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Fate and transport of emerging contaminants in groundwater: A chemometric approach.

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Introduction

Groundwater serves as a critical source of drinking water for nearly half the global population. However, its quality is increasingly threatened by the infiltration of emerging contaminants (ECs)—a diverse group of synthetic and naturally occurring compounds, including pharmaceuticals, personal care products, endocrine-disrupting chemicals, and microplastics. These substances often escape traditional water treatment processes and enter aquifers through agricultural runoff, industrial discharge, and wastewater leakage. Understanding the fate and transport of these contaminants in groundwater systems is essential for effective risk assessment and remediation strategies [1].

Unlike conventional pollutants such as nitrates or heavy metals, emerging contaminants are characterized by their low concentrations, varied sources, and complex chemical structures. Many of these compounds are biologically active even at trace levels, raising concerns about long-term ecological and human health effects. As new substances are continually introduced into the environment, the list of ECs evolves, making their monitoring and analysis a moving target for scientists and regulatory agencies [2].

Groundwater systems are inherently complex due to their subsurface nature, variability in hydrogeological conditions, and interactions between physical, chemical, and biological processes. The transport of ECs is influenced by factors such as soil composition, porosity, pH, redox conditions, microbial activity, and organic matter content. These variables collectively determine whether a contaminant will degrade, adsorb to soil particles, or migrate with the groundwater flow [3].

Conventional monitoring methods often fail to detect ECs at environmentally relevant concentrations. However, advances in chromatography-mass spectrometry (e.g., LC-MS/MS, GC-MS) have improved the detection and quantification of a wide range of trace contaminants. While these analytical tools are powerful, the large volumes of complex, multivariate data they generate require sophisticated analysis techniques. This is where chemometrics becomes an essential component of environmental chemistry [4].

Chemometrics refers to the application of mathematical and statistical methods to extract relevant information from complex chemical data. In the context of groundwater contamination, chemometric tools help interpret patterns, relationships, and trends in environmental datasets. Techniques such as Principal Component Analysis (PCA), Cluster Analysis (CA), and Partial Least Squares Regression (PLSR) are commonly used to reduce dimensionality, classify contamination sources, and predict the behavior of ECs [5].

Conclusion

The growing presence of emerging contaminants in groundwater represents a significant environmental challenge. Understanding their fate and transport is critical for protecting public health and maintaining ecosystem integrity. By combining advanced analytical chemistry with powerful statistical modeling, chemometrics provides a promising framework for deciphering the complex behavior of ECs in subsurface environments. As analytical capabilities and computational tools continue to evolve, the chemometric approach will play an increasingly vital role in sustainable groundwater management and pollution mitigation.

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