EBNet
Environmental Biotechnology

Engineering and Physical Sciences Research Council

Biotechnology and Biological Sciences Research Council

# ENVIRONMENTAL BIOTECHNOLOGY NETWORK

## PFAS ‘Forever Chemicals’ WG

# PFAS 'Forever Chemicals' (PFAS WG)

Led by Dr Tao Lyu, Cranfield University

Per- and Polyfluoroalkyl Substances (PFAS), known as 'forever chemicals', are extensively used in industrial and consumer applications due to their exceptional persistence properties. Attributed to the enduring characteristics, these substances have a detrimental impact on human health when their residues persist in the environment. While current remediation approaches primarily rely on physical adsorption and chemical oxidation processes, recent studies have emerged regarding the potential of microbial degradation as a cost-effective solution. However, the effectiveness of this approach is still subject to debate, necessitating further investigations. The WG aims to bring together experts from multidisciplinary fields and to collaborate on researching, developing, and promoting cutting-edge bioremediation strategies that target PFAS contamination across various environmental matrices, including water, wastewater and soil.

This WG has fostered new partnerships between academia and industry and serves as a platform to facilitate the development of early career researchers

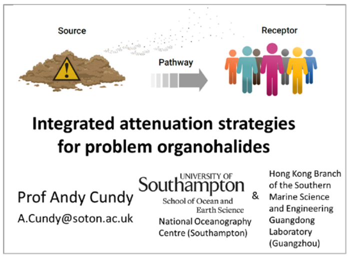
## ACTIVITY SYNOPSIS

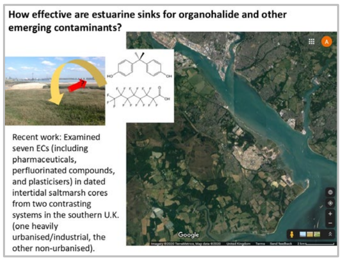
Activity in this area started with proof-of-concept (POC) funding for a project on Enhancing PFASs Attenuation in Coastal brownfield Soils (EPACS): enhancing natural system attenuation capacity for a key emerging contaminant. Led by Prodf Andy Cundy with Prof Frederic Coulon as Co-Investigator. Results from this fed into the EU H2020 EiCLAR project, and a paper on assessing the role of the 'estuarine filter' for emerging contaminants: pharmaceuticals, perfluoroalkyl compounds and plasticisers in sediment cores from two contrasting systems in the southern UK.

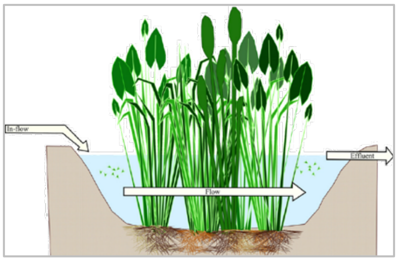
The POC findings were also presented in a webinar chaired by Prof Tony Gutierrez with invited speakers Dr Sophie Holland, University of New South Wales and Professor Andy Cundy, National Oceanography Centre (NOC), University of Southampton

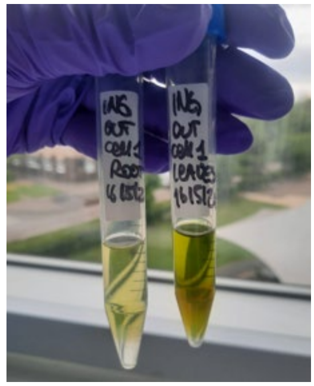
*Webinar* Organohalide Bioremediation – Current Approaches in Environmental Biotech

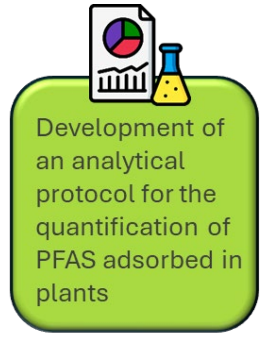
There was not much further activity in the Network on this topic area for a while, as PFAS degradation is a notoriously difficult area: but then in 2024 another POC was awarded and the PFAS WG was formally established led by Dr Lyu, with Prof Coulon and Prof Gutierrez as core team members.



