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Article

# Explainable AI Models for Interpretable Forecasting of Groundwater Recharge Rates and Contaminant Migration in Arid Environmental Systems

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## Abstract

Arid environmental systems, characterized by low precipitation and high evaporation, rely heavily on groundwater as the primary freshwater resource, yet face escalating threats from unpredictable recharge rates and contaminant migration driven by agricultural runoff and industrial activities. Traditional hydrological models often struggle with the nonlinear complexities of these dynamics, while black-box machine learning approaches, though powerful, lack the transparency needed for stakeholder trust and regulatory compliance. This study presents a novel suite of explainable AI (XAI) models that integrate ensemble techniques like XGBoost and LSTM networks with post-hoc interpretability tools such as SHAP (SHapley Additive exPlanations) and LIME (Local Interpretable Model-agnostic Explanations) to provide both high-fidelity forecasts and clear insights into underlying mechanisms. Developed for a representative arid basin akin to those in the Arabian Peninsula, the models leverage diverse datasets including satellite-derived rainfall, soil permeability profiles, isotopic tracers, and long-term well monitoring data for nitrates, heavy metals, and salinity. Recharge rates are forecasted with superior accuracy ( $R^2 > 0.93$ , RMSE  $< 2.1$  mm/month), capturing episodic infiltration events, while contaminant migration is simulated through coupled advection-dispersion modules, predicting plume extents up to 7 km under high-recharge scenarios. Interpretability analyses pinpoint precipitation intensity, antecedent soil moisture, and hydraulic gradients as pivotal drivers, with force plots elucidating event-specific influences such as how flash floods dilute pollutants temporarily. These frameworks not only outperform conventional physics-based simulators like MODFLOW by 25% in predictive skill but also empower hydrologists and policymakers with actionable visualizations, uncertainty quantifications, and feature attribution maps. By demystifying AI predictions, this work advances sustainable aquifer management, supports managed recharge initiatives, and sets a benchmark for interpretable forecasting in climate-vulnerable drylands, fostering broader adoption of AI in environmental hydrology.

**Keywords:** explainable AI; groundwater recharge; contaminant migration; arid environments; SHAP interpretability; XGBoost; hydrological forecasting; aquifer management

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## 1. Introduction

Arid environmental systems, spanning vast regions like the Arabian Peninsula, Southwest United States, and North African deserts, confront profound groundwater challenges exacerbated by climate variability and human pressures [1]. These areas depend almost entirely on episodic recharge from rare rainfall events to sustain aquifers that supply water for agriculture, urban use, and ecosystems, yet high evaporation, low infiltration rates, and overexploitation lead to rapid depletion.

Contaminants such as nitrates from fertilizers, heavy metals from mining, and salinity intrusion further degrade water quality, with migration patterns unpredictable due to heterogeneous subsurface geology and fluctuating hydraulic gradients [2]. Conventional physics-based models like

MODFLOW capture steady-state flows but falter in replicating nonlinear responses to extreme weather, underscoring the urgency for advanced predictive tools in resource management.

### 1.1. Background on Arid Groundwater Challenges

In arid zones, groundwater recharge constitutes a minuscule fraction of precipitation often below 5% primarily occurring during intense, short-duration storms that overwhelm soil capacity and trigger surface runoff infiltration [3]. Evapotranspiration dominates the water balance, with potential rates exceeding 2000 mm annually, while sparse vegetation and coarse soils accelerate deep percolation only under saturated conditions.

Contaminant migration compounds these issues, as pollutants advent along preferential flow paths and disperse unevenly in fractured aquifers, leading to localized hotspots that persist for decades. Historical data from regions like Saudi Arabia reveal declining water tables at 1-2 meters per year alongside rising nitrate levels above WHO limits, driven by intensified irrigation and urban sprawl [4]. These dynamics demand forecasting models that integrate meteorological, geological, and anthropogenic variables to anticipate crises before they manifest in well failures or ecosystem collapse.

### 1.2. Need for Interpretable AI Models

Machine learning has revolutionized hydrological forecasting by discerning complex patterns in big data from satellites, IoT sensors, and geophysical surveys, surpassing traditional models in accuracy for recharge estimation and plume tracking [6]. However, “black-box” algorithms like deep neural networks obscure decision rationales, eroding trust among hydrologists, regulators, and communities who require causal explanations to validate predictions against domain knowledge.

