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Investigating FAIMS Response to Trihalomethanes with Respect to Humidity

A.K.R. Morris1, R. Parris2, S. Sheridan1, T. Ringrose1, I. P. Wright1, G. H. Morgan1

1PSSRI, The Open University, Milton Keynes, MK7 6AA
2Owlsolve Ltd, 127 Cambridge Science Park, Milton Road, Cambridge, CB4 0GD

1. Introduction

The development of volatile organic compounds (VOCs) can interact with the decomposition processes to form Deformation By-Products (DBPs) [1]. One group of DBPs are Trihalomethanes (THMs) with several compounds of the group being suspected carcinogens. Within the UK the total concentration of all THMs within drinking water need not exceed 100μg/l.

As present water authorities take samples of the water supply and return them to a central laboratory for analysis. This provides an accurate test but one which can involve a long lead time in discovering a potential hazard to public health.

A Field Atactic Ion Mobility Spectrometer (FAIMS) sensor may be ideally placed to perform in situ continuous monitoring at particular sites. As part of a PhD co-supervised by The Open University and Owlsolve Nanotech Plc an investigation is ongoing to discover how sensitive a FAIMS device is with respect to THMs and humidity when sampling. Initial results and the method of data processing, which involves peak fitting to evolving spectra are presented.

2. Trihalomethanes and FAIMS

The formation of THMs is dependent on the location of the water reserve. Open air reservoirs and bore holes will have different exposure to sources such as agricultural run-off and therefore the formation of a particular THM will vary from one location to the next. There are four THMs of particular interest since they are frequently the most abundant halogenated hydrocarbons: Chloroform and Bromoform, their structures are presented below.

As mentioned within the introduction the total permitted abundance of THMs within UK drinking water is 100μg/l [1] (80μg/l in the US under new regulations [2]). Therefore it is a requirement that all THMs can be detected.

There have been previous studies of systems incorporating FAIMS with the detection of THMs within drinking water. Of particular note are the extremely sensitive readings from Elnik et al [3]. Those studies however used a FAIMS system as a preliminary stage to a mass spectrometer. To provide a significant step to what is already accomplished through sampling and analysis within the lab is required that this detection be completed in situ. This will reduce the time taken to take appropriate action given an excessively high level of THMs within the potable water supply.

A stand alone FAIMS system may provide the ideal solution. While the system would not be as sensitive as when used in conjunction with additional technologies such as gas chromatography and mass spectrometry it would be able to operate at ambient conditions of temperature and pressure. The system used within this investigation incorporated the Owlsolve Nanotech FAIMS chip [4] which is a miniaturised solid state device. The sensor's micro sensor response mechanism was not adversely affected in a small size, low power requirement and high reliability.

3. Experimentation

The limit of detection of the THMs and the FAIMS response with respect to concentration were quantities that were to be determined. It was therefore the case that an exponential distribution (EDF) experiment [5] was used for the investigation. Analysis of the data will be continuously flushed by the incoming flow. The concentration within the EDF is expressed through the equation:

\[ C = C_0 \exp \left( -\frac{t}{\tau} \right) \]

It is therefore possible to easily generate a large range of known concentrations. An Owlsolve Lonestar unit was used to sample the EDF which allows the response of a FAIMS system with respect to varying concentration of THMs to be observed.

The sample line from the EDF to the Lonestar and the EDF itself were maintained at an elevated temperature throughout data collection.

Two airflows were passed into the EDF. One was a clean and dry air line while the second was a clean and dry air line which was passed through a bubbling water bottle. Through the control of needle valves the humidity within the EDF was maintained.

The Lonestar system required a carrier gas of clean dry air. While the system can operate by drawing air from ambient air, the unit was provided with clean and dry air to remove any deviation from the scrubbing during the investigation. Initial testing was performed through a 55mmBar of H2 source.

Through initial testing a suitable dispersion field was discovered which provided good separation of ion species at an acceptable sensitivity. Data was recorded with the dispersion field as a constant to minimise the variation. It was therefore possible to observe the formation and evolution of separate ion species across a large concentration range.

In between experiments the instrumentation was left to flush through to mitigate against any residual analyte from the previous data collection affecting later runs.

4. Data Processing

The response from the FAIMS device is made up of many compensation voltage (CV) spectra. Each sweep of compensation voltage provides a snapshot of the ion species present at that particular time of scanning. These spectra contain Gaussian peaks due to the ion species present.

The response is gathered through a Paradox cap which provides a summed response of the Gaussian curves. The compensation voltage of the Gaussian peaks within a FAIMS device are known to be dependent upon the identity of the ion species present. It is therefore of special interest to obtain the most accurate determination of component ratio possible as possible.

Since the response from each ion species is summed, any response which results in two or more Gaussian curves overlapping with one another will result in the low point and intensity of the peaks being a result of the mixing Gaussian. Deconvolution of the signal is required to obtain the true CV position and intensity of the mixed responses. Peak fitting can be used to discover the most likely initial Gaussian responses which have resulted in the amalgamated response provided by the FAIMS system.

Within FAIMS studies the observation of a Gaussian peak is often attributed to a single ion species. When FAIMS has been used as a preliminary stage to mass spectrometry it is often observed that there are in fact several ion species responsible for a single Gaussian observed.

With this knowledge it is tempting to fit as many Gaussian on as possible to the data in the hope of being able to uncover underlying features. The result of this process is often to create fits which no longer correspond to the features of the raw data.

It is important to know the number of peaks to fit to the readily identifiable number of peaks present from the raw data and from known or anticipated chemical reality [6]. This will mean mass spectrometry will always be required to identify the exact constitution of peaks. However, in the process of fitting a low number of peaks allows us to identify trends within a data set. Also the improved CV positions and ion intensity values are still extremely relevant for investigations.

The spectra shown in section 5 are single CV sweeps. If the relevant values of CV position and ion intensity are recorded for each single sweep and plotted with respect to time we can observe how they evolve over time. Two important quantities can now be discerned from each EDF run, the CV position of peaks resulting from THMs and the limit of detection of the system.

5. Peak Fitting

(a) The raw data undergoes a stage where the baseline is corrected back to zero. This is required due to the effects of the electronics of the system.

(b) The data is then automatically deconvoluted by an algorithm which determines the maximum number of Gaussian peaks and also includes the likely CV position, ion intensity and FAIMS of each peak. This information is then used to fit an advanced model allowing an advanced fitting procedure. This provides the final peak fit.

(c) The final deconvoluted data can be exported to a file [7] and can be used from the second files that the fitted peaks are easily controllable to the main peaks in the raw data.

6. Discussion and Further Work

An initial surprise was the strong positive polarity response to the introduction of the THMs. The strongest signal was found from one single and symmetrical Chloroform compound. After this however the system appears to be more sensitive with increasing amounts of bromine present.

The limits of detection are too high to be immediate to the water industry. Modest pre-concentration, such as purge and trap, may provide the required LOD and provide the method of sampling needed to remove the THMs from the water for analysis [8].

This investigation was constructed to investigate not only the FAIMS response to THMs but also the effect humidity has on this response. Unfortunately the experimental setup resulted in a very small range of humidity which proved stable. The EDF was therefore held dry (5% O2 vapour water) or saturated.

(a) Initially starts with low humidity and then later saturated levels. The high humidity appears to stabilise the data across any given temperature.

(b) Displays the unique CV positions resulting from each THM. Future studies are being prepared which provide a consistent flow of analyte via a pressurisation source and no water can be injected into the EDF providing the well characterised humidity variation.

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