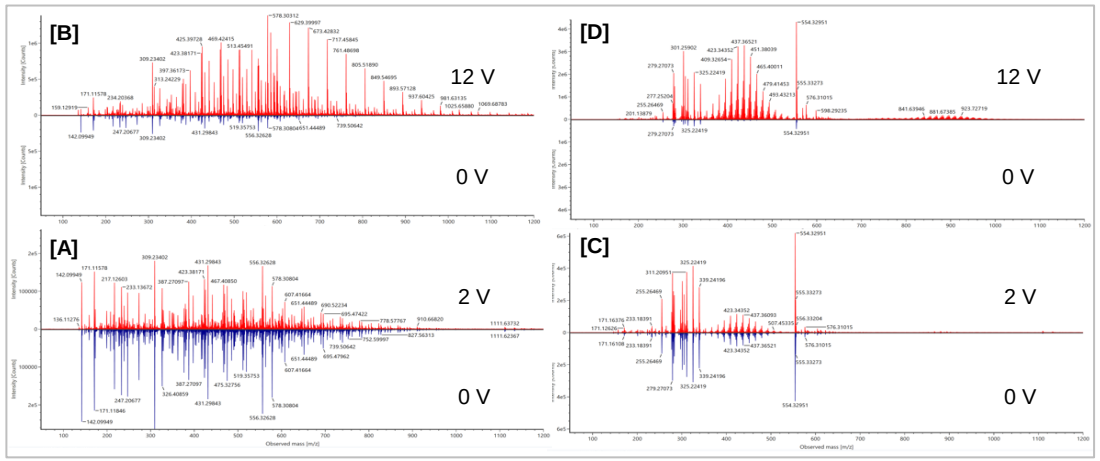

Figure 3. [A] Soaked plate, positive ion mirrored spectra with linked axes, 0 V compared with 2 V. [B] Soaked plate, positive ion mirrored spectra with linked axes, 0 V compared with 12 V. [C] Soaked plate, negative ion mirrored spectra with linked axes, 0V compared with 2 V. [D] Soaked plate, negative ion mirrored spectra with linked axes, 0V compared with 12 V.