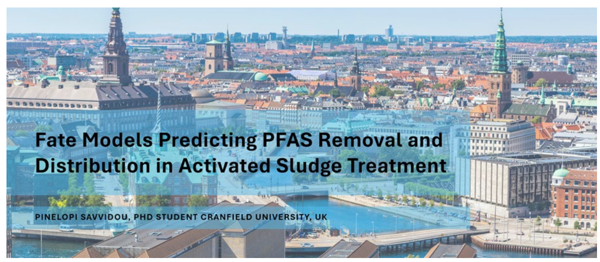





## ACTIVITY SYNOPSIS ctd

In 2024 EBNet funded a second POC project on Molecular docking and molecular dynamics simulations for assessing biodegradation of PFAS, headed by WG Lead Dr Tao Lyu. Outputs include an animated video available on EBNet's YouTube channel. This POC received follow-on funding from Cranfield University's Global Research Fund for work on '*Engineering biotechnology enabled innovative nature-based solutions to tackle emerging contaminants*', while the results also contributed to two larger proposals to NERC and the Royal Academy of Engineering (in review at the time of writing).

The group also benefitted from an EBNet Travel Bursary supporting an ECR to attend the *IWA Young Water Professionals European Conference 2024*: a video on the presentation is available on YouTube.




The WG prepared a position statement on 'Addressing PFAS 'Forever Chemicals' Contamination in the Environment which outlines the challenges and identifies research needs.

- Optimising analytical methods to detect PFAS sources, precursors, and degradation products
- Understanding PFAS behaviour and toxicity in different environmental compartments
- Improving modelling approaches to predict distribution, bioavailability and ecological risks
- Enhancing knowledge of toxicity mechanisms for ecologically relevant exposure thresholds

## WG Journal Papers

Sarti, C., Souleymane, A.A., Dotro, G., Cincinelli, A. and Lyu, T., 2025. Partitioning and removal of per-and polyfluoroalkyl substances (PFAS) in full-scale surface flow treatment wetlands with different upstream wastewater treatment. Journal of Water Process Engineering, 71, p.107236.

Ma, M., Coulon, F., Tang, Z., Hu, Z., Bi, Y., Huo, M. and Song, X., 2025. Unveiling the Truth of Interactions between Microplastics and Per-and Polyfluoroalkyl Substances (PFASs) in Wastewater Treatment Plants: Microplastics as a Carrier of PFASs and Beyond. Environmental Science & Technology.

Savvidou, P., Dotro, G., Campo, P., Coulon, F. and Lyu, T., 2024. Constructed wetlands as nature-based solutions in managing per-and poly-fluoroalkyl substances (PFAS): Evidence, mechanisms, and modelling. Science of the Total Environment, 934, p.173237.

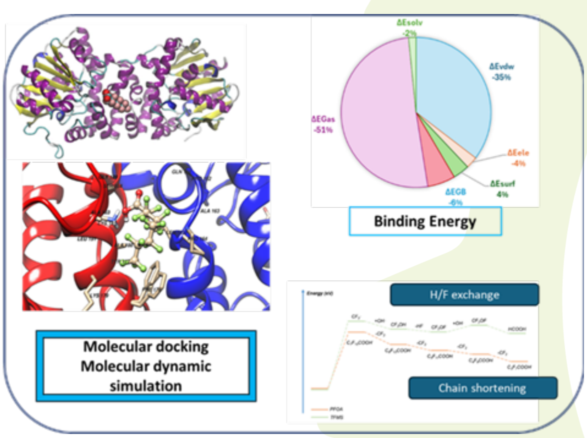
**Dr Tao Lyu**
Senior Lecturer in Green Technologies,
Cranfield University
**POC202413**

# Molecular docking and molecular dynamics simulations for assessing biodegradation of PFAS

## AIM

Per- and poly-fluoroalkyl substances (PFAS) have recently gained growing regulatory attention as emerging micropollutants, recognised for their exceptional resistance and environmental hazard to both human health and ecosystems. Often referred to as 'forever chemicals', PFAS compounds exhibit extremely stable chemical structures. While numerous treatment technologies have been investigated to mitigate PFAS contamination, final remediation stages typically rely on thermal or incineration processes to achieve complete chemical breakdown. Recently, the *biodegradation* of PFAS has shown potential as a cost-effective alternative. This study employed molecular docking and molecular dynamics simulations as in silico tools to investigate interactions between enzymes (proteins) and PFAS compounds (ligands) and elucidate the biodegradation mechanisms of PFAS, bridging the gap between theoretical exploration and experimental validation.

The study focused on the microbial fluoroacetate dehalogenase enzyme (RPA1163) and its interaction with perfluorooctanoic acid (PFOA) as a long chain PFAS containing an acetate functional group; and with a short chain PFAS (trifluoromethanesulfonic acid or TFMS) which lacks an acetate functional group for comparison. Molecular docking was performed using AMBER 99SB force field to investigate the enzyme's binding affinity for PFAS, while molecular dynamic simulations provided insights into the stability and dynamics of the enzyme-ligand complex. The results revealed that van der Waals and gas-phase energy are the driving force of binding interaction between the enzyme and PFAS.