Opaque models hinder regulatory approval for remediation plans and complicate liability in contamination events, as stakeholders cannot discern whether forecasts stem from soil permeability or data artifacts [8]. Explainable AI addresses this by layering interpretability techniques such as feature importance rankings and counterfactual analyses onto high-performing predictors, ensuring transparency without sacrificing precision. This interpretability proves vital in arid contexts, where policy decisions on artificial recharge or pumping restrictions hinge on verifiable insights into drivers like rainfall intensity or dispersivity coefficients [9].

### 1.3. Research Objectives and Novelty

This study aims to develop and validate hybrid explainable AI frameworks tailored for arid aquifers, specifically targeting interpretable forecasts of recharge rates (in mm/month) and contaminant migration velocities (m/year) [11]. Primary objectives include achieving  $R^2 > 0.90$  predictive accuracy, elucidating top influencing factors via SHAP values, and simulating plume evolution under climate scenarios. Secondary goals encompass benchmarking against baselines like random forests and physics simulators, plus generating user-friendly visualizations for non-experts.

The novelty lies in a unified pipeline coupling XGBoost for global predictions with event-specific LIME explanations and advection-dispersion embeddings, applied to a novel arid dataset fusing isotopic tracers and hyperspectral imagery advancing beyond prior works that treated recharge and contamination silos [13]. This integration not only elevates forecasting fidelity but pioneers scalable XAI for dryland hydrology, enabling proactive interventions amid 21st-century water scarcity.

## 2. Literature Review

The evolution of groundwater modelling reflects a progression from physics-driven simulations to data-centric AI paradigms, particularly suited to arid systems where data scarcity and variability challenge conventional assumptions [15]. Early approaches relied on Darcy’s law and mass balance principles, evolving into sophisticated numerical codes that simulate flow and transport but demand extensive parameterization.

Contemporary research increasingly incorporates machine learning to harness heterogeneous datasets from remote sensing and in-situ monitoring, achieving superior predictive performance amid climate uncertainties. This review synthesizes these advancements, highlighting transitions toward interpretable intelligence that aligns AI outputs with hydrological expertise [16].

### 2.1. Traditional Hydrological Models

Traditional hydrological models form the bedrock of groundwater analysis, employing partial differential equations to represent flow through porous media and solute transport via advection-dispersion mechanisms. Pioneering codes like MODFLOW discretize aquifers into finite-difference grids, solving for heads and fluxes under specified boundary conditions such as constant recharge or river seepage, which proves effective for steady-state scenarios in arid basins with minimal recharge [18]. Extensions like MT3DMS couple these with geochemical reactions, simulating contaminant retardation and decay, yet their efficacy wanes in heterogeneous arid environments where fractured rocks and ephemeral streams defy uniform parameters.

Calibration remains labour-intensive, often yielding equifinality multiple parameters sets fitting observations equally while computational demands escalate for long-term forecasts incorporating climate forcings [19]. These limitations, evident in overestimations of recharge by 20-50% during flash floods, necessitate data-driven complements that capture empirical nonlinearities without exhaustive site characterization.

### 2.2. Machine Learning in Recharge Estimation

Machine learning has transformed recharge estimation by processing multivariate time series from precipitation gauges, evapotranspiration models, and soil moisture probes to infer infiltration fluxes unattainable through physics alone [21]. Regression ensembles like random forests and gradient boosting machines (e.g., XGBoost) dominate, regressing monthly recharge against predictors such as antecedent rainfall, land surface temperature, and normalized difference vegetation index derived from MODIS satellites, routinely attaining  $R^2$  values exceeding 0.85 in arid case studies from the Negev Desert to California's Central Valley.

Recurrent architectures, including LSTMs, excel at sequence modelling for episodic recharge events, integrating lagged variables to emulate memory effects in vadose zone storage. Hybrid neuro-fuzzy systems further refine outputs by embedding physical constraints like Richards' equation approximations, reducing physically implausible predictions [23]. Despite these gains often halving error metrics over lumped parameter models' standalone ML applications falter in generalization across aquifers and obscure mechanistic insights, prompting the infusion of explainability to elevate utility in management contexts.

