Goldschmidt 2025 Abstract
https://doi.org/10.7185/gold2025.27135

Integrating CSIA and reactive transport modeling to characterize DNAPL Source Zone Architecture during natural attenuation in biogeochemically heterogeneous aquifers

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The heterogeneity of aquifers plays a critical role in the spatial distribution of dense non-aqueous phase liquid (DNAPL) contaminants. Previous research has focused on physical heterogeneity (e.g., hydraulic conductivity and porosity) in static characterization of DNAPL source zone architecture (SZA), while biogeochemical properties have often been assumed to be homogeneous due to limited data availability. However, in DNAPL-contaminated sites, biodegradation kinetics are typically heterogeneous, influencing the migration and transformation of contaminants under natural attenuation (NA) [1]. The homogeneous assumption may result in inaccurate estimates of DNAPL SZA longevity and remediation efficiency. Sparse data and traditional measurement limitations (e.g., concentration data) hinder the identification of biogeochemical heterogeneity. The potential of compound-specific isotope analysis (CSIA) to reveal the spatial variability of biodegradation process based on its enhanced sensitivity compared with concentration data has been noted [2].

This study proposes a novel “Two-stage” framework to dynamically characterize DNAPL SZA during NA. In Stage 1, short-term downstream measurements including concentration and CSIA data are integrated using a principal component geostatistical approach (PCGA) to identify biogeochemical heterogeneity. In Stage 2, these inversion results are applied to predict long-term NA efficacy. A synthetic case study demonstrates the framework’s effectiveness, revealing that CSIA data provides complementary diagnostic insights that significantly improve the identification of biogeochemical heterogeneity compared to concentration data alone. This led to a reduction in SZA characterization errors by up to 47.1%. Our framework offers a promising approach for improving long-term NA predictions, enhancing remediation strategy design in heterogeneous aquifers.

[1] Yang, L. et al. (2021), Water Resources, 193, 116842.
[2] Wanner, P. et al (2016), Environmental Science & Technology, 50(11), 5622-5630.