MSCA-ETN

InnovEOX

Training a new generation of researchers in **Innov**ative **E**lectrochemical **OX**idation processes

EU H2020 MSCA-ETN

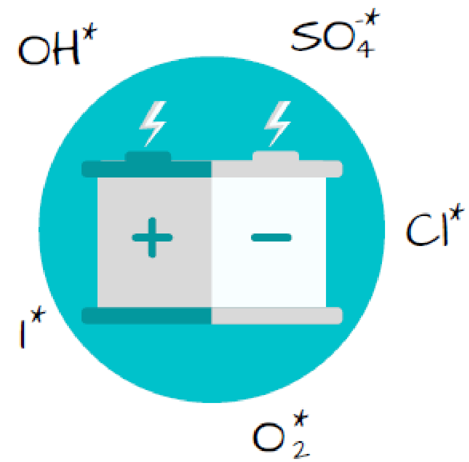
Project Introduction

InnovEOX at a glance

Our purpose

The presence of hazardous micro-pollutants in water streams has become a **worldwide concern**

Advanced Oxidation Processes (AOPs) are a well-known class of technologies for the degradation of micropollutants in water, among which **Electrochemical AOPs (eAOPs)** stand out as a **promising sustainable and effective solution**



Our goal

Training of a new generation of researchers in **Innov**ative **E**lectrochemical **OX**idation processes for the removal and analysis of micro-pollutants in water streams

Beneficiaries & Partners

Beneficiaries

KU LEUVEN
UNIVERSITY OF PATRAS
UCL
UNIVERSITEIT GENT
INERIS
UNIVERSITY OF LIVERPOOL
TU Delft
INOPSYS SIDE STREAM SOLUTIONS
nijhuis INDUSTRIES
Agilent Technologies

Partner Organizations

VLAAMSE MILIEUMAATSCHAPPIJ
IRIS
euronovia
LABORATOIRE WATCHFROG
AAQUA AQUAPROX Water & Waste Water Technology
DOW
xylem

MSCA-ETN
InnovEOX
Training a new generation of researchers in Innovative Electrochemical OXidation processes

Organization

WP 7. Project Management

WP 5. Training

eAOP technology advancements

WP 1. Enhancing eAOP via the generation of alternative radicals

WP 2. Combined electrochemical and (photo-) catalytic oxidation

Removal and analysis of micro-pollutants in water streams

Characterization of treatment effects

WP 3. Innovations in chemical analysis of degradation products by eAOPs

WP 4. Effects of eAOP treatment on environment / toxicity

WP 6. Dissemination, exploitation and communication

MSCA-ETN
InnovEOX
Training a new generation of researchers in Innovative Electrochemical OXidation processes

Early-Stage Researchers

WP 1


Sara Feijoo Moreira
ESR 1


Gagandeep Singh Matharoo
ESR 2


Amir Jabbari
ESR 3


Nadia Gadi
ESR 4

WP 2


Agha Zeeshan Ali
ESR 5


Rebecca Dhawle
ESR 6


Zhongda Liu
ESR 7


Izba Ali
ESR 8

WP 3

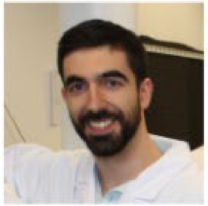

Quynh Khoa Pham
ESR 9


Allisson Barros de Souza
ESR 10


Elena Bandini
ESR 11


Ardiana Kajtazi
ESR 12

WP 4


Rafael Reis
ESR 13


Barbara Brusca
ESR 14


Gema Amaya
ESR 15

Research topics

Electrochemical AOP with *in-situ* generation of sulfate radicals

MSCA-ETN InnovEOX
Training a new generation of researchers in Innovative Electrochemical OXidation processes

ESR: Sara Feijoo Moreira
Main Supervisor: Prof. Raf Dewil
Host: KU Leuven

ESR 1

Sulfate-radical Advanced Oxidation Processes (SR-AOPs) are a novel AOP approach where **$SO_4^{\bullet -}$ radicals** are promoted over conventional $HO^{\bullet -}$ as oxidizing agent of recalcitrant pollutants in wastewater.

$$SO_4{}^{2-} \rightarrow SO_4{}^{\bullet -} + e^-$$

Why sulfate radicals?