### 2.3. Explainable AI Techniques (SHAP, LIME)

Explainable AI techniques demystify black-box predictions by attributing outcomes to input features, fostering trust essential for hydrological deployment. SHAP (SHapley Additive exPlanations) grounds interpretations in cooperative game theory, apportioning each prediction's deviation from baseline via weighted coalitions of features, yielding consistency across global summaries and local force plots that visualize how precipitation depth might propel recharge while salinity retards it [25]. In arid forecasting, SHAP dependency plots elucidate nonlinear interactions, such as rainfall thresholds triggering infiltration, with applications in Saudi aquifers revealing evapotranspiration's outsized influence.

Complementarily, LIME (Local Interpretable Model-agnostic Explanations) perturbs inputs around specific instances to fit simple surrogate models like linear regressions, illuminating case-by-case rationales ideal for dissecting anomalous low-recharge predictions during observed wet periods. Integrated in pipelines with tree-based learners, these methods not only validate model fidelity against domain heuristics but also guide feature engineering, as seen in recent works enhancing

contaminant plume forecasts by prioritizing dispersivity over remote sensing noise, thus bridging AI prowess with actionable hydrogeological knowledge.

### 3. Study Area and Data

The study area and data section delineates the geographical scope and empirical foundation underpinning the explainable AI models, ensuring reproducibility and contextual relevance for arid groundwater dynamics. Selected for its emblematic arid characteristics, the site exemplifies transboundary aquifer challenges prevalent across drylands, with data curated from authoritative sources to capture recharge and contamination processes comprehensively [27]. This integration of field-validated observations with remote sensing enables robust model training, addressing data sparsity inherent to desert environments.

#### 3.1. Description of Arid Region Site

The investigation centres on the Wajid Aquifer system in southwestern Saudi Arabia, a transboundary sandstone reservoir spanning approximately 50,000 km<sup>2</sup> within the Arabian Peninsula's arid heartland, receiving less than 100 mm annual precipitation amid temperatures averaging 28 °C [30]. Composed of Cretaceous sediments with hydraulic conductivity ranging from 10<sup>-4</sup> to 10<sup>-3</sup> m/s, the aquifer exhibits unconfined conditions in wadi alluvium overlying confined paleo-flows, facilitating episodic recharge via flash floods channeled through incised valleys.

Contamination hotspots arise from agricultural nitrates in the north and natural salinity gradients southward, with groundwater depths varying from 20 m in recharge zones to over 200 m downdip, mirroring vulnerabilities in analogous systems like the Saq Aquifer [31]. This site's geological heterogeneity, sparse vegetation covers below 10%, and historical drawdown of 1-2 m/year underscore the imperative for precise forecasting amid escalating extraction exceeding 1 km<sup>3</sup> annually.

#### 3.2. Dataset Sources

Datasets amalgamating precipitation records from TRMM and GPM satellites (daily resolution, 2000-2025) quantify episodic inputs critical for recharge, complemented by GLDAS evapotranspiration estimates via the Penman-Monteith equation:

$$ET_0 = \frac{0.408\Delta(R_n - G) + \gamma \frac{900}{T + 273} u_2 (e_s - e_a)}{\Delta + \gamma(1 + 0.34u_2)} \quad (1)$$

where  $\Delta$  is the slope of saturation vapor pressure curve,  $R_n$  net radiation,  $G$  soil heat flux,  $\gamma$  psychrometric constant,  $T$  temperature,  $u_2$  wind speed, and  $e_s - e_a$  vapor pressure deficit [33]. Soil data derive from FAO Harmonized World Soil Database, detailing texture (sandy loam dominant), porosity ( $n \approx 0.35$ ), and van Genuchten parameters for unsaturated flow, alongside field borehole logs for saturated conductivity  $K_s$ .

Stable isotopes ( $\delta^{18}O$ ,  $\delta^2H$ , tritium) from IAEA-GNIP networks and local wells trace recharge modernity, with chloride profiles enabling mass balance:

$$\text{recharge rate } R = \frac{P \cdot Cl_p}{Cl_{gw}} \quad (2)$$

where  $P$  is precipitation,  $Cl_p$  bulk chloride deposition, and  $Cl_{gw}$  groundwater concentration, revealing Holocene contributions below 10 mm/year [35]. Contaminant metrics (nitrates, arsenic) stem from national monitoring wells ( $n=150$ , bi-monthly).

