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Data-Driven Method for Groundwater-Level Mapping and Monitoring- Well Network Optimization at Hanford

September 2025

Xuehang Song
Tse-Chun Chen
Grigoriy Kondyukov
Zhangshuan Hou
Inci Demirkanli

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Pacific Northwest National Laboratory
Richland, Washington 99354

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Summary

This report summarizes the initial results and outcomes of a physics-informed, data-driven groundwater-level (GWL) mapping capability for the Hanford Site. GWL mapping at Hanford is typically conducted annually and requires a significant amount of computational and expert resources, and it does not allow assessment of the informational value of specific monitoring wells. The proposed method produces spatially and temporally resolved fields consistent with sparse, irregularly sampled, and nonuniformly distributed well measurements. Implemented successfully, this capability will allow rapid mapping of groundwater levels and provide an opportunity to optimize monitoring activities (both location and sampling frequency) based on data information value evaluation.

The approach integrates a diffusion-based generative model – trained on MODFLOW simulation data from the Plateau-to-River (P2R) model – with score-based data assimilation (SDA), allowing observation-conditioned mapping without retraining for each monitoring-network layout. The diffusion prior captures dominant spatiotemporal structure – including regional gradients, barrier effects, and capture zones – while SDA infuses current observations to generate full-domain GWL fields that are both physically consistent and measurement-informed. Uncertainty is represented through an ensemble of reconstructions, each reflecting independent realizations of the diffusion model conditioned on observed data. A geospatial sampling pipeline harmonizes unstructured simulation outputs and point-well data onto a common rasterized grid, providing consistent model-ready input throughout the workflow.

Preliminary results show stable reconstruction accuracy [mean absolute error (MAE) ≈ 0.12 – 0.24 m], with spatial uncertainty concentrated in high-gradient or data-sparse areas. A remove-well demonstration quantifies marginal information value and illustrates how targeted adjustments to the monitoring network can reduce reconstruction error. A prior-only forecast establishes a baseline for error growth when no new observations are assimilated, providing guidance on monitoring frequency and scenario screening (e.g., pump-and-treat operational or hydrologic perturbations). Work planned for fiscal year 2026 will focus on fine-tuning the diffusion–SDA model hyperparameters, expanding robustness testing, developing the monitoring-network assessment workflow, completing formal quality assurance and validation, and preparing a manuscript. Together, these developments offer a scalable, physics-aware, and uncertainty quantified mapping capability to support adaptive groundwater management at Hanford.

Background & Objectives

The Hanford Site requires long-term management of comingled contaminant plumes spanning decades of remedial activity. GWL maps are critical inputs to the conceptual site model, remedial decisions and actions, and performance monitoring, providing essential information to establish hydraulic gradients and flow directions, evaluate pumping strategies to prevent aquifer overdraw, delineate contaminant migration pathways, and assess groundwater–river interactions. In this report, GWL refers to hydraulic head (elevation) in unconfined (water-table), perched, semi-confined, and confined aquifers across the site.

Generating these GWL maps relies on a large monitoring network – more than 1,000 wells – with measurements obtained from manual groundwater sampling (periodic and the annual synoptic event) and from automated water-level or pressure records, such as the Automated Water Level Network (AWLN). However, these GWL measurements exhibit spatial and temporal irregularities that require mapping approaches capable of integrating data across both dimensions while handling irregular sampling patterns. In parallel, a capability is needed to identify where additional measurements would reduce mapping errors the most and quantify the marginal information value of existing wells, supporting cost-effective monitoring network optimization.

Hanford’s contractor presently uses two complementary workflows to produce GWL maps. First, a geostatistical workflow – multi-event universal kriging (MEUK) – interpolates irregularly spaced water-level measurements; the MEUK outputs are then assembled with other inputs using ArcGIS to create the annual sitewide GWL map (Heil, 2024). Second, for the low-gradient 200 East Area, a simplified single-layer, two-dimensional, steady-state groundwater-flow simulator (MODFLOW-USG with PEST) is calibrated to monitoring well heads to produce mass-conserving elevation grids used for quarterly GWL mapping and particle tracking (Nordberg, 2025).