- Better selectivity
- Higher redox potential
- Longer lifetime in water
- Efficiency is pH-independent
- Lower self-scavenging effect

Why is it relevant?

- Generating **sulfate radicals from sulfate ions already present** in the wastewater avoids the need for additional chemicals and the generation of waste, while operating at ambient conditions.
- It is a more **environmentally-friendly and energy-efficient** treatment

MSCA-ETN
InnovEOX
Training a new generation of researchers in Innovative Electrochemical OXidation processes

ESR: Gagandeep Singh Matharoo
Main Supervisor: Prof. James Walsh
Host: University of Liverpool

Manipulation of plasma species generation in an AOP

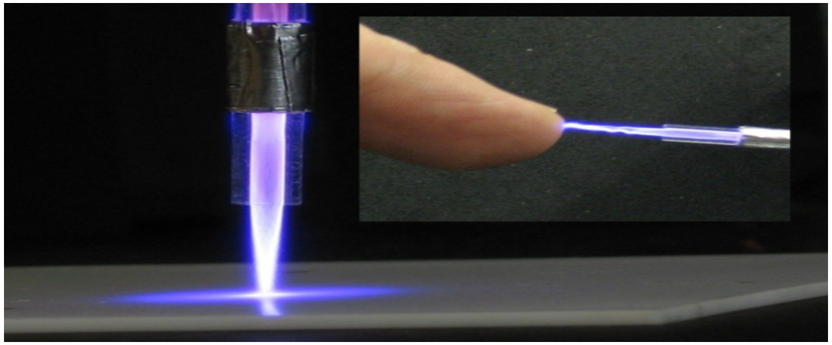
ESR2

Concept

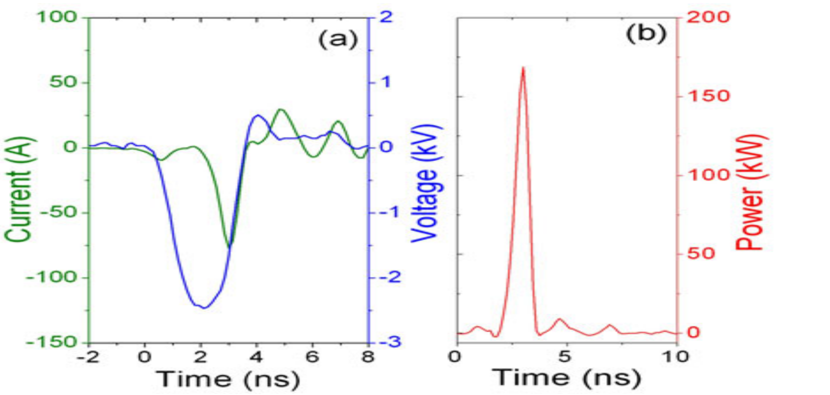
The energy of electrons in the plasma dictate its chemical composition, and it can be controlled to optimize production of reactive species

Main objective

To test the hypothesis that nanosecond pulsed excitation can exert a level of control over electron energy and therefore control plasma chemistry



$e + N_2 \rightarrow N_2^+ + e + e$	$1 \times 10^{-16} \varepsilon^{1.90} \exp(-14.6/\varepsilon)$
$e + N \rightarrow N(^2D) + e$	$5.06 \times 10^{-15} \exp(-10.8/\varepsilon^{3.95})$
$e + N \rightarrow N^+ + e + e$	$1.45 \times 10^{-17} \varepsilon^{2.58} \exp(-8.54/\varepsilon)$
$e + O_2 \rightarrow O + O + e$	$2.03 \times 10^{-14} \varepsilon^{-0.10} \exp(-8.47/\varepsilon)$
$e + O_2 \rightarrow O(^1D) + O + e$	$1.82 \times 10^{-14} \varepsilon^{-0.13} \exp(-10.7/\varepsilon)$
$e + O_2 \rightarrow O_2(a\,^1\Delta) + e$	$1.04 \times 10^{-15} \exp(-2.59/\varepsilon)$



Enhancing mass transport in plasma AOP via liquid spray reactor

ESR: Amir Jabbari
Main Supervisor: Prof. James Walsh
Host: University of Liverpool

ESR3

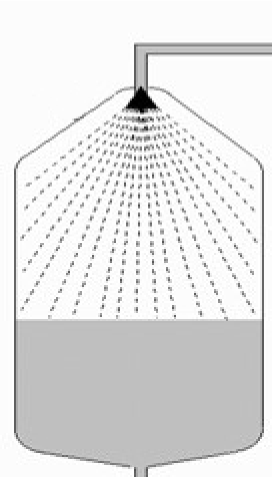
Challenges:
Enhancing the mass transfer and overcoming the disruption caused by interation of liquid and plasma

How?

