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The road to rejuvenation: using FT-ICR mass spectrometry to investigate renewal of roads by rejuvenation of bitumen.

BENEDICT GANNON[1], ANCY KUMAR[1], LATIFA ALOSTAD[1], RORY P DOWNHAM[1], DERYA KAYA OZDEMIR[1], TONY MCNALLY[1], ANAND SREERAM[2], GORDON AIREY[2], CHRISTOPHER H VANE[3] AND MARK P BARROW[1]

[1]University of Warwick
[2]University of Nottingham
[3]British Geological Survey

Bitumen binder is a complex organic mixture that holds together most roads in Britain. When it is laid at high temperatures and over time with UV exposure and traffic, the bitumen undergoes a chemical aging that changes the distribution of molecule classes it comprises, changing its physical properties and making it more prone to rutting and cracking. Renewal of bitumen rather than replacement is a more sustainable approach to maintenance of road networks.

A rejuvenator is a substance that can be added to used bitumen to restore its useful properties, allowing it to be re-used in roads. One potential rejuvenator is waste cooking oil.

Presented here is analysis by ultra-high resolution Fourier transform ion cyclotron mass spectrometry (FT-ICR) of virgin, aged, and subsequently rejuvenated bitumen samples. These samples have been rejuvenated by both commercial rejuvenator and by waste cooking oil at various concentrations to determine the change in the chemical make-up of the bitumen, and how this can correlate with its physical properties.

Briefly, the spectra contain species within the range of *m/z* 200-1200. The resolving power was sufficient to differentiate species that differ by a mass of 3.4 mDa, which is essential for the analysis of complex mixtures with sulfur-containing species. Between 12,000 and 18,000 species were assigned in each spectrum, with root mean squared (RMS) errors of less than 0.2 ppm. Samples were ionised by atmospheric pressure photoionisation in positive-ion mode (APPI(+)).

Assignments were categorised using three criteria: heteroatom class, that is number of non-hydrocarbon elements contained within each assigned species, double bond equivalents (DBE) which indicates the number of carbon-associated rings and double bonds contained within a species from an elemental formula, giving some insight into structure and particularly what kinds of structures are first targeted during ages and then replenished during rejuvenation, and carbon number. The data was then visualised by percentage contribution to signal intensity for each sample using in-house software.

Indications of aging were successfully established in the molecular make-up of the bitumen, and the identified pathways of rejuvenation at the molecular level gave insights into the action of rejuvenators in bitumen.