## OUTCOME

These findings provide critical insights into the molecular mechanisms underpinning PFAS biodegradation, which could contribute to the development of cost-effective biotechnologies for PFAS remediation. The deeper understanding of the catalytic mechanism can guide the rational engineering of enzymes to enhance the degradation of fluorochemicals, fostering more sustainable and effective approaches for environmental remediation of persistence pollutants.

### Highlights

- Molecular docking simulations reveal the binding mechanisms of PFAS with the dehalogenase enzyme.
- PFOA exhibits stronger binding affinity with the enzyme but presents slower degradation.
- TFMS biodegradation relies on electron beam irradiation, which is limited in natural environments.
- Chain shortening of PFOA leads to the formation of less harmful and biodegradable carboxylic acids.
- Future engineering biotechnology approaches should focus on optimising the binding pocket geometry.

*Research Team* : Mahsa Baniasadi, Frederic Coulon, Tao Lyu

This POC project led to follow-up funding from Cranfield University, two further submitted proposals, a conference abstract, a dissemination video and a journal paper (in preparation)

**Professor Andy Cundy**
University of Southampton
POC202001

# EPACS: ENHANCING PFAS ATTENUATION IN COASTAL BROWNFIELD SOILS:
## ENHANCING NATURAL SYSTEM ATTENUATION CAPACITY FOR A KEY EMERGING CONTAMINANT

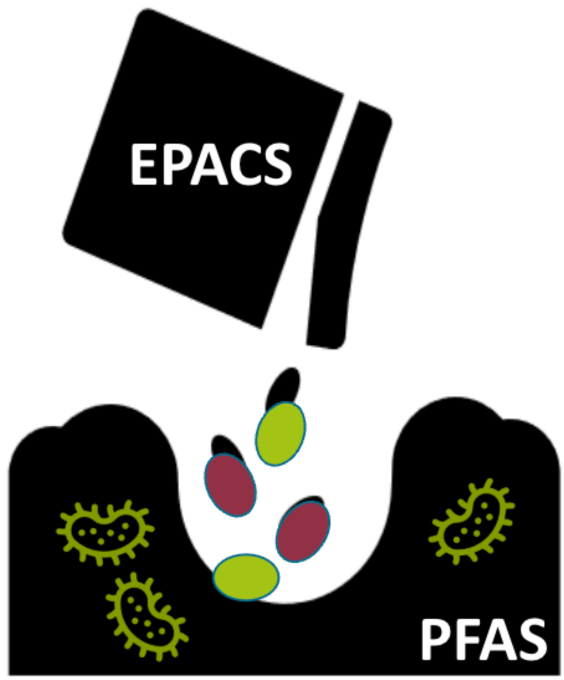
*"EBNet support has allowed the generation of key data which we can use to assess the natural capacity of coastal soils to adsorb and degrade PFAS, and how we can enhance this natural capacity to design more effective PFAS removal and management processes."*
**Prof Andy Cundy, University of Southampton**

## THE PROBLEM

Perfluoroalkyl substances (PFASs) are key emerging contaminants which have been used for over 60 years in a wide range of industrial applications. They are now ubiquitous in environmental matrices. Several bioaccumulate in marine food webs, so their presence in coastal brownfield soils is of significant concern, particularly given their recalcitrant and mobile nature. Current remediation technologies involve highly invasive interventions such as soil removal and off-site landfilling or incineration, sorption/stabilization through ex-situ soil mixing, and ex-situ thermal desorption with off-gas destruction.

## OUR APPROACH

We assessed the capability of zero-valent iron (ZVI) combined with highly sorptive biochar to enhance PFASs attenuation, improve soil functionality and stimulate local microbial communities to enhance breakdown of PFASs.




## THE RESULTS

Hypotheses were tested via a series of controlled microcosm experiments carried out over 20- and 60-day periods, using artificially spiked and natural or control soils and intertidal sediments collected from the Hamble estuary. This was followed by materials characterisation (including surface area measurements, N%, C%, and C and N isotopes), and PFAS and targeted DNA analysis. Results were used to assess the validity of enhanced natural attenuation approaches for PFAS management and trapping/degradation in these and similar coastal settings, including the impact of PFAS contamination on local microbial populations. These results form the focus of subsequent larger proposals to UKRI examining enhanced ‘treatment train’ approaches for PFAS management.