Plasma source

Plasma volume
Plasma stability

Spray-type reactor



Flow rate
Aerosol size

Techniques

- ✓ Particle Imaging Velocimetry (PIV) system
- ✓ Fluid-dynamics properties
- ✓ Computational fluid dynamics modelling
- ✓ Characterisation

Reactor and process design for industrial implementation of eAOP

MSCA-ETN **InnovEOX**
Training a new generation of researchers in Innovative Electrochemical OXidation processes

ESR: Nadia Gadi
Main Supervisor: Nadine Boelee
Host: Nijhuis Industries

ESR4

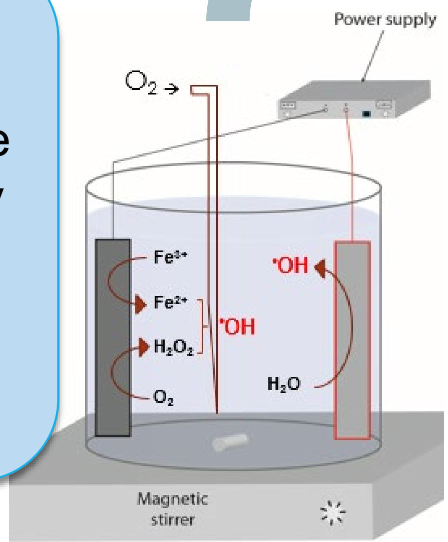
Lab scale

Scale up

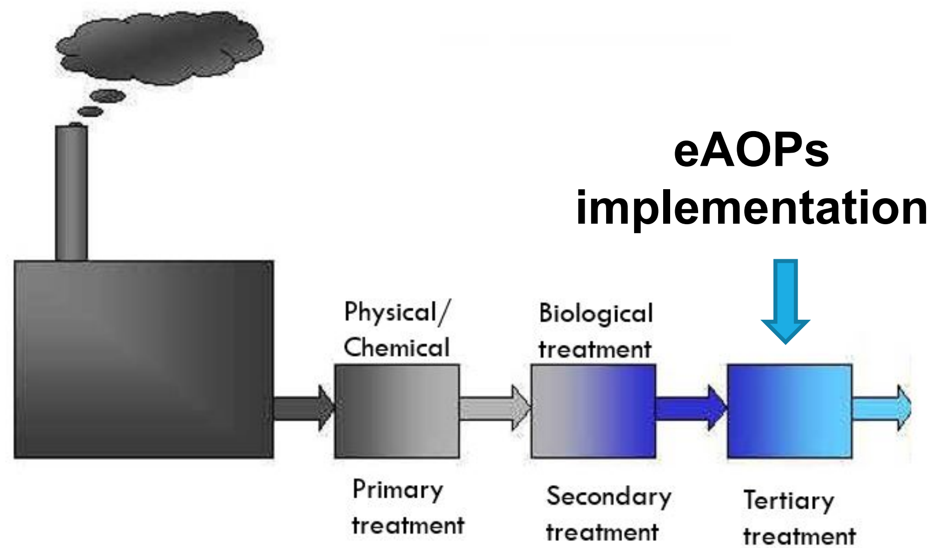
Industrial scale

Investigate the effect of the parameters[1] on the process efficiency

([1]Current density, Anode material, Concentration of pollutants …)



