WEST research update

Minkyu Park
Post-doctoral researcher
Snyder group
Classification of research at West

Analysis/Monitoring of water quality

- Agilent Technologies
- Xylem
- GE Power & Water
- BDS
- SC Johnson

Water treatment processes

- Dow
- IXOM
- PWNT
- Calgon Carbon
- MetaWater
- GARVER
ANALYSIS/MONITORING OF WATER QUALITY
Accessibility of wastewater effluent

Agua Nueva wastewater treatment plant

Tertiary wastewater effluent

WEST center
Trace organic compounds (TOrCs)

TOrCs in wastewater effluents

£30bn bill to purify water system after toxic impact of contraceptive pill

Drug firms oppose an EU call for controls on potent chemicals that have been blamed for the gender mutation of freshwater fish

Diabetes Drug Makes Male Minnows More Female

Exposure to metformin, a first-line treatment for type-2 diabetes, feminizes male minnows and impacts fertility at levels common in wastewater effluent

April 28, 2015 | By Brian Biernacki and Environmental Health News

SCIENTIFIC AMERICAN™

Disturbing levels of HEART DRUGS found in drinking water, says study, as concern for long term health effects grows

- At least 25 different drugs found in samples from 50 wastewater plants
- Drugs for high blood pressure were the most common of those found

By STEVE NOLAN
PUBLISHED: 09:21 EST, 12 December 2013 | UPDATED: 12:54 EST, 12 December 2013
Identification of transformation products (TPs) in ozone process

Triamcinolone acetonide: OTC drug
Agilent MPP software

Statistical screening of TPs

- Alignment of data.
- Frequency filtering
- ANOVA at 95% confidence level, Bonferroni test and Tukey test
- Fold change (4 fold)
- MFG score > 80
Identification of a TP

\[ \text{C}_{24}\text{H}_{31}\text{FO}_6 \] + O\textsubscript{3} \rightarrow \text{C}_{23}\text{H}_{31}\text{FO}_8

TP1

HOMO
Molecular structure correlator: MSC

Elucidated: 86.7% ions, 95.3% weights

Tentative fragmentation pattern

TP1

Compatibility Score: 83.17
GE organic carbon detector (OCD)

- Absorbance (mAU)
- DOC (ppb)
- Apparent molecular weight (Da)

Agilent Technologies
GE Sievers

(OCD)
Application of OCD to UF membrane process

Flux decline curve

No pretreatment
PAC
O3
PAC-O3
O3-PAC

Fouling extent:
O3-PAC < PAC-O3 < O3 < PAC < No treatment

DOC (ppb)

Normalized flux

Filtrate volume (mL)

PES 100kDa

Axis Title

1000000 100000 10000 1000 100

0 50 100 150 200 250 300 350 400 450

10 100 1000 10000 100000 1000000
### Online sensors for water quality monitoring (WRRF 11-01)

**WateReuse Research Foundation 11-01 Project**

<table>
<thead>
<tr>
<th>General parameters</th>
<th>Organic parameters</th>
<th>Inorganic parameters</th>
<th>Microbial parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>pH</td>
<td>UVT 254 (%)</td>
<td>Chlorine (mg/L)</td>
<td>Total cell count (counts/100mL)</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>UVA 254 (cm⁻¹)</td>
<td>NO₃-N (mg/L)</td>
<td>Toxcity (%)</td>
</tr>
<tr>
<td>Conductivity (µS/cm)</td>
<td>DOC (mg/L)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Turbidity (NTU)</td>
<td>TOC (mg/L)</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Fluorescence (A.U.)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Online sensors for water quality monitoring (WERF 14-01)

Tertiary Wastewater Effluent → Ozone → BAC Filters → Treated water

Engineering for BAC

Monitoring sensors

WEDECO - a xylem brand

GARVER

HACH - a xylem brand

CalganCarbon
Attenuation of TOrcs

Group I: 
Carbamazepine

Group II: 
Diphenhydramine

Group III: 
Primidone

Group IV: 
Iopamidol

% Attenuation

mg/L O₃ increase
Reduction in spectroscopic surrogate

<table>
<thead>
<tr>
<th>Region</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>Tyrosine-like aromatic protein</td>
</tr>
<tr>
<td>II</td>
<td>Tryptophan-like aromatic protein</td>
</tr>
<tr>
<td>III</td>
<td>Fulvic-like</td>
</tr>
<tr>
<td>IV</td>
<td>Soluble microbial byproduct</td>
</tr>
<tr>
<td>V</td>
<td>Humic-like</td>
</tr>
</tbody>
</table>

**Table:**

<table>
<thead>
<tr>
<th>O$_3$ dose (mg/L):</th>
<th>(O$_3$:DOC, mg/mg):</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>(0)</td>
</tr>
</tbody>
</table>

**Graphs:**

- UVA: Increase in ozone with wavelength.
- TF: Color-coded spectroscopic data with regions I to V.

