Development and mathematical modeling of a Membrane Inlet Mass Spectrometer for environmental monitoring

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Online monitoring of analytes in marine environments is receiving increased attention for a range of applications, including the detection of dissolved gases and volatile organic compounds (VOC's) in water. Some of the analytes of interest are dissolved carbon dioxide, methane, benzene, toluene, tetrachloroethane, trichloroethylene, dimethylsulphide, chloroform and bromoform. In addition to being a main concern of environmental protection agencies, these compounds are also of interest to the oceanographic and atmospheric community. Produced water from active oil and gas fields contains many such dissolved VOC's. It is important to monitor these analytes to not only to mitigate their environmental impact but also to maximise the extraction of oil reserves.

A widely used monitoring method is membrane inlet mass spectrometry (MIMS) which is capable of detecting trace organics in aqueous solutions [1].

The technique is simple and sensitive, provides detection limits in the low ppb range, has no need for pre-concentration. Further, multi-component mixtures can be simultaneously analysed in a few minutes.

Our MIMS system consisted of a PDMS probe inlet, coupled to a portable quadrupole mass spectrometer (QMS) system. Two different QMSs were investigated to monitor analyte concentrations in the range from 10 ppb to 2000 ppm.

In this paper, we present a novel approach for the simulation of MIMS data obtained from monitoring crude oil constituents, such as benzene, toluene and xylene (BTX), both in the laboratory and in the field. By using QMS2-Hyperbolic and QMS-Ion simulation programs, which are multi-ion (>107) trajectory simulations [2], we were able to simulate the performance of the complete system including the MIMS probe and the QMS. The model is therefore capable of modelling full mass spectra across the mass range from 0-200 Da. To test the model, experimental results are compared with the theoretical predictions in each case.

[1] Bell, R.J., Short, R.T., van Amerom, F.H.W. & Byrne, R.H., 'Calibration of an In Situ Membrane Inlet Mass Spectrometer for Measurements of Dissolved Gases and Volatile Organics in Seawater Environ. Sci. Technol. 41, 8123-8128 (2007)

[2] T.J.Hogan and S.Taylor, 'Performance simulation of a quadrupole mass filter operating in the first and third stability zones' IEEE Trans. on Instrumentation and Measurement, 57 (3) pp.498-508 (2008)