eAOPs implementation



Optimal conditions

Electro-Fenton Process

*Anode M + H_2O → **HO*** (MHO*)*

$O_2 + 2H^+ + 2e^- \rightarrow H_2O_2$

$Fe^{3+} + e^- \rightarrow Fe^{2+}$

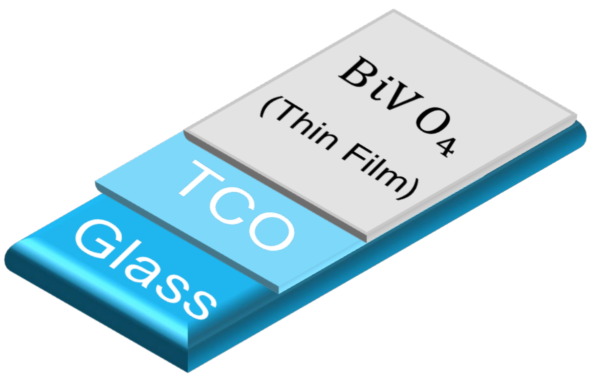
$Fe^{2+} + H_2O_2 \rightarrow Fe^{3+} + HO^* + HO^-$ *(Fenton's reaction)*

- Overcome the limitations: Mass transfer Electrodes fouling…
- Optimize the system

Catalyst evaluation for anode selectivity in photo-electrochemical system

ESR: Agha Zeeshan Ali
Main Supervisor: Prof. J.P. van der Hoek
Host: TU Delft

ESR 5



Photoanode (Components)

Goals

- Use of Bismuth Vanadate ($BiVO_4$) as photocatalyst
- Fabrication & testing of $BiVO_4$ based photoanodes
- Identifying the degradation pathways of micro-pollutants
- Integration of photoanodes in a reactor design

Aim: Use of Solar Energy

Hybrid photo-electrochemical processes

MSCA-ETN
InnovEOX
Training a new generation of researchers in Innovative Electrochemical OXidation processes

ESR: Rebecca Dhawle
Main Supervisor: Prof. Dionisios Mantzavinos
Host: University of Patras

ESR6

Objective: Combine Solar Photocatalysis and Electrochemical Oxidation to achieve synergy

GOALS

- Immobilization of TiO_2 on anodes and sensitization to visible light
- Enhance degradation in comparison to individual processes
- Cathode selection to promote H_2O_2 production
- Compare the H_2O_2 production and process efficiency with different cathodes
- Kinetic analysis of the process to identify the by products

Electrochemical modification of catalytic activity for water treatment

MSCA-ETN InnovEOX

Training a new generation of researchers in Innovative Electrochemical OXidation processes

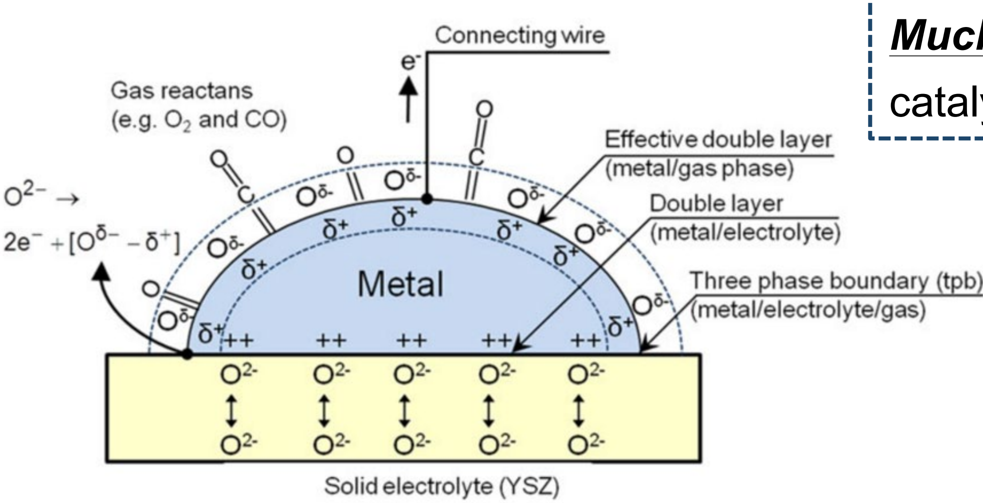
ESR: Zhongda Liu
Main Supervisor: Prof. Alexandros Katsaounis
Host: University of Patras

ESR7

Using Electricity Wisely!

