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Tracing Water-Rock Interactions and Contaminant Pathways in Acid Mine Drainage (AMD) Systems: Insights from Geochemical and Multi-Isotope Approaches

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Acid Mine Drainage (AMD) presents a severe environmental challenge in mining regions. To analyze the complex water-rock interactions and pollutant pathways in AMD systems, this study integrates hydrochemical fingerprinting with multiple isotope techniques (δD-$\delta^{18}O$, $^{87}Sr/^{86}Sr$) to develop a comprehensive "source-pathway-sink" model for pollutant apportionment. Combined with long-term monitoring and PHREEQC modeling, our research quantifies the contributions of key reactions like pyrite oxidation and carbonate dissolution to water quality evolution, identifying the dominant processes controlling AMD formation.

Significant spatial gradients were observed along the groundwater flow path: pH and temperature decreased, while electrical conductivity (EC), Na^+, K^+, Mg^{2+}, oxidation-reduction potential (ORP), SO_4^{2-}, and NO_2^- concentrations markedly increased. Hydrogen and oxygen isotope analysis confirms atmospheric precipitation as the primary recharge source, revealing complex interactions among mine, surface, and groundwater that create preferential pathways for pollutant migration. Sulfur and oxygen isotope data clearly indicate that sulfate originates from sulfide oxidation, with H_2O as the principal oxygen source.

Metagenomic analysis highlights the critical role of microorganisms in pollutant transformation. In acidified downstream waters, microbial diversity significantly decreased, while the abundance of acid-tolerant, sulfur-cycling genera like *Acidithiobacillus* and *Acidulodesulfobacterium* substantially increased. A strong correlation between functional genes and hydrogeochemical parameters revealed a synergistic relationship between sulfur oxidation and nitrate reduction, indicating a tightly coupled nitrogen-sulfur (N-S) biogeochemical cycle. Furthermore, 158 high-quality metagenome-assembled genomes (MAGs) confirmed that core microbes possess complete N and S cycling genes, identifying them as the primary biological drivers of pollutant transformation.

By integrating these techniques, this research systematically elucidates the hydro-geochemical-microbial coupling mechanisms that govern pollutant formation, migration, and transformation in AMD systems. This provides a crucial scientific basis for the precise assessment and remediation of aquatic environments in mining areas.