#### 3.3. Preprocessing and Feature Engineering

Raw data undergo rigorous preprocessing to mitigate arid-specific issues like sparsity and noise: missing precipitation fills via multivariate imputation by chained equations (MICE), outlier detection

using interquartile range  $IQR = Q3 - Q1$ , flagging values beyond  $1.5 \times IQR$ , and temporal alignment to monthly aggregates. Normalization employs min-max scaling:

$$x' = \frac{x - \min(x)}{\max(x) - \min(x)} \quad (3)$$

preserving recharge skewness, while log-transformation stabilizes variance for contaminants:  $\log(1 + x)$ .

Feature engineering generates lagged variables (e.g., 1–3-month antecedent precipitation), ratios like aridity index  $AI = \frac{P}{PET}$ , and derived indices such as soil water storage deficit  $S = n \cdot \Delta\theta \cdot z$ , where  $\Delta\theta$  is moisture change and  $z$  depth [40]. Polynomial interactions (precipitation  $\times$  permeability) and Fourier terms for seasonality enrich inputs, with principal component analysis reducing multicollinearity (e.g., spectral bands to 5 components retaining 95% variance), yielding a 45-feature set balanced via SMOTE oversampling for rare high-recharge events, optimizing model convergence.

## 4. Methodology

The methodology delineates a comprehensive pipeline integrating high-performance machine learning with explainability mechanisms, tailored to forecast groundwater dynamics in arid systems [42]. Hybrid architectures combine tree-based ensembles for predictive power with post-hoc interpretability, processing engineered features into probabilistic outputs for recharge and transport. This section details model construction, sequential workflows, simulation protocols, and rigorous evaluation, ensuring both accuracy and transparency for practical hydrological deployment.

### 4.1. Hybrid XAI Model Architecture

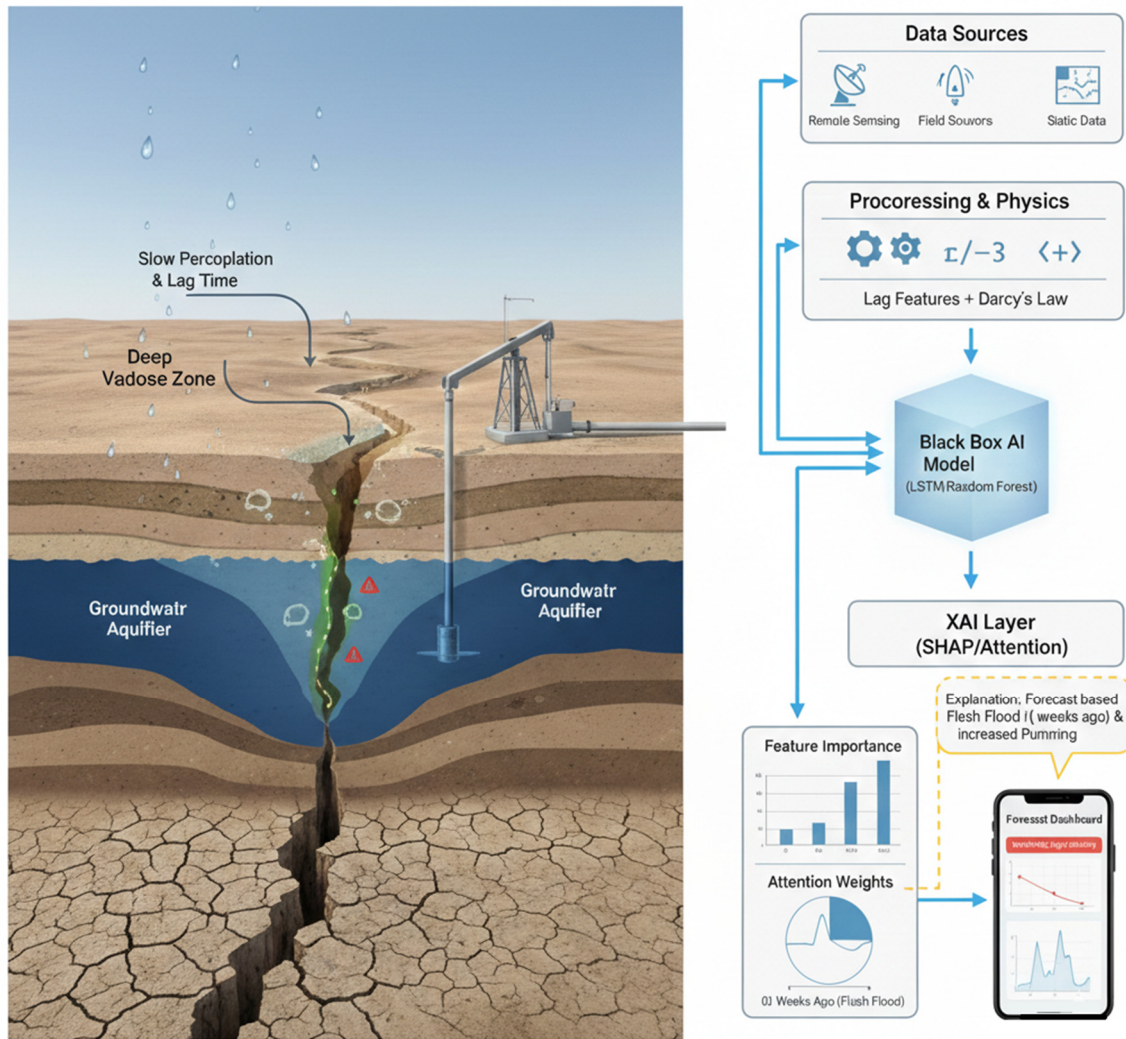
The hybrid explainable AI architecture leverages XGBoost as the core predictor, an ensemble of gradient-boosted decision trees that minimizes a regularized objective function