Idea:

EPOC: supplying ions to modify the catalyst surface, bringing a Faradaic efficiency of ***~10⁷%***.



EPOC in gaseous phase
(Electrochemical Promotion of Catalysis)

Challenge:

First attempt to bring EPOC in aqueous phase for catalytic wet air oxidation (CWAO). ***Much more complex interactions*** between catalyst, pollutants and intermediates.

Goal:

Promoting catalysis for CWAO in a ***pronounced***, ***reversible***, ***predictable*** and ***controllable*** manner.

In-situ production of H_2O_2 at the cathode in catalytic wet air oxidation

MSCA-ETN
InnovEOX
Training a new generation of researchers in Innovative Electrochemical OXidation processes

ESR: Izba Ali
Main Supervisor: Kwinten Van Eyck
Host: InOpSys

ESR 8

Background

The formation of H_2O_2 is dependent of the process conditions in the system, and very specifically, on the **composition of the cathode**. In general, **carbonaceous cathodes** are beneficial for H_2O_2 generation.

Goals

- **AOP process based on H_2O_2** will be further developed and optimized.
- A beneficial **catalytic coating** for the cathode will be designed, for the production of H_2O_2.
- Influential parameters will be determined and an **optimization** of the process will be carried out.

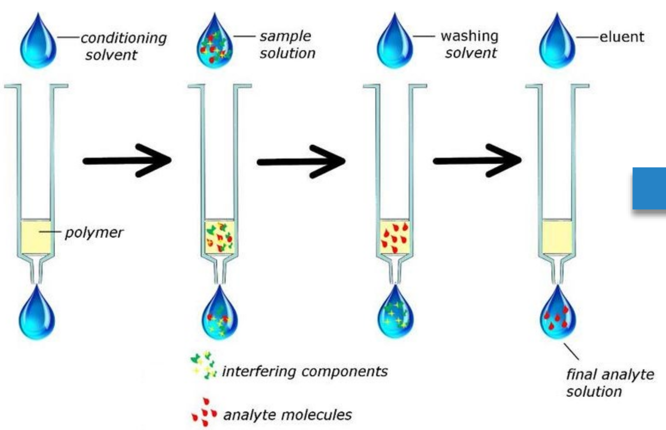
MSCA-ETN
InnovEOX
Training a new generation of researchers in Innovative Electrochemical OXidation processes

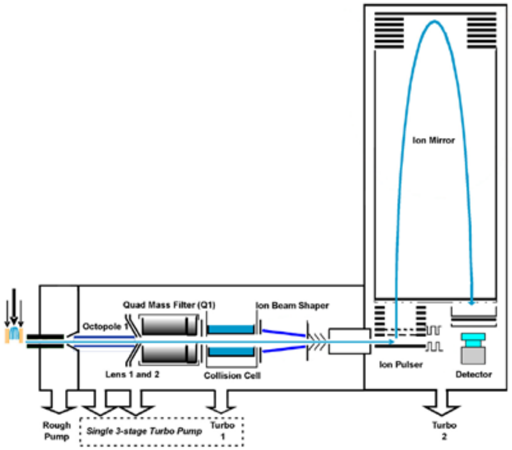
Evaluating sample preparation methods to monitor eAOP degradation products

ESR: Quynh Khoa Pham
Main Supervisor: François Lestremau
Host: INERIS

ESR9

AOPs





Multi-mode SPE cartridges
- Analyte enrichment
- Removal of matrix compounds

LC-MS-QTOF
- Sensitivity increase
- Identification strength

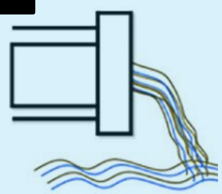
Identification
- Database (online and in-house)
- Reference standards

Multidimensional LC separations with MS as a generic method to study eAOP degradation products

