



Research article



NeutroChem Fusion: an uncertainty-aware source diagnosis framework for mining impacted waters in West Africa

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ARTICLE INFO

Keywords:

Mining impacted waters
Heavy metal source diagnosis
Neutrosophic logic
Dezert-Smarandache theory
Screening level remediation decision support

ABSTRACT

Mining impacted waters in West Africa are mixed chemical systems in which mining-derived Hg-Pb-Cd signals, geogenic As-Fe-Mn mobilisation, acid mine drainage, agricultural runoff, domestic inputs and sediment remobilisation may coexist. Existing water-quality indices, receptor models, geochemical models and machine-learning classifiers are useful for screening and apportionment, but they may compress overlapping mechanisms into dominant factors or exclusive labels. This study develops NeutroChem Fusion as a neutrosophic-Bayesian constrained DSMT framework for uncertainty-aware source-mechanism diagnosis and treatment-pathway decision support. The framework was internally evaluated on 720 field-water-system records from Ghana, Burkina Faso, Mali, Guinea, Côte d'Ivoire, Senegal and Niger sampled from January to May 2026. The full model showed source-label concordance of 0.9023 in the internal test set and 0.8730 in the workbook-held-out country-transfer subset. Pooled fixed-validation concordance was 0.8880 (95% bootstrap interval 0.8494–0.9228) and pooled macro-F1 was 0.8786. On the same fixed split and field/reference labels, multinomial logistic regression, PCA-logistic regression and random forest achieved concordances of 0.7568, 0.7606 and 0.8147, respectively; these comparisons are internal supervised benchmarks rather than proof of external superiority. The engineering chemistry layer was experimentally calibrated using standardised bench-scale adsorption, precipitation, electrocoagulation and membrane tests. The variables `biochar_pct`, `iron_oxide_adsorption_pct`, `lime_precipitation_pct`, `electrocoagulation_pct` and `membrane_rejection_pct` are measured removal or rejection percentages, while the associated 0–1 process scores are normalised indices calibrated against those experiments. Experimental treatment outcomes for internal test and workbook-held-out records were masked during pathway prediction. NeutroChem Fusion therefore provides a transparent route from exceedance screening to uncertainty-aware source diagnosis, confirmatory-sampling priority and experimentally supported treatment-pathway selection, while independent field validation and site-specific pilot assessment remain necessary. Established method comparisons yielded source-label concordances of 0.8649 for XGBoost-SHAP, 0.6988 for APCS-MLR score mapping and 0.5985 for uncertainty-weighted PMF score mapping. A PHREEQC input-completeness audit found that 0 of 720 records contained the full temperature, major cation, inorganic carbon and redox speciation inputs required for defensible charge balanced simulation.

1. Introduction

Mining impacted waters in West Africa should be understood as mixed chemical systems rather than as isolated exceedance events. Across artisanal, small-scale and industrial mining environments, water

chemistry is shaped by interacting inputs from ore extraction, mineral processing, tailings and waste rock weathering, acid generation, lithologic metal release, seasonal runoff, agricultural drainage, settlement pressure and sediment disturbance. Evidence from Ghanaian mining districts and wider sub-Saharan artisanal gold mining settings shows

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