Both workflows are designed for periodic (annual/quarterly) updates and reporting. Generating these maps requires nontrivial effort, including data preparation, parameter selection, and assembly steps (e.g., MEUK input generation, variogram fitting, control-point integration, and model calibration). Neither workflow directly quantifies the information value of individual wells, which is critical for improving the monitoring efforts. These considerations motivate a more flexible spatiotemporal mapping capability that supports rapid GWL mapping and facilitates evaluation and optimization of monitoring activities – both location and sampling frequency – based on data-value evaluation.

Data Sources

GWL records for this study are drawn from the Hanford Environmental Information System (HEIS, <https://ehs.hanford.gov/eda/>), which houses a comprehensive archive of water-level measurements dating back to July 1948. After applying quality control (QC) filters, the dataset contains 187,361 observations from 2,151 groundwater monitoring wells, out of 204,899 total entries spanning 2,517 unique well locations. These measurements extend through December 2024 and reflect highly variable sampling frequencies: Half of all wells contribute fewer than 57 readings, while the top decile exceeds 218 measurements. This uneven distribution in space and time poses challenges for interpolation and uncertainty quantification, yet the long temporal record and broad spatial coverage also capture localized hydrogeologic effects that are critical for model conditioning and validation. Given the labor and cost to acquire and maintain these measurements, improving mapping efficiency increases the monitoring program’s return on investment.

The filtered, cleaned dataset was archived as a data package for reproducible analysis and future reference. Figure 1 summarizes annual well counts and highlights the early-1990s expansion and sustained coverage thereafter. Figure 2 provides spatial snapshots showing how the monitoring footprint evolved relative to the Columbia River and management areas.

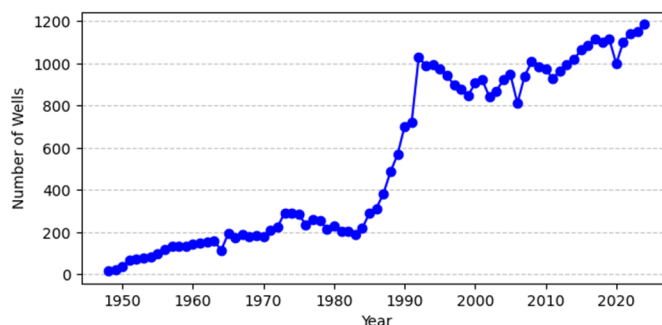


Figure 1. Annual number of unique HEIS wells with at least one groundwater-level measurement, 1948-2024 (QC-filtered).

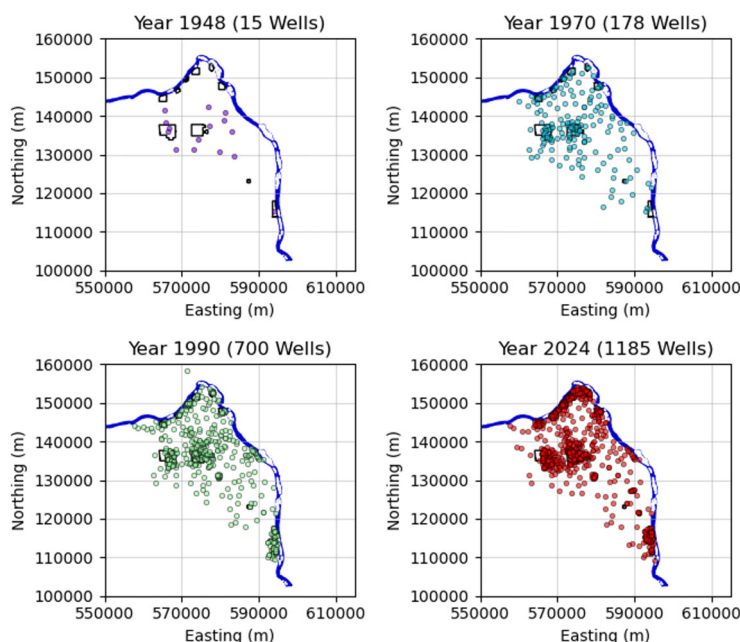


Figure 2. Representative snapshots of the GWL monitoring network (QC-filtered): 1948 (15 wells), 1970 (178), 1991 (718), and 2024 (1,185). Circles indicate wells with ≥ 1 reading in the indicated year, the blue line represents the Columbia River, and the squares outline site management areas for context.

