Investigating TriHaloMethanes with respect to humidity

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Version: Version of Record

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1. Introduction

The detection of potable water has dramatically reduced the instances of cholera and similar ailments within a population due to unclean water sources. Here we demonstrate that natural organic matter (NOM) can interact with the disinfection compound to form Disinfection By-Products (DBP) [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 must not exceed 100µg/l.

At 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 Amperometric Ion Mobility Spectrometer (FAIMS) sensor may be ideally placed to perform in situ continuous monitoring at particular sites. As part of a PhD co-sponsored by The Open University and Ovaltube Nanotech Pvt; 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 upon the location of the water reservoir. Open air reservoirs and tank roofs will have different compositions in leachates due to different water bodies in contact with the leachates. Chlorine and bromine, their structures are presented below.

As mentioned in 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 BIS et al. [3] whose 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 complete 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 under ambient conditions of temperature and pressure. The system used within this investigation incorporated the Ovaltube Nanotech FAIMS chip [4] which is a miniaturised static dielectric device. The sensory nano-electronic transceiver system was very attractive because of its 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 quantified to be determined. It was therefore the case that an exponential dilution flow (EDF) experiment [5] was used for the investigation. EDF experiments consist of a sample tank which is continuously flushed with a flow. Analytes are introduced into the flask, typically through an injection, and over time the concentration of the analyte will be diluted by the incoming flow. The concentration within the EDF is expressed through the equation:

\[ C = C_0 \exp \left( -\frac{V}{F} \right) \]

It is therefore possible to easily generate a large range of known concentrations.

An Ovaltube Lonesensor unit was used to sample the EDF allowing the response of a FAIMS system with respect to varying concentration of THMs to be observed.

The sample line from the EDF to the Lonesensor and the EDF itself was 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 passed through a bubbling water bottle. Through the control of needle valves the humidity within the EDF was maintained.

The Lonesensor system required a carrier gas of clean dry air. While the system can operate by drawing an ambient air, the unit was provided with clean and dry air to remove the possibility of any degradation to the carrier during the investigation. Illumination was provided through a 55W lamp as a THM 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 observed that the dispersion and evolvement of separate ion species across a large concentration range

In between experiments the instrumentation was left to flushing 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 contains Gaussian peaks due to the ion species present. The response is gathered through a Faraday cup 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 compensating voltage possible as process.

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 loss of position and intensity of the peaks being a result of the mixing Gaussian. Decoupling of the signal is required to obtain the true CV position and intensity of the respective species. 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 rule out the number of peaks fit to the easily 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 the 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 3.5 is an example of these fits. 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

The CV data underwater is a stage where the baseline is essentially black to zero. This is required due to the effects of the electronics of the system.

The data is then inputted automatically by an algorithm which determines the maximum peak and also removes all high CV peaks, CV intensity and FAIMS of each peak. This information is then used to fit an advanced weather-function allowing an automated dispersion-flow-free method. This provides the final peak CV.

A FAIMS system has the ability to fit many peaks, but there is a need to be careful as fitting too many peaks can be detrimental to the final results of the analysis.

6. Discussion and Further Work

This investigation was conducted to investigate not only the FAIMS response to THMs but also the effect humidity has on this response. Unfortunately the experimental set-up resulted in a very small range of humidities which proved stable. The EDF was therefore either very dry (50 parts water) or saturated.

A) initially starts with low humidity and then later saturated levels. The high humidity appears to stabilise the system.

B) displays the unique CV positions resulting from each THM. Future studies are being prepared which produce a constant flow of ion analysis via a termination source and no water can be injected into the EDF providing the well-characterised humidity variation.