ESR: Allisson Barros de Souza
Main Supervisor: Tom Van de Goor
Host: Agilent

ESR10

1



Parent pollutants

AOP →
Water treatment

2

Degradation products

LC →
Analytical separation

Complex samples

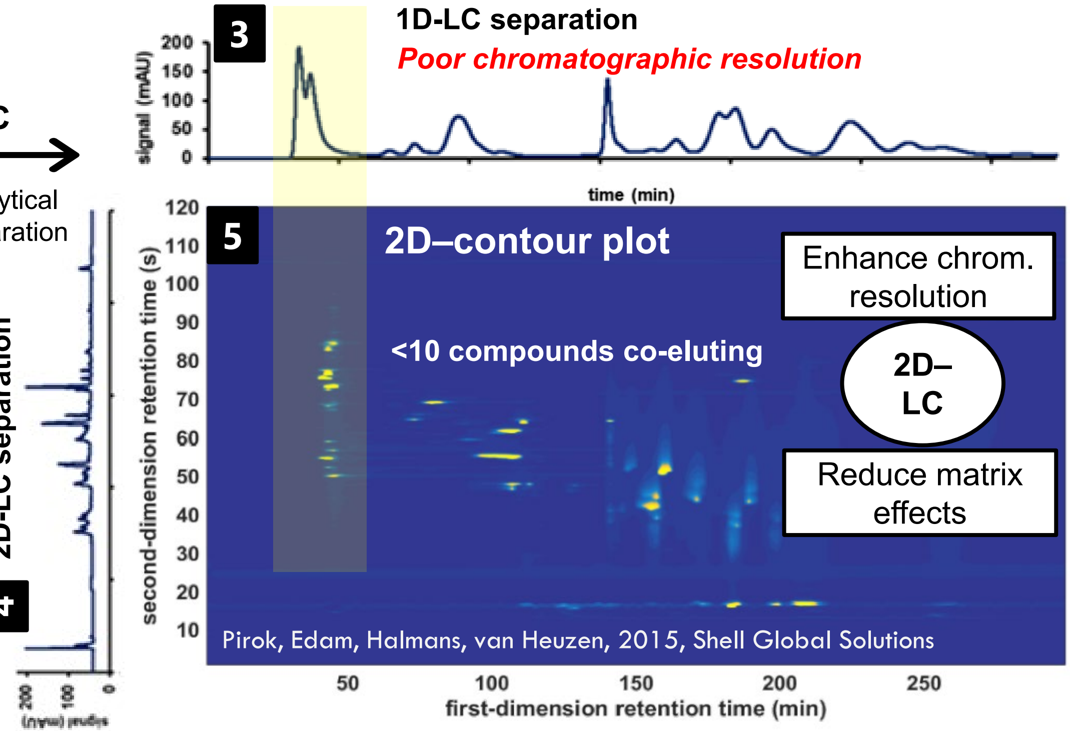
Challenge

Large number of compounds with a broad range of physicochemical properties, e.g.:
- ○ Molecular size
- ○ Polarity
- ○ Ionizability

Opportunity

Multidimensional liquid chromatography
+
High resolution mass spectrometry (HRMS)

4 **2D-LC separation**



6 **Objectives**

- Provide a universal 2D–LC/MS separation system
- Support the structure elucidation of the degradation products

MSCA-ETN
InnovEOX
Training a new generation of researchers in Innovative Electrochemical OXidation processes

Evaluating alternative chromatographic strategies for enhanced eAOPs analysis

ESR: Elena Bandini
Main Supervisor: Prof. Frédéric Lynen
Host: University of Ghent

ESR11

TRLC-RID

Pure water as mobile phase with thermo-responsive polymer based colums

Universal detection with Refractive Index Detector

GCxGC image recognition

Functional group type classification using deep learning methods

Construction of Neural Networks for the interpretation of contour plots

Combination of chromatographic and spectroscopic data to enhance the identification of eAOP products

MSCA-ETN
InnovEOX
Training a new generation of researchers in Innovative Electrochemical OXidation processes

ESR: Ardiana Kajtazi
Main Supervisor: Prof. Frédéric Lynen
Host: University of Ghent

ESR12

Goals

1. Setting up LC-MS and GC-MS platforms for analysis of advanced oxidation products.

2. Combining *in silico* prediction of retention times to enhance the quality of the predicted elemental compositions.

3. Developing comprehensive multidimensional platforms for analysis of advanced oxidation products.

4. Developing phase optimized liquid chromatography (POPLC) for small molecule analysis.

Toxicity assessment of degradation products using zebrafish and advanced LC-MS techniques