Complementing the field data, we use simulated GWL snapshots from the Plateau-to-River (P2R) MODFLOW model (Budge & Nichols, 2020), calibrated against historical well observations. The baseline P2R configuration outputs GWL on a 274×201 grid with variable horizontal resolution over a 75-year history-matching interval (1943–2018) and a 122-year projection interval (2015–2137), with time-varying stress periods (monthly to yearly). We reconfigured the model to output monthly fields for both periods and extracted consistent time series of recharge, discharge, and well-pumping rates, together with hydraulic conductivity fields, from the model inputs. Recharge, discharge, and pumping series were then quantile-transformed to standardize their marginal distributions. All post-processed products are stored as HDF5 files (~2,385 monthly steps in total). Training the diffusion prior on these physically consistent, fully gridded sequences captures dominant spatiotemporal structure (regional gradients, barrier effects, low-flow zones), while HEIS observations provide measurements for score-based conditioning during inference.

Method

We employed a spatiotemporal mapping framework that combines a diffusion model with SDA to reconstruct temporal sequences of GWL fields that honor both physics-informed site patterns and well measurements. Figure 3 summarizes the workflow: Physics-based simulations provide training sequences for the diffusion prior; during reconstruction, SDA assimilates measurements as spatiotemporal constraints; ensemble reconstructions quantify uncertainty; and add/drop experiments evaluate monitoring-network configurations. The subsections that follow briefly describe the reconstruction procedure, the uncertainty and well-information analyses, and the data-preparation steps.

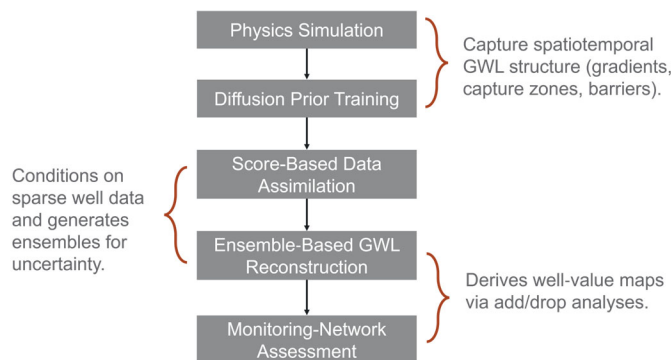


Figure 3. Diffusion-SDA workflow for groundwater-level reconstruction and monitoring assessment.

Diffusion-SDA Framework for GWL Reconstruction

- **Training (diffusion prior).** Train a generative prior on monthly sequences of P2R simulations (Song et al., 2021). The prior captures dominant hydrogeologic structure – regional gradients, capture zones, barrier effects, and river influence – without overfitting to individual snapshots.
- **Inference (observation conditioning).** At reconstruction, SDA guides reverse-time diffusion (Rozet & Louppe, 2023a, 2023b) trajectories toward HEIS well measurements at their recorded locations and times, enforcing observation consistency under sparse, irregular sampling.
- **Outputs.** Running the conditioned reverse-diffusion process multiple times with independent (noise) initializations produces an ensemble of plausible GWL reconstructions.

Uncertainty Quantification and Well Information Value Analysis

- **Ensemble uncertainty.** Multiple SDA-conditioned reconstructions with independent initializations form an ensemble; the ensemble mean is the best-estimate GWL field and the ensemble spread (standard deviation across members) indicates where predictions are less certain in space and time.
- **Information-value analysis.** Leave-one-out and add/drop experiments compare errors (e.g., MAE) against the full-network reconstruction to quantify each well's marginal information value and reveal under-monitored areas for potential network adjustments.