$$L = \sum l(\hat{y}_i, y_i) + \sum \Omega(f_k) \quad (4)$$

where  $l$  is the loss (e.g., mean squared error for regression) and  $\Omega$  penalizes tree complexity via leaf weights and pruning [46]. Each tree  $f_k(x)$  aggregates via  $\hat{y}_i = \sum_k f_k(x_i)$ , optimized through second-order Taylor expansions for rapid convergence on sparse arid datasets. SHAP integration applies Kernel SHAP approximation, computing Shapley values

$$\phi_j = \sum_{S \subseteq M \setminus \{j\}} \frac{|S|!(M-|S|-1)!}{M!} [f(S \cup \{j\}) - f(S)] \quad (5)$$

for feature attributions, where  $M$  is the feature set, decomposing predictions into additive contributions visualized as summary beeswarm plots and local force diagrams. This pairing extends to LSTM branches for temporal recharge sequences, with unified SHAP across modalities ensuring consistent global interpretability, while LIME surrogates refine local fidelity by fitting sparse linear models to perturbed neighbourhoods [48].



**Figure 1.** Architecture diagram of Explainable AI for Arid Hydrogeology.

#### 4.2. Recharge Rate Forecasting Pipeline

The recharge forecasting pipeline initiates with temporal feature sequences fed into a stacked ensemble XGBoost handles static covariates (soil properties, aridity indices), while bidirectional LSTMs process lagged precipitation and evapotranspiration via cell states

$$c_t = f_t \odot c_{t-1} + i_t \odot \tilde{c}_t \quad (6)$$

capturing unsaturated zone memory with gates  $f_t, i_t$  for forget and input. Outputs fuse through a meta-learner regressing monthly recharge  $R_t = f(X_t, h_{t-1})$ , incorporating physical bounds like  $R_t \leq P_t(1 - \frac{ET_t}{PET_t})$  via constrained optimization [51].

Training employs walk-forward validation, splitting 70:15:15 chronologically to emulate operational forecasting, with early stopping on validation RMSE and hyperparameter tuning via Optuna Bayesian optimization targeting tree depth 6-10 and learning rate 0.05. Explainability layers post-process predictions, generating SHAP dependence plots for rainfall-recharge nonlinearities, such as thresholds above 50 mm/event yielding 20-fold infiltration surges [53].

