Assessing the Fate of Organic Contaminants During Water Treatment Using TOF Mass Spectrometry and Sample Profiling

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Introduction & Objective

Context and Background

- Water scarcity due to climate change and the increasing water demand leads a growing number of large cities worldwide to consider potable water reuse.
- Most potable water reuse strategies involve advanced oxidation processes (AOPs) for the attenuation of trace organic contaminants.
- While water treatment processes are often evaluated by monitoring the concentration of selected contaminants, little is known about the fate of unknowns and by-products.

Objective

- Use QTOF analysis and sample profiling to assess the attenuation of known and unknown contaminants by AOPs along with the formation of by-products.

Sample Preparation & Analysis

Sample Preparation

- Filtration on GFF filter
- Solid Phase Extraction
  - Dionex Autotrace
  - HLB cartridges (Waters)
  - Sample volume: 375 mL
  - Final Extract: 0.5 mL

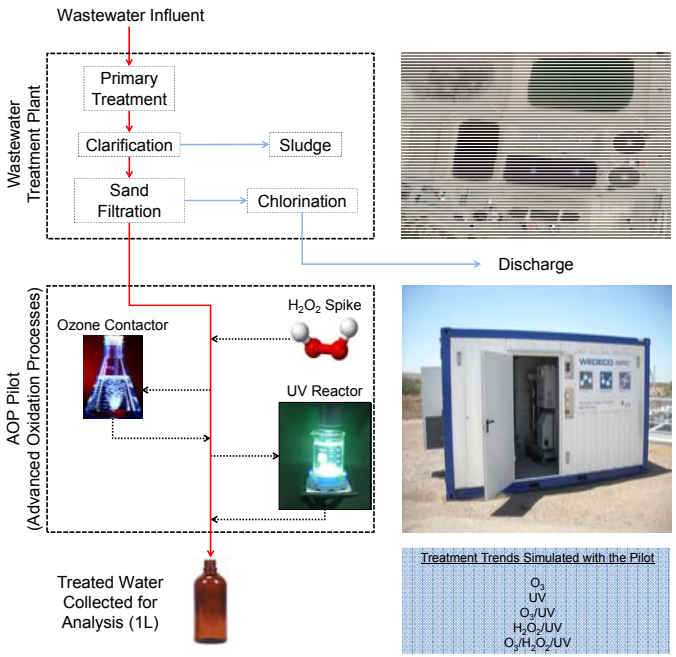
LC-QTOF Analysis

- Liquid chromatography
  - Agilent 1290 series
  - Zorbax C18 column
  - 3 µL injection (triplicate)
  - Mobile phase H_2O/C_2H_3N
- Mass Spectrometry
  - Agilent 6540 QTOF
  - ESI Positive
  - MS scan m/z 100-3200

Data Processing

- MassHunter software
  - Extraction of chromatograms
  - Extraction of molecular features
- Mass Profiler Professional software
  - Filtration of molecular features
  - Principal Component Analysis
  - Visualization of sample profile

Sample Collection



Treatment Trends Simulated with the Pilot

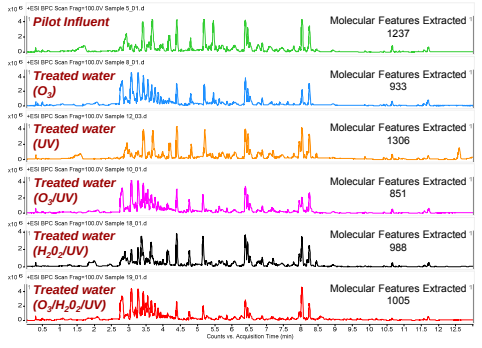
O_3
UV
O_3/UV
H_2O_2/UV
O_3/H_2O_2/UV

Chromatograms & Extraction of Molecular Features

Most of the chromatograms appeared similar.

Close to 1000 molecular features extracted in each chromatogram.

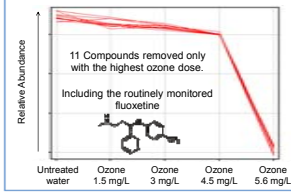
Software essential for further data processing.

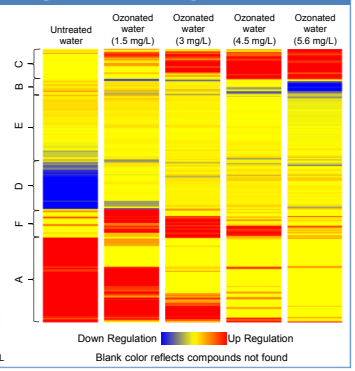


Sample Profiling & Clustering

The heatmap of ozonated samples clearly reveals compounds that are attenuated (A&B), formed (C & D), recalcitrant (E) or intermediates (F).

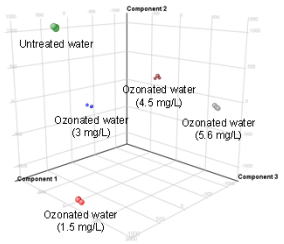
Further clustering will isolate compounds with the same behavior.



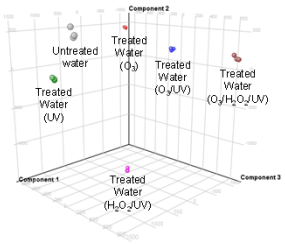


Principal Component Analysis

PCA Plot for Different Ozone Doses



PCA plot for Different Treatments



Sample replicates were closely clustered on the PCA Plot.
Samples treated by different processes or different doses of oxidant could be distinguished

Conclusion

QTOF analysis showed AOPs attenuate multiple unknowns beyond target organic compounds commonly monitored.

Advanced data processing with Mass Profiler Professional allows the clustering of compounds with the same behavior during water treatment

Compounds with similar behavior could be used as indicator in order to limit the amount of target analytes for the assessment of treatment efficiency.

Further sampling campaigns are required to confirm the identification of robust clusters around contaminants routinely analyzed.

Acknowledgment

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