The results of the project were presented in an EBNet webinar and went forward as input into a UKRI proposal and the EU H2020 EiCLAR project

**REFERENCES:**
Assessing the role of the “estuarine filter” for emerging contaminants: pharmaceuticals, perfluoroalkyl compounds and plasticisers in sediment cores from two contrasting systems in the southern U.K. By: Omar Celis-Hernandez, Andrew B. Cundy, Ian W. Croudace, Raymond D. Ward, Rosa Busquets, John L. Wilkinson. In: Water Research Volume 189, 1 February 2021, 116610

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# Addressing PFAS 'Forever Chemicals' Contamination in the Environment

**Position statement by the PFAS Working Group, EBNet**
Prepared by Tao Lyu, Frederic Coulon, and Tony Gutierrez

Per- and polyfluoroalkyl substances (PFAS) are a class of synthetic chemicals widely used in industrial and consumer products due to their water and grease-resistant properties. Despite their relatively low market price of ~£15 per kilogram, the true cost of PFAS is far greater when societal impacts are considered (nearly 1000 times higher) (ChemSec, 2023)[1]. Their persistence, mobility, and bioaccumulative nature have triggered global alarm, leading to stringent regulatory limits in drinking water, now measured in nanograms per litre. A widely circulated report from the Europe Forever Lobbying Project warns that cleaning up PFAS contamination could surpass £1.6 trillion across the UK and Europe over the next two decades, with the UK alone facing annual costs of £9.9 billion. As the number of sites contaminated with PFAS continues to rise, urgent action is required to mitigate environmental and human health risks.

### Scientific Bases to Address PFAS Challenges

Despite growing evidence of the prevalence and harmful effects of PFAS, significant knowledge gaps remain regarding their environmental fate, transport, transformation, and degradation. Moreover, the structural diversity of PFAS compounds further complicates efforts to predict their behaviour and ecological impacts. The first PFAS list hosted by the NORMAN Network in 2015 consisted of ~4700 PFAS species. In 2021, the Organisation for Economic Co-operation and Development (OECD) revised the definition of PFAS, and consequently, over 7 million PFAS were summarised in one of the largest open chemical collections, PubChem. Recent drinking water regulations have included only a small portion of these compounds, with the EU and Scotland focusing on 20 PFAS and the rest of the UK on 48 PFAS. Although the statutory PFAS list is limited, previous studies from the PFAS WG attempted to develop an AI-driven model to simulate the removal performances of PFAS in contaminated water. This effort was still significantly inhibited by the lack of revealed basic chemical characteristics of those PFAS. The following urgent research needs were summarised and recommended by the UK Research Council through a specific call named 'Addressing Environmental Challenges' in 2024:

- Optimising analytical methods to detect PFAS sources, precursors, and degradation products
- Understanding PFAS behaviour and toxicity in different environmental compartments
- Improving modelling approaches to predict PFAS distribution, bioavailability, and ecological risks
- Enhancing knowledge of PFAS toxicity mechanisms to establish ecologically relevant exposure thresholds

### Evidence-Supported Technologies

Numerous treatment technologies have been explored to mitigate PFAS contamination, including granular activated carbon, ion exchange resins, membrane processes, and chemical oxidation. In these approaches, the final steps typically involve thermal/incineration processes for the complete breakdown of chemical structures. The development of cost-effective approaches capable of efficiently reducing PFAS or achieving complete mineralisation of PFAS remains a significant challenge. The key obstacle is the stability of the carbon-fluorine (C-F) bond, which requires substantial energy (526 kJ/mol) to break. Exploring biotechnology-based solutions, such as microbial degradation and enzymatic breakdown, offers a promising avenue for PFAS remediation.

Encouragingly, some studies have demonstrated the feasibility of PFAS biodegradation. However, further research is needed to improve efficiency and long-term viability. To achieve meaningful progress, it is essential to develop sustainable and scalable technologies for PFAS removal and destruction. These efforts should be integrated with broader strategies, such as implementing PFAS bans and reducing the flow of these contaminants into the environment at their source.

The PFAS Working Group, as part of the Environmental Biotechnology Network, is committed to advancing scientific research, developing innovative solutions, and informing policy to mitigate the impacts of PFAS pollution. By addressing the challenges outlined in this position paper and prioritising the identified research needs, we can work towards a cleaner, safer, and more sustainable future.

1. https://chemsec.org/reports/the-top-12-pfas-producers-in-the-world-and-the-staggering-societal-costs-of-pfas-pollution/

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