Geospatial Sampling and Data Preparation

Training the diffusion prior and applying SDA require consistent spatiotemporal tensors that preserve domain geometry and observation metadata. To handle heterogeneous inputs – unstructured P2R meshes with time-variable stress periods, aquifer hydraulic-property fields, and sparse, irregular well

measurements – we developed a lightweight geospatial toolkit (*geosamplerite*) for fast data rasterization and lazy loading. The toolkit harmonizes sources by rasterizing model outputs (e.g., heads, recharge/discharge, pumping) and static fields (e.g., hydraulic conductivity), together with point-well observations, onto a uniform grid, while retaining boundary masks and inactive cells and aligning records to a common monthly time base. Using this toolkit, we produce model-ready time series with minimal information loss for the diffusion–SDA workflow.

Results

Results are organized into three parts: (1) observation-conditioned GWL mapping, (2) impact of reducing well coverage, and (3) GWL forecast. Performance is evaluated against physics-based reference (“truth”) fields from the P2R model: Spatial accuracy is assessed with cellwise residuals, uncertainty with ensemble spread, and temporal behavior with the domain-wide monthly MAE.

Observation-Conditioned GWL Mapping

To evaluate spatial accuracy under observation conditioning, a representative month (March 2023) is analyzed in detail. The physics-based reference (Figure 4a) and the diffusion–SDA reconstruction (Figure 4b) exhibit close agreement across the domain, with the residual field (Figure 4c, prediction – reference) predominantly within -1 to 1 m. Observation locations (dots in Figure 4c) show the impact of measurement conditioning: Denser clusters correspond to smaller residuals. The ensemble standard-deviation map (Figure 4d) mirrors these patterns – higher spread co-locates with larger residuals – indicating that the uncertainty metric is well calibrated to local prediction difficulty.

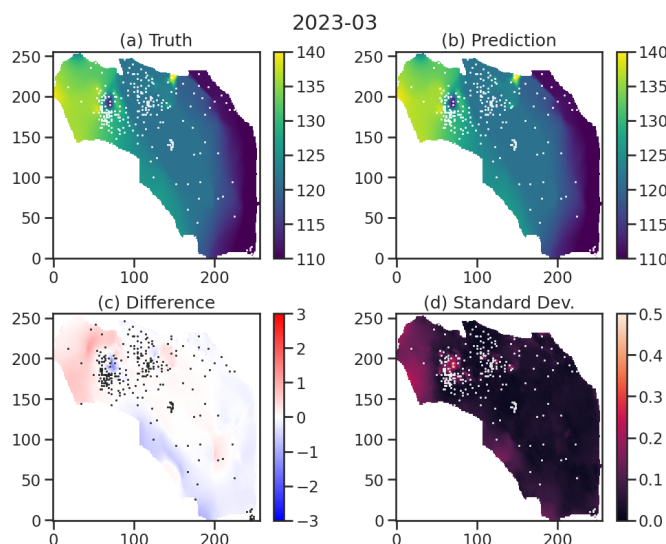


Figure 4. Observation-conditioned GWL mapping. Panels (a–b) show water-table elevation in meters above sea level: (a) reference field from the physics-based simulator; (b) diffusion–SDA prediction; (c) prediction minus reference (red = overprediction, blue = underprediction), m; (d) ensemble standard deviation (“spread”), m. Points indicate wells with observations.

Figure 5 summarizes the month-to-month model performance (Jan 2022–Dec 2024). Monitoring coverage varies substantially (Figure 5, top), and mapping accuracy tracks it (Figure 5, bottom): The domain-wide monthly MAE between diffusion–SDA and the P2R reference is typically 0.12–0.24 m – lower in months with more reporting wells (e.g., ~400) and higher when coverage drops.

These results demonstrate that the proposed framework quantitatively links monitoring-network size and spatial placement to GWL mapping accuracy.

