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# Development of alternative method for PFAS detection

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**Abstract:** The global water supply crisis is worsening due to climate change, population growth, and poor economic conditions. Compounding this issue is the rise of contaminants of emerging concern (CECs), such as per- and polyfluoroalkyl substances (PFAS). Widely used in industry and household products, PFAS are resistant to degradation, accumulating in wastewater systems and waterbodies. Current wastewater treatment technologies are inadequate for removing these complex compounds, leading to heightened environmental and health concerns. Despite regulatory progress, challenges persist in monitoring PFAS due to the limitations of conventional methods, such as chromatography, which are costly, time-intensive, and unsuitable for real-time analysis. Electrochemical methods offer promise due to their sensitivity but are hindered by high costs, low selectivity, and reliance on expensive materials. This research explores the use of soft sensors as a cost-effective solution for real-time PFAS monitoring. Soft sensors utilize physical online water quality sensors (e.g., pH, conductivity) and advanced data analytics to estimate hard-to-measure parameters. A sampling campaign across wastewater treatment plants in Oslo analyzed water quality parameters, fluorescence, and absorbance spectra. The developed model prediction revealed strong correlations ($R^2 = 0.96$) between PFAS concentrations and water quality parameters. The findings demonstrate that soft sensors, combined with spectral data and analytics, provide a viable, affordable method for real-time PFAS monitoring, addressing critical gaps in current technology.

**Keywords**: contaminants of emerging concern, online monitoring, machine learning

The problem of inadequate water supply is getting more severe in recent years due to major factors such as climate change, population growth and poor economic conditions worldwide. In addition, due to more intense industrialization processes world started facing the problem of new, previously unknown, pollutants, contaminants of emerging concern (CECs). These chemicals were historically present in water in low concentrations and, therefore, were not a subject for regulations. However, in recent years the occurrence of these chemicals has been increased and so did the concern regarding the effect of these chemicals on health and environment. One of the most discussed representatives of CECs is per- and polyfluoroalkyl substances (PFAS).

PFAS substances are widely used in industry, and in production of various household products. Due to their complex structure, PFAS compounds are resistant to degradation and, therefore, end up in the wastewater system. However, the current wastewater treatment technologies are not able to remove such complex compounds as PFAS, they end up in waterbodies in high concentrations (Kasprzyk-Hordern et al., 2009; Tong et al., 2022). In order to control this problem, EU Commission proposed to revise the list of surface and groundwater pollutants, that should be monitored (EU legislation in progress, 2023). The revision includes adding several different substances to the watch list, among which are 24 PFAS compounds (EU legislation in progress, 2023). Additionally, EU Council recently adopted a new urban wastewater directive that requires implementing of quaternary treatment of micropollutants (The European parliament, 2024).

Despite adding contaminants of emerging concern to the watch list, the challenges with monitoring of these substances remain, primarily due to the lack of appropriate technological solutions. The conventional method, such as chromatographical methods, offer good detection limits of PFAS. However, the main disadvantage of such methods is the time consumption related to the sample preparation. Moreover, the instrumentation for the standard analytical detection methods is extremely expensive and requires specialized training of the personnel. Additionally, sample preparation is required, and the analytical processes itself are time-consuming. This leads to a delay in results, which makes it impossible to use such methods for online monitoring.

Among other solutions, the use of electrochemical methods for detection of contaminants of emerging concern have been studied (Manivannan et al., 2022). Electrochemical approaches offer good sensitivity for detecting these contaminants (Qian et al., 2021; Lahcen et al., 2020; Manea et al., 2012). However, these techniques often require the use of expensive nanomaterials, quantum dots, or precious metals, which can limit their practicality and widespread use. Additionally, despite their sensitivity, electrochemical methods have low selectivity, making it challenging to distinguish between different contaminants in complex environmental samples (Manivannan et al., 2022).

Considering the above-mentioned need for the online monitoring of contaminants of emerging concern, and the challenges that come with it, it was decided to explore the possibility of the application of a soft sensor concept for the detection of PFAS. The soft sensors approach combines utilizing of physical online sensors (pH, conductivity, turbidity, etc.) and advanced data analytics for finding the correlation of simple water quality parameters with concentrations of hard-to-measure parameters, like Total Phosphorus, Chemical Oxygen Demand, etc (Nair et al., 2022).

