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Unraveling Hydrogen Induced Geochemical Reaction Mechanisms through Coupled Geochemical Modeling and Machine Learning

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Subsurface hydrogen storage has emerged as a prospective large-scale energy storage solution, yet ensuring adequate recovery of stored hydrogen remains a critical challenge. Within subsurface reservoirs, hydrogen undergoes intricate geochemical interactions with the brine and host rock, potentially leading to hydrogen losses. This study presents an integrated approach by coupling geochemical modeling with, non-negative matrix factorization (NMF) based an unsupervised machine learning technique, to unravel the complex H_2-brine-rock geochemical processes governing hydrogen losses, with a particular focus on sulfate reduction reactions.

NMF is applied to simulated mineral evolution and fluid component profiles, and it revealed hidden patterns and relationships within the simulation dataset. This approach enables the decoupling of overlapping equilibrium reactions, facilitating the separation of redox processes, dissolution fronts, and secondary precipitation while accounting for simulation parameters such as salinity, temperature, and total H_2 pressure. NMF successfully disentangle these competing effects in nonlinear manners and effectively identifies four distinct reaction stages, enabling robust interpretation. Furthermore, it unveils subtle coupled mineral associations and reaction fronts that are obscured in conventional model analyses.

Finally, a feature importance framework based on NMF results is employed to enhance the explainability of the analysis by exploiting correlations among attributes of the basis matrix. This study highlights the efficacy of synergistically combining geochemical modeling with machine learning techniques to enhance the interpretability of intricate geochemical simulation outputs by deciphering overlapping reaction pathways, a task unachievable through conventional analysis of geochemical models alone.