

Smart monitoring of contaminants of emerging concern in wastewater treatment

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The current analytical and monitoring systems for detecting trace contaminants of emerging concern (CECs), such as pharmaceutical compounds (PhCs) and antimicrobial resistance (AMR), are expensive and time-consuming, posing challenges for routine application in wastewater treatment plants (WWTPs) and water quality monitoring. These limitations hinder real-time decision-making and operational efficiency. Smart monitoring solutions, such as soft sensors, offer a transformative approach by enabling continuous, cost-effective, near-real-time estimation of contaminant levels through advanced algorithms and data integration. This reduces reliance on labour-intensive laboratory analyses, supporting proactive management and enhancing treatment process efficiency while addressing the growing demand for sustainable water management.

In this context, the EU-funded LIFE Fitting project (lifefitting.lnec.pt/) aims to develop and demonstrate, at full scale in three large WWTPs, an innovative set of tools (PLAN-DO toolbox, TRL 7, ready for professional software production) for strategic planning, monitoring, and intelligent operation of WWTPs. This includes the “MonitorTool,” designed to produce simplified protocols for routine use by water utilities to monitor WWTPs for emerging contaminants (e.g., PhCs, AMR) based on online bulk parameters and AMR biomarkers.

Field water quality data from 27 monitoring campaigns conducted at the WWTPs and their receiving waters were used as inputs for MonitorTool. These data included analyses of over 54 PhCs, microbial indicators, AMR biomarkers, and regular (e.g., BOD5, COD, nitrogen, phosphorus, colour) and non-regular (e.g., T254, alkalinity) bulk indicator parameters.

Correlations between CEC concentrations/removals and other water quality parameters are being explored using Projection to Latent Structures regression (PLSR), a versatile multivariate data analysis method increasingly applied in fields such as bioinformatics, machine learning, and chemometrics, including water and wastewater treatment.

Results confirm that water spectroscopic data are key surrogates for CEC concentrations and removals. Specifically, absorbance at 254 nm, an indicator of organic matter aromaticity and C=C bonds characteristic of several PhCs, emerges as the most prominent surrogate. Other key surrogates include nitrogen species and parameters, such as ammonia nitrogen and total nitrogen, related to nitrification/denitrification conditions in WWTPs, as expected. Furthermore, fluorescence spectroscopy through excitation-emission matrices with parallel factor analysis (EEM-PARAFAC) is being explored as a high-resolution proxy for CECs.

The correlations underway constitute a practical and cost-effective way of supporting on a continuous basis the routine monitoring of the WWTP effectiveness towards CECs.

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