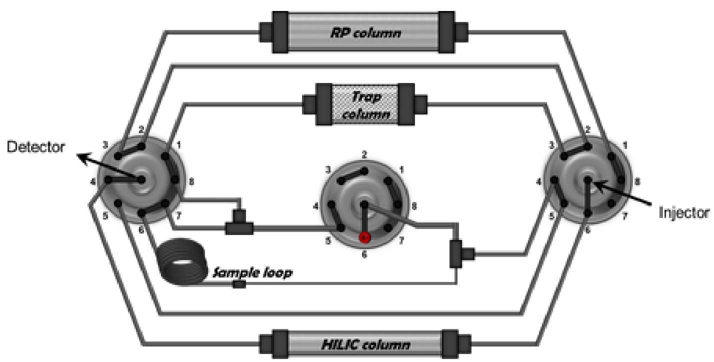
MSCA-ETN
InnovEOX
Training a new generation of researchers in Innovative Electrochemical OXidation processes

ESR: Rafael Reis
Main Supervisor: Prof. Deirdre Cabooter
Host: KU Leuven

ESR13

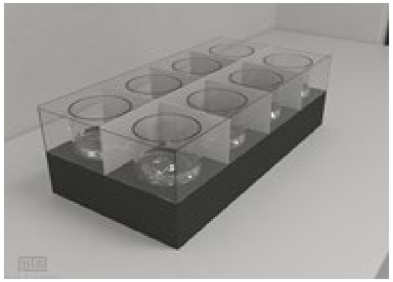
Goals:

1. Development of robust, easy-to-operate multi-dimensional LC techniques for the analysis of complex samples;
2. Application of the developed methods to samples generated during this project by other partners in the consortium and also in local WWTP's and surface waters;
3. Toxicological assessment of the identified compounds using zebrafish models.



Single heart-cutting multidimensional UHPLC

Danio rerio



Zebrafish test plates

Combined electrochemical oxidation and biological wastewater treatment

MSCA-ETN
InnovEOX
Training a new generation of researchers in Innovative Electrochemical OXidation processes

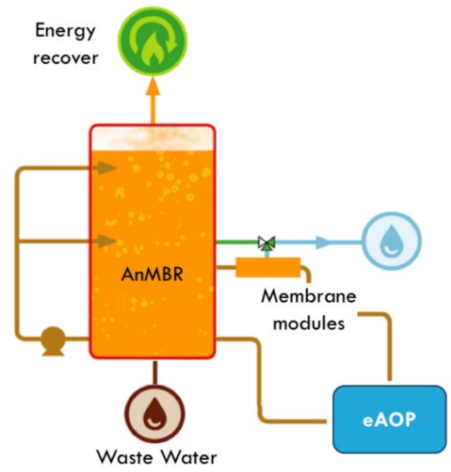
ESR: Barbara Brusca
Main Supervisor: Prof. Lise Appels
Host: KU Leuven

ESR14

GOAL **Implementation** of the eAOP-techniques developed in the other WPs in **biological wastewater treatment processes.**

- **Partial eAOP** degradation
  - Micropollutants are transformed into biodegradable components
  - Toxic components may still be present → affect the biological step

  Evaluation of the influence of the eAOP treatments and of the formed degradation products on subsequent aerobic and anaerobic treatments



- **eAOP + aerobic treatment**: already researched
  - Partial oxidation impact on the long term is unknown
  - Toxicity reduction of the influent
- **eAOP + anaerobic** treatment: more effective biodegradation “totally new concept “
  - H_2 will end up in the biogas
  - O_2 will create micro-aerobic conditions in the reactor (reducing unwanted H_2S)
  - Energy neutral or even an energy producer

MSCA-ETN
InnovEOX
Training a new generation of researchers in Innovative Electrochemical OXidation processes

Life-cycle assessment & cost analysis of emerging eAOP technologies

ESR: Gema Amaya
Main Supervisor: Prof. Paola Lettieri
Host: University College London

ESR15

- Which strategy is more **sustainable**?
- Which technology could be **implemented full scale**?
- What is the **environmental impact** of its implementation?
- Is it **feasible**?

Q&A

Questions?

This project has received funding from the European Union's
EU Framework Programme for Research and Innovation
Horizon 2020 under Grant Agreement No 861369.