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From legacy to emerging groundwater contaminants: Advancing monitoring tools to assess sources and remediation of contaminated sites

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Aquifers worldwide are under increasing pressure from the widespread use of synthetic chemicals, many of which, alone or as a mixture, are persistent, mobile, and toxic. Legacy and emerging organic contaminants pose major challenges for groundwater remediation, often involving substantial cleanup costs and requiring efficient monitoring strategies to trace their sources and transformation mechanisms. Various legacy contaminants, such as petroleum and chlorinated hydrocarbons, have been successfully removed from contaminated aquifers, *e.g.*, via natural attenuation (biodegradation). However, the biotransformation of emerging contaminants, such as novel pesticides, their transformation products and per- and polyfluoroalkyl substances (PFAS), remains only partially understood.

Integrating conventional hydrogeochemical monitoring with multi-element compound-specific isotope analysis (ME-CSIA), biomolecular tools, and reactive transport modeling have proven useful in evaluating sources, transport and transformation mechanisms of various groundwater contaminants *in situ* [1]. Such integrative approach holds great potential to provide decisive information on contaminant removal processes and enhance the selection of remedial actions and the evaluation of remediation efficiency. In particular, ME-CSIA can provide evidence of contaminant transformation mechanisms at contaminated sites. However, the structural complexity of many polar emerging contaminants, combined with their typically low environmental concentrations, necessitates the development of advanced high-resolution mass spectrometry (HRMS) techniques to accurately resolve and quantify isotope fractionation in environmental samples. In our recent study, HRMS techniques like QTOF-MS were proposed to evaluate Cl isotope fractionation of the pesticide chlordecone, allowing insights into the remediation challenges of contaminated soils from the French West Indies [2]. Advancing monitoring tools like ME-CSIA using HRMS will open new avenues to understand the complex challenges posed by the pervasiveness of (emerging) contaminants in soils and groundwater and develop suitable remediation and monitoring strategies.

[1] Prieto-Espinoza, M., Hohener, P., & Imfeld, G. (2025). From Legacy to Emerging Groundwater Contaminants: Combining Advanced Monitoring Tools to Assess Sources and In Situ (Bio) Transformation. *ACS ES&T Water*, *5*(12), 7088-7104.

[2] Prieto-Espinoza, M., Malleret, L., Durand, A., & Hohener, P. (2024). Elucidating the fate of the organochlorine pesticide chlordecone under abiotic reductive and oxidative processes: kinetics, transformation products, and C vs Cl isotope fractionation. *Environmental Science & Technology*, *58*(43), 19475-19485