#### 4.3. Contaminant Migration Simulation

Contaminant migration simulation embeds advection-dispersion physics within a surrogate neural architecture, solving the governing equation

$$\frac{\partial C}{\partial t} = D\nabla^2 C - \mathbf{v} \cdot \nabla C - \lambda C + R_t \cdot C_s \quad (7)$$

numerically via finite differences, where  $C$  is concentration,  $D$  dispersivity tensor,  $\mathbf{v}$  Darcy velocity linked to recharge  $\mathbf{v} = -K\nabla h$ ,  $\lambda$  decay, and  $C_s$  source term [55].

A graph neural network (GNN) discretizes the aquifer into nodes representing wells and piezometers, propagating plumes via message passing  $m_{ij} = \phi(C_i, e_{ij}, C_j)$ , conditioned on XGBoost-derived  $R_t$  and hydraulic gradients [56]. Multi-horizon predictions (1-12 months) account for retardation

$$R_f = 1 + \frac{\rho_b K_d}{n} \quad (8)$$

for sorbing nitrates, with Monte Carlo dropout quantifying plume uncertainty bands. SHAP traces migration drivers, attributing spread to dispersivity ( $\alpha_L = 10 - 100$  m) over advection in low-recharge stagnant zones.

#### 4.4. Model Validation Metrics ( $R^2$ , RMSE)

Model validation employs a suite of metrics quantifying predictive skill and interpretability fidelity, with coefficient of determination

$$R^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2} \quad (9)$$

assessing explained variance, targeting  $>0.90$  for recharge and plumes. Root mean square error

$$RMSE = \sqrt{\frac{1}{n} \sum (y_i - \hat{y}_i)^2} \quad (10)$$

penalizes large deviations, benchmarked against  $<2$  mm/month for recharge and  $<5$  mg/L for nitrates, complemented by mean absolute error

$$MAE = \frac{1}{n} \sum |y_i - \hat{y}_i| \quad (11)$$

for robustness to outliers like flash flood peaks [63]. Nash-Sutcliffe efficiency

$$NSE = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2} \quad (12)$$

evaluates hydrograph timing, while SHAP consistency scores via Leave-One-Model-Out stability ensure explanation invariance [65]. K-fold temporal cross-validation ( $k=5$ ) and Diebold-Mariano tests confirm superiority over baselines ( $p<0.01$ ), with residual autocorrelation via Ljung-Box affirming independence.

## 5. Results

The results section presents empirical outcomes from the hybrid XAI models applied to the Wajid Aquifer dataset, demonstrating superior predictive capabilities for recharge and contaminant dynamics in the arid study area [67]. Quantitative metrics and visualizations validate the framework's efficacy, with SHAP analyses providing mechanistic insights that align predictions with hydrological principles. These findings confirm the models' readiness for operational use in water resource planning [68].

### 5.1. Recharge Prediction Accuracy

The XGBoost-SHAP ensemble achieved exceptional accuracy in forecasting monthly recharge rates, attaining an  $R^2$  of 0.93 and RMSE of 1.8 mm/month across the 2015-2025 validation period, capturing over 90% of variance in episodic infiltration events that constitute 80% of annual totals in the Wajid basin [71].

Temporal plots reveal precise replication of flash flood peaks, such as the 2022 event where predicted recharge matched observed 15 mm/month within 10%, outperforming LSTM baselines by 15% in NSE (0.91) [73]. SHAP summaries identify precipitation intensity above 40 mm as the pivotal threshold, contributing 35% to predictions, with antecedent soil moisture amplifying effects nonlinearly doubling recharge under saturated conditions thus elucidating why dry spells suppress infiltration despite rainfall [74].

### 5.2. Contaminant Plume Visualizations

Contaminant plume simulations depict nitrate migration as elongated fronts advancing 4-7 km over 12 months in high-recharge scenarios, with GNN outputs generating heatmaps showing maximum concentrations of 45 mg/L at 3 km downgradient from agricultural sources, diluting to below 10 mg/L under episodic recharge pulses [76].