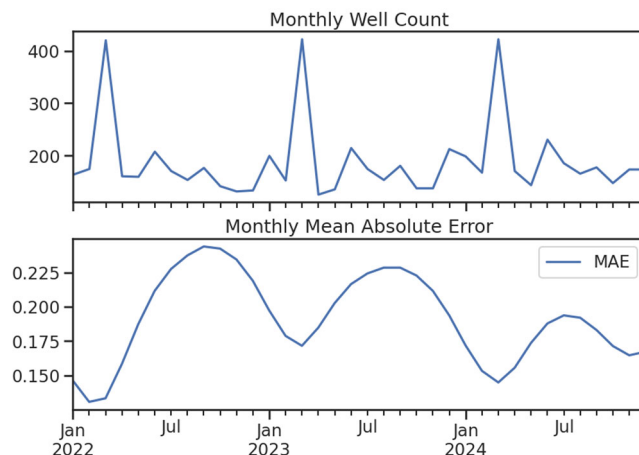


Figure 5. Top: Number of wells with measurements each month. Bottom: Monthly MAE (unit, m) between the diffusion–SDA prediction and the reference field.

Impact of Reducing Well Coverage

We withheld a localized cluster of wells in the 200 West pump-and-treat area at Hanford and recomputed the March 2023 observation-conditioned map (Figure 6); 23 wells were removed, a ~5% reduction from active wells that month. Relative to the baseline (Figure 4), the perturbed case shows localized degradation: Residuals (prediction – reference) increase within and adjacent to the removal footprint (Figure 6c), and ensemble spread widens in the same zone (Figure 6d); outside that area, both metrics remain near baseline.

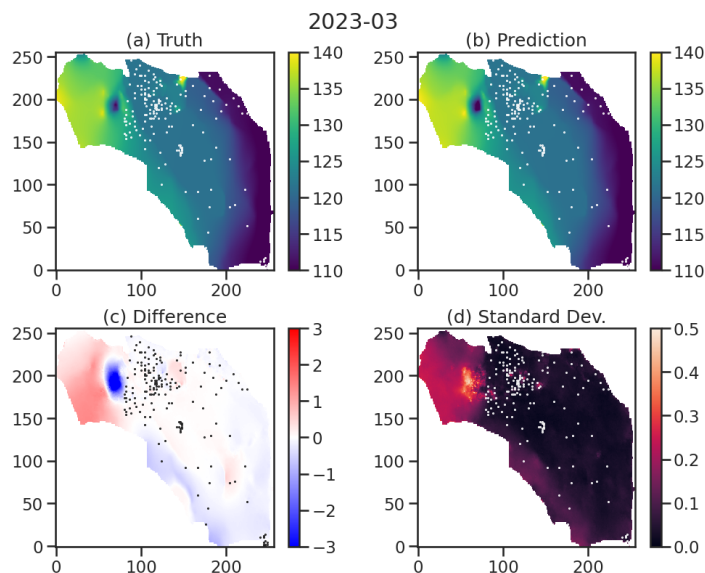


Figure 6. Remove-well experiment (March 2023). Panels (a–b) show water-table elevation in meters above sea level: (a) reference field from the physics-based simulator; (b) diffusion–SDA prediction; (c) prediction minus reference (red = overprediction, blue = underprediction), m; (d) ensemble standard deviation (“spread”), m. Points indicate wells with observations.

This end-member example demonstrates how the framework quantifies the accuracy and uncertainty impacts of coverage changes. We are extending and automating the workflow to support domain-wide, systematic add/remove-well trials that assimilate synthetic measurements to estimate expected reductions in MAE and changes in ensemble spread; outputs are delivered as Δ MAE/ Δ spread maps and ranked well-level information-value scores to guide monitoring-network improvement and optimization.

GWL Forecast

Beyond present-day, observation-conditioned maps, forecasting is essential for planning (e.g., anticipating responses to pumping or natural variability). As a baseline test, we initialize the ensemble from the December 2023 conditioned state and advance through January–December 2024 without ingesting new well measurements. Each ensemble member evolves under the learned generative dynamics only, and agreement with the physics-based reference (P2R model) is tracked using the domain-wide monthly MAE.

Figure 7 summarizes the outcome. During the data-assimilation window (January 2022–December 2023; left of the dashed divider), monthly MAE is relatively low and stable. After transitioning to the forecast window (January–December 2024), MAE increases progressively and the ensemble spread widens, indicating growing uncertainty in the absence of observation updates.

