Assessing the potential of fluorescence spectroscopy to track the presence of contaminants in water reuse systems

Joseph Wasswa, Natalie Mladenov

Dept. of Civil, Construction and Environmental Engineering San Diego State University





Methods

Results

Conclusion

MOTIVATION

Water Stress by Country: 2040



NOTE: Projections are based on a business-as-usual scenario using SSP2 and RCP8.5.

For more: ow.ly/RiWop

🌞 WORLD RESOURCES INSTITUTE

- A way forward is water reuse
 - Non-potable
 - Potable
 - indirect and direct















Methods

Conclusion

UV/H₂O₂

(Source: Rodrigo Tackaert)





Fluorescence spectroscopy (FS) and the excitation emission matrices (EEMs)

Results

Methods



Advantages of FS

Introduction

- Sensitive and selective
- No sample preparation needed



Conclusion

MONITORING EQUIPMENT

3D Benchtop fluorometer



Insitu C3 fluorometer



- Spike contaminants into several water sources
 - VOCs (Diesel and Gasoline)
 - PPCPs (Ibuprofen, Caffeine and Lopinavir)
 - Pesticides (Isoxathion)



Monitor the changes
in DOM fluorescence
intensities and
characteristics



WATER SOURCES USED

Results

Advanced Water Purification Facility, San Diego, CA

Methods



Photo by City of SD Public Utilities Department

E

Collection points:

- Before ozonation (Pre-ozone) •
- After ozonation (Post-ozone) •
- After UV (UV-AOP) •



Alvarado Creek, San Diego, CA

Conclusion





Creek water

Methods

Conclusion

CREEK WATER





- All contaminants fluorescein the tryptophan-like peak region.
- But can we distinguish them against the background?

Methods

Results

Conclusion

300



3D benchtop fluorometer

Results of titration with contaminants

- Strong linear and significant relationship relationship between peak B intensities and contaminant concentration
- Ibuprofen peak not tracked well with Peak T or B fluorescence



Methods

Conclusion

C3 submersible fluorometer

Results of titration with contaminants

- Strong linear and significant relationship relationship between tryptophan intensities and contaminant concentrations
- C3 allows a wider range of fluorescence to be captured hence better R2 values







Concentration (ppm)

600

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 Adjusting the algorithm to track a specific Ibuprofen peak

Peak I (Ex/Em 260/(290-300 nm)



(a) UV-AOP water, (b) post-ozone water, (c) Creek water and (d) Pre-ozone water

Methods

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LIMIT OF BLANK AND LIMIT OF DETECTION FOR A C3 SUBMERSIBLE FLUOROMETER

Tryptophan

The limit of Blank (LOB) and the Limit of detection (LOD) were calculated based on 10 replicates following Armbruster and Pry (2008)

Water source	LOD (RFU)
UV-AOP	163
Post-Ozone	148
Pre-Ozone	242
Creek Water	224



1000

• Tryptophan-like peak is the best choice for contaminant monitoring

Methods

• Applications:

Introduction

- Source water monitoring (contaminant spills, industrial discharges...)
- Monitoring performance of treatment steps (barriers) in water reuse systems

Results

Conclusion

- Advantage of in-situ instrument:
 - Optical filters on C3 cover a "range" of excitation and emission wavelengths
 - Capture multiple contaminants (VOCs, pesticides, PPCPs,...)
 - Ratio of TRP peak to CDOM peak could discriminate contaminant from background

 Benchtop instrument could provide superior monitoring if peak corresponding to every chemical is tracked

Methods

3D EEM visualization

Introduction

• Algorithm to track peaks



Results

Conclusion

Post-ozone water

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Thanks for listening! Any questions?