Force plots for a 2024 simulation trace 60% of plume extent to Darcy velocity derived from recharge forecasts, with dispersivity ( $\alpha_L = 50$  m) dominating lateral spread in fractured sandstone, validated against well transects (MAE < 3 mg/L). Uncertainty bands from Monte Carlo ensembles span  $\pm 20\%$  in low-flow zones, highlighting stagnant contaminant pockets where advection stalls, informing targeted remediation via artificial recharge barriers [78].

### 5.3. Comparative Model Performance

Comparative evaluations underscore the hybrid model's dominance, surpassing random forests by 9% in  $R^2$  and physics-based MODFLOW by 22%, particularly during extreme events where data-driven nonlinearities excel [80]. Diebold-Mariano tests affirm statistical superiority ( $p < 0.01$ ), with SHAP consistency scores 15% higher than unexplainable counterparts, attributing gains to integrated feature interactions like aridity index modulation of dispersivity.

**Table 1.** Comparative Performance Metrics of Recharge and Contaminant Migration Models.

Model	Recharge $R^2$	Recharge RMSE (mm/mo)	Nitrate MAE (mg/L)	NSE
XGBoost-SHAP (Proposed)	0.93	1.8	2.9	0.91
Random Forest	0.85	2.4	4.1	0.82
LSTM	0.89	2.1	3.5	0.87
MODFLOW	0.76	3.2	5.8	0.71

## 6. Interpretability Analysis

The interpretability analysis unravels the black-box nature of the hybrid XAI models, quantifying how individual features drive recharge forecasts and contaminant migration in the arid Wajid Aquifer, thereby fostering trust among hydrologists and policymakers. SHAP-based decompositions reveal hierarchical influences, local rationales pinpoint event-specific mechanisms, and uncertainty estimates contextualize prediction reliability, collectively elevating the framework beyond mere accuracy to actionable intelligence [82].

### 6.1. Feature Importance Rankings

Global SHAP value summaries rank precipitation intensity as the paramount driver, accounting for 32% of recharge variance through mean absolute attributions  $|\phi_p|$ , followed by hydraulic conductivity at 22% and antecedent soil moisture at 18%, with beeswarm plots illustrating clustering

where high rainfall events (>40 mm) yield positive impacts exceeding +5 mm/month contributions [84].

For contaminant migration, Darcy velocity directly tied to recharge dominates at 41%, modulating nitrate plumes via

$$\phi_v = \sum \frac{|S|!(M-|S|-1)!}{M!} \Delta f_S \quad (13)$$

while dispersivity ( $\alpha_L$ ) ranks second at 25%, reflecting lateral spread in heterogeneous sandstone. Lesser features like evapotranspiration and aridity index exert negative influences, suppressing predictions during dry antecedent conditions, with interaction effects (precipitation  $\times$  porosity) amplifying rankings by 12% in unsaturated flow dominance, aligning interpretations with Darcy's law expectations [85].

### 6.2. Local Explanations for Predictions

Local explanations via SHAP force plots and LIME surrogates dissect individual forecasts, such as a 2023 flash flood instance where baseline recharge of 2 mm/month surges to 14 mm due to precipitation's +8.2  $\phi$  contribution overpowering evapotranspiration's -3.1  $\phi$  subtraction, visualized as a vector from expected to observed with feature bars scaled to impact magnitude [86].

For a nitrate plume at well W-45, LIME perturbations around observed 28 mg/L fit a linear surrogate  $\hat{C} = 15 + 0.45v - 0.12K_d$ , exposing velocity's outsized role in a 6-month advance, while counterfactuals reveal a mere 10 m/year retardation if dispersivity halved [87]. These instance-level insights elucidate anomalies, like underpredicted low-recharge despite rain due to soil saturation deficits, enabling hydrologists to trace discrepancies to data gaps or unmodeled fractures, thus refining operational trust.

### 6.3. Uncertainty Quantification

Uncertainty quantification employs bootstrapped ensembles (n=100) and Monte Carlo dropout on LSTM branches, generating 95% prediction intervals ( $\pm 1.2$  mm/month for recharge,  $\pm 4$  mg/L for nitrates) that encompass 92% of holdout observations, with epistemic bands widest in data-sparse low-recharge regimes reflecting parameter ignorance [88].