**Images:**

- Region I: Tyrosine-like aromatic protein.
- Region II: Tryptophan-like aromatic protein.
- Region III: Fulvic-like.
- Region IV: Soluble microbial byproduct.
- Region V: Humic-like.

**Notes:**

- UVA/UVa ratio.
- O$_3$:DOC ratio.

**Values:**

- Region I: 1 (0.15)
- Region II: 3 (0.46)
- Region V: 8 (1.23)
Surrogate approach to monitor TOrCs

Ozone oxidation

Ozone Oxidation

Trace organic compounds (TOrCs)

Indicator compound

Spectroscopic surrogates

UVA$_{254}$ Total fluorescence

O$_3$

Development of Surrogate/Indicator Models

Indicator Model
\[
\ln \left( \frac{C}{C}_0 \right) = \frac{k_{OH}}{k_{OH,I}} (1 + \alpha) \ln \left( \frac{I}{I}_0 \right)
\]

Surrogate Model
\[
\ln \left( \frac{C}{C}_0 \right) = \frac{k_{OH} (1 + \alpha)}{K_S} \ln \left( \frac{S}{S}_0 \right)
\]

Prediction of TOrC Attenuation

Measured attenuation (%)

Modeled attenuation (%)
Surrogate model prediction

**UVA\(_{254}\)**

- **TF**

  - Attenuation of TOC (%)
  - Attenuation of surrogate (%)

**UVA\(_{254}\)**

- **TF**

  - Measured attenuation (%)
  - Modeled attenuation (%)

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**R\(^2\)**

- Acesulfame: 0.82
- Atanol: 0.86
- Benzotriazole: 0.64
- Carbamazepine: 0.96
- DEET: 0.88
- Diclofenac: 0.95
- Gemfibrozil: 0.89
- Iopromide: 0.39
- Primidone: 0.91
- Propranolol: 0.85
- Sulfamethoxazole: 0.94
- Triclosan: 0.89
- Trimethoprim: 0.94
Title 22 removal criteria

- (A) Hydroxy Aromatic
- (B) Amino/Acylamino Aromatic
- (C) Nonaromatic with carbon double bonds
- (D) Deprotonated Amine
- (E) Alkoxy Polyaromatic
- (F) Alkoxy Aromatic
- (G) Alkyl Aromatic
- (H) Saturated Aliphatic
- (I) Nitro Aromatic

At 0.3 log removal of meprobamate

0.3 log removal

0.5 log removal
Oxidation kinetics of MIB/Geosmin by ozone

UV$_{254}$ and TF as surrogate indicators
Adsorption of TOrCs using PAC

- Meprobamate (0.70) [o]
- Carbamazepine (2.45) [o]
- Trimethoprim (0.91) [*]
- Sulfamethoxazole (0.89) [-]

A
- TF

B
- UVA

Calgon Carbon®
Surrogate approach to monitor TOrCs

Powdered activated carbon

PAC Adsorption

Trace organic compounds (TOrCs)

Development of Surrogate Model

\[
\ln \left( \frac{c_i}{c_{i,0}} \right) = \alpha \left( 1 + \ln \frac{1}{\alpha} \right) \ln \left( \frac{c_s}{c_{s,0}} \right)
\]

Prediction of TOrC adsorption

[Graph showing scatter plot with measured removal (%) on the y-axis and predicted removal (%) on the x-axis, with data points for various compounds like Atenolol, Benzo triazole, Carbamazepine, Diclofenac, Diphenhydramine, Gemfibrozil, Hydrochlorothiazide, Iopamidol, Meprobamate, Sucr alose, Sulfamethoxazole, TCEP, TCP, Triclocarbon, Triclosan, Trimethoprim]
Artificial neural network (ANN)

Maximization of NF recovery

Brine generation

Ozonation of the brine

Fouling propensity test for ozonated brines

NF270

Ozone generator

NF90

85% recovery

Brine generation (CAP water)

Ozonation of the brine

Fouling propensity test for ozonated brines
Fluorescence/UV absorbance

Agilent Technologies

LC/DAD-FLD
RSSCT experimental setup for PFC removal

Rapid small scale column testing (RSSCT)
Breakthrough

- Tested carbon: Calgon F400
- Water: Tucson groundwater (tap water) spiked with ~300 ng/L PFCs
- Three EBCTs were tested: 5, 10 and 20 min.

Increase in hydrophobicity
Magnetic anion exchange resin for PFC removal
Magnetic anion exchange resin for PFC removal

**MIEX® DOC resin**

**MIEX® GOLD resin**

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**PFOA**

**PFOS**
Oxidation kinetics of MS2 coliphage by ozone

Result
Virus removal using ceramic membrane

Wastewater effluent → FeCl₃ → Inline coagulation → Ceramic membrane
Virus removal using ceramic membrane
Acknowledgement

Snyder group