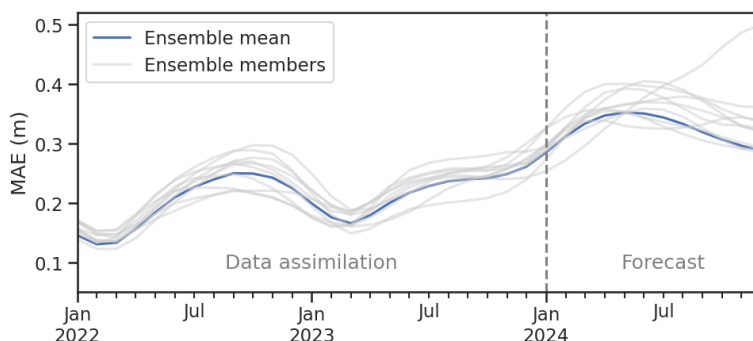


Figure 7. Monthly MAE from January 2022 to December 2024. Gray traces are individual ensemble members; the blue curve is the ensemble mean. The vertical dashed line marks the transition from the observation-conditioned period to the prior-only forecast period with no observation updates, unit m.

As an exploratory test, this establishes a baseline for error growth and uncertainty in the absence of new data, demonstrating the framework’s potential to determine the minimum measurement frequency needed to meet specified accuracy targets.

Ongoing Evaluations and Expected Outcomes

- Continue to improve diffusion–SDA accuracy via targeted hyperparameter tuning (e.g., noise schedule, network capacity, learning rate) and refinement of the observation-error model.
- Develop an automated add/drop toolkit for well information value assessment that runs rolling leave-one-out and add-one-in experiments, generates well information value scores and ranked recommendations, and conducts quality assurance with documented acceptance criteria.
- Deliver a manuscript summarizing methods and the monitoring-network assessment workflow.

- Inform water-level monitoring decisions: Use these outputs to (1) identify well information value based on quantified information value; (2) set minimum measurement frequency by area to meet accuracy targets; and (3) adjust the spatial distribution of monitoring to reduce uncertainty in high-gradient or under-constrained zones.

Quality Assurance

This work was performed in accordance with the Pacific Northwest National Laboratory Nuclear Quality Assurance Program (NQAP). The NQAP complies with the DOE Order 414.1D, *Quality Assurance*. The NQAP uses NQA-1-2012, *Quality Assurance Requirements for Nuclear Facility Application*, as its consensus standard and NQA-1-2012, Subpart 4.2.1 as the basis for its graded approach to quality. Any data presented in this document is preliminary, for information only (FIO), and subject to revision.

References

- Budge, T., & Nichols, W. (2020). *Model Package Report: Plateau to River Groundwater Model Version 8.3* (No. CP-57037-Rev.2). Hanford Site (HNF), Richland, WA (United States).
<https://doi.org/10.2172/1601635>
- Heil, E. (2024). *Preparation of the March 2023 Hanford Site Water Table Map* (Technical report No. ECF-HANFORD-23-0109, Rev 0) (p. 114). INTERA Inc. Retrieved from
<https://pdw.hanford.gov/document/AR-28423>
- Nordberg, A. W. (2025). *Groundwater Elevation Mapping for 200 East Area: Quarter 4 Calendar Year 2024* (Technical report No. ECF-200E-25-0002, Rev 0). Richland, WA: Central Plateau Cleanup Company. Retrieved from <https://pdw.hanford.gov/document/AR-35643>
- Rozet, F., & Louppe, G. (2023a, October 31). Score-based Data Assimilation. arXiv.
<https://doi.org/10.48550/arXiv.2306.10574>
- Rozet, F., & Louppe, G. (2023b, November 2). Score-based Data Assimilation for a Two-Layer Quasi-Geostrophic Model. arXiv. <https://doi.org/10.48550/arXiv.2310.01853>
- Song, Y., Sohl-Dickstein, J., Kingma, D. P., Kumar, A., Ermon, S., & Poole, B. (2021, February 10). Score-Based Generative Modeling through Stochastic Differential Equations. arXiv.
<https://doi.org/10.48550/arXiv.2011.13456>

Pacific Northwest National Laboratory

902 Battelle Boulevard
P.O. Box 999
Richland, WA 99354

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