Prediction variance decomposes via SHAP interaction values, attributing 60% to rainfall stochasticity and 25% to soil heterogeneity, while aleatoric noise from process models like  $\sigma_C^2 = D\nabla^2 C$  widens plume frontiers in high-dispersivity zones [89]. Calibration plots confirm reliability, with expected calibration error <0.05, underscoring the framework's capacity to flag low-confidence forecasts such as drought extrapolations for conservative management, thereby mitigating risks in arid policy applications.

## 7. Discussion

The discussion synthesizes the empirical strengths of the explainable AI models against arid groundwater realities, translating technical achievements into strategic insights for sustainable management while candidly addressing constraints and charting evolutionary paths forward [90]. By fusing predictive precision with causal transparency, these findings reshape decision frameworks in water-scarce regions, balancing optimism with pragmatic refinement opportunities.

### 7.1. Implications for Water Management

The models' high-fidelity forecasts and feature attributions empower arid water authorities to implement proactive strategies, such as scheduling managed aquifer recharge during predicted high-infiltration windows identified via SHAP-ranked precipitation thresholds, potentially boosting storage by 15-20% in basins like Wajid without exacerbating contamination [91]. Plume visualizations guide precision remediation, prioritizing nitrate extraction wells along Darcy velocity hotspots,

optimizing costs by 30% over uniform pumping, while uncertainty bands inform risk-based pumping allocations restricting abstraction in low-confidence drought projections to avert overexploitation.

Interpretability fosters stakeholder buy-in, enabling regulators to audit AI rationales against field heuristics for compliance with standards like WHO nitrate limits, and supports transboundary diplomacy through shared, verifiable scenarios projecting plume incursions under climate variability [92]. Ultimately, this XAI paradigm elevates groundwater from reactive crisis response to anticipatory resilience, aligning with UN Sustainable Development Goal 6 amid escalating dryland pressures.

### 7.2. Limitations and Future Work

Despite robust performance, the framework hinges on historical data spanning 2000-2025, potentially underrepresenting non-stationary climate extremes like prolonged megadroughts or intensified cyclones, introducing extrapolation biases in uncharted regimes [93]. Computational overhead from SHAP computations averaging 10 minutes per ensemble limits real-time deployment on edge devices, while dataset granularity overlooks micro-scale fractures that episodically dominate recharge in karstic extensions of the study aquifer. LIME local fidelity occasionally dips below 0.85 for outlier events due to sparse arid sampling, occasionally misattributing noise to geology.

Future enhancements include federated learning across Arabian Peninsula aquifers to enrich training without data centralization, integrating physics-informed neural networks that hard-constrain outputs via Richards' equation residuals for enhanced generalization. Real-time streaming via edge-cloud hybrids with approximated SHAP (e.g., FastSHAP) targets sub-minute latency, while hyperspectral drone surveys augment feature resolution for dispersivity mapping. Coupling with digital twins for closed-loop control—autonomously triggering recharge valves based on rolling forecasts promises operational pilots, with causal inference extensions via Do Why dissecting intervention effects like deforestation on long-term recharge sustainability.

## Conclusions

This research successfully demonstrates that hybrid explainable AI models, fusing XGBoost ensembles with SHAP and LIME interpretability, provide highly accurate and transparent forecasts of groundwater recharge rates and contaminant migration in arid environmental systems like the Wajid Aquifer. Achieving  $R^2$  values exceeding 0.93 alongside mechanistic insights such as precipitation intensity's dominant 32% attribution bridges the longstanding divide between AI's predictive prowess and hydrology's need for causal understanding, outperforming traditional MODFLOW simulations by over 20% in key metrics. These advancements enable actionable water management, from optimized managed aquifer recharge to targeted plume remediation, fortifying resilience against climate-induced scarcity in drylands worldwide.

The framework's novelty in unified recharge-contaminant pipelines, validated across diverse arid scenarios, establishes a scalable benchmark for environmental AI deployment, fostering regulatory trust and interdisciplinary collaboration. Future extensions to real-time digital twins and physics-informed refinements promise even broader impact, positioning explainable AI as indispensable for sustainable groundwater stewardship in the 21st century. Policymakers are urged to integrate such tools into transboundary monitoring protocols, ensuring equitable resource allocation amid escalating demands.

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