A sampling campaign across different wastewater treatment plants in Oslo region was conducted for obtaining data for model development, The collected samples were analysed for a range of water quality parameters. Additionally, the spectral properties (fluorescence and absorbance) of the collected samples were examined. The collected fluorescence EEMs underwent decomposition using Principal Component Analysis and Parallel Factor Analysis (PARAFAC). The obtained data was further analysed to establish a correlation between the measured parameters and the concentration of PFAS in the analysed matrix.

The developed model prediction has shown a good correlation (R2=0.96) (Figure 1.1) with the concentration of PFAS. The results have shown the soft sensors can be used for estimation of PFAS concentrations in wastewater using simple water quality parameters and spectral data in combination with advanced data analytics. This gives opportunity to monitor the concentration of PFAS in real-time without high expanses for instrumentation.

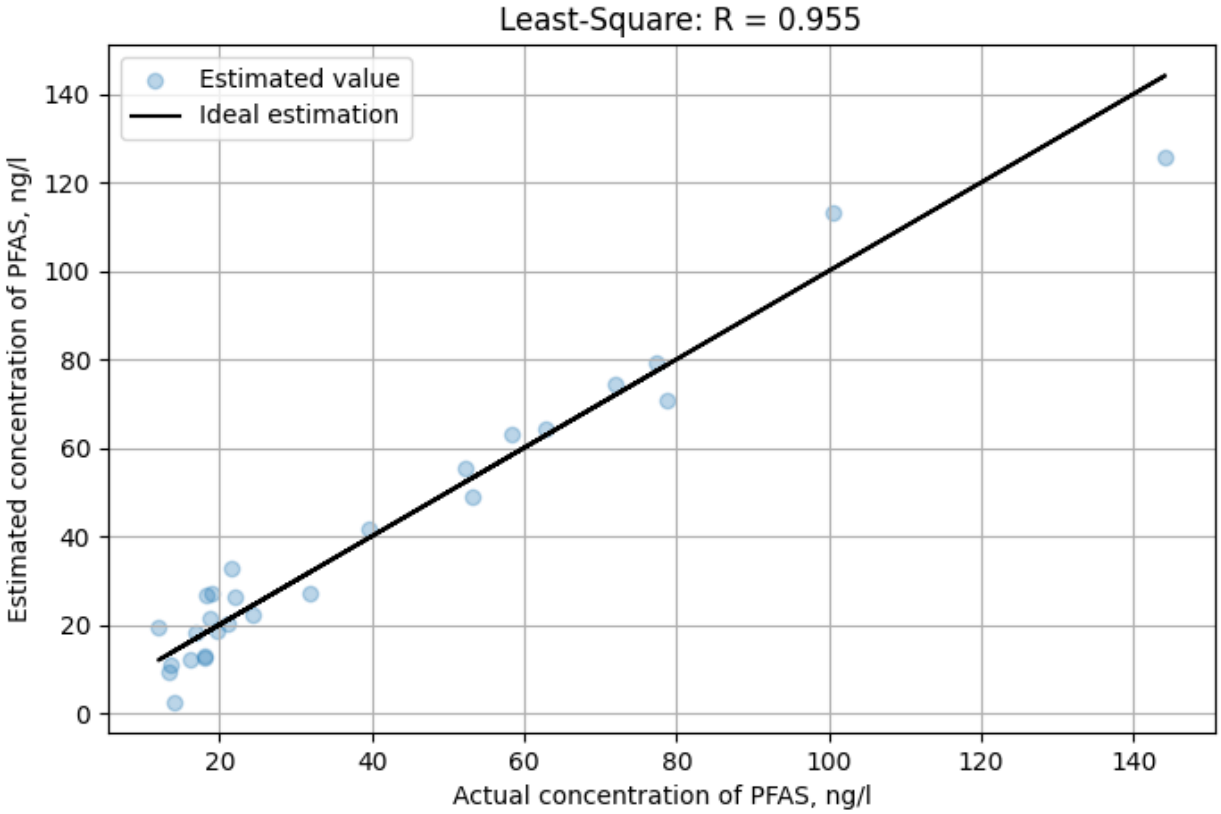


**Figure 1.1** Correlation between soft sensor prediction and concentration of PFAS in wastewater

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