DEEP VADOSE ZONE PROGRAM @PNNL

Computational Tools for Supporting Pump-and-Treat Optimization at the Hanford Site

Xuehang Song[1], Inci Demirkanli[1], Jason Hou[1], Xinming Lin[1], Byan[1] He, Mark Rockhold[1] Marinko Karanovic[2], Matt Tonkin[2], and Rob Mackley[1]

[1]Pacific Northwest National Laboratory
[2]S.S. Papadopulos and Associates Inc

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November 11, 2025

Outline

- **OPTIMA Framework Overview** – Overview of the integrated optimization approach.
- **Modeling Components** – Site model setup, surrogate design, and validation.
- **Optimization Demonstrations** – Single- and multi-objective results.
- **Deployment and Next Steps** – Web-based implementation and future use.

OPTIMA Tool Framework

1 Optimization/scenario setup:

- Optimization objectives
- End-state/cleanup performance criteria
- Optimization constraints

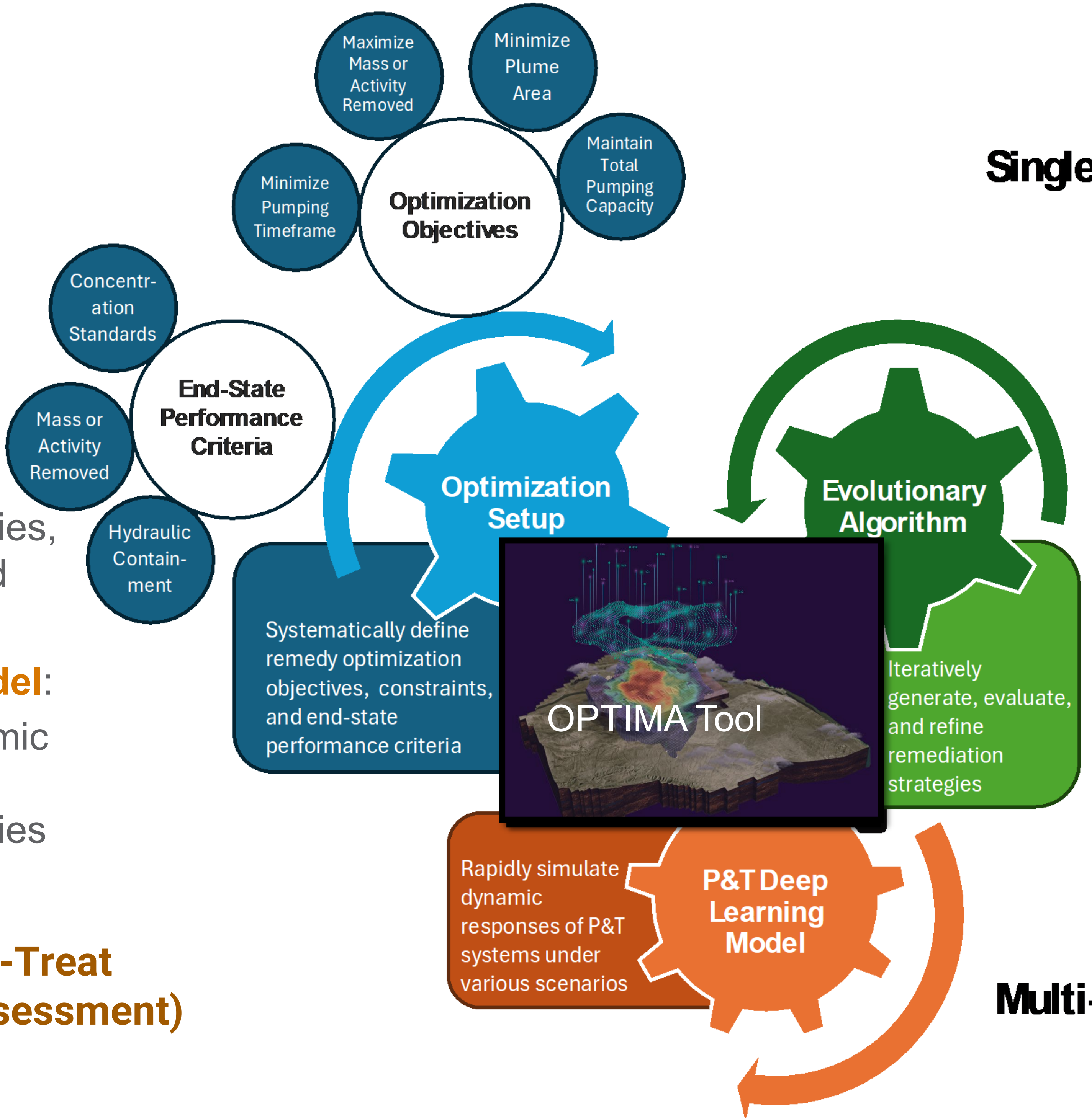
2 Evolutionary algorithm:

- Iterative evaluations of extraction-injection strategies, converging to an optimized solution

3 F&T Model or Deep-learning model:

- Rapid simulations of dynamic subsurface responses to extraction-injection strategies

OPTIMA (Optimization for Pump-and-Treat Implementations: Management & Assessment)

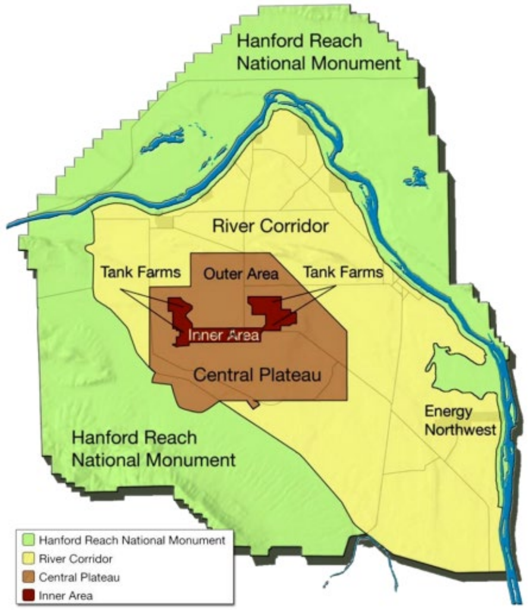


Single-
- Objective
- Contaminant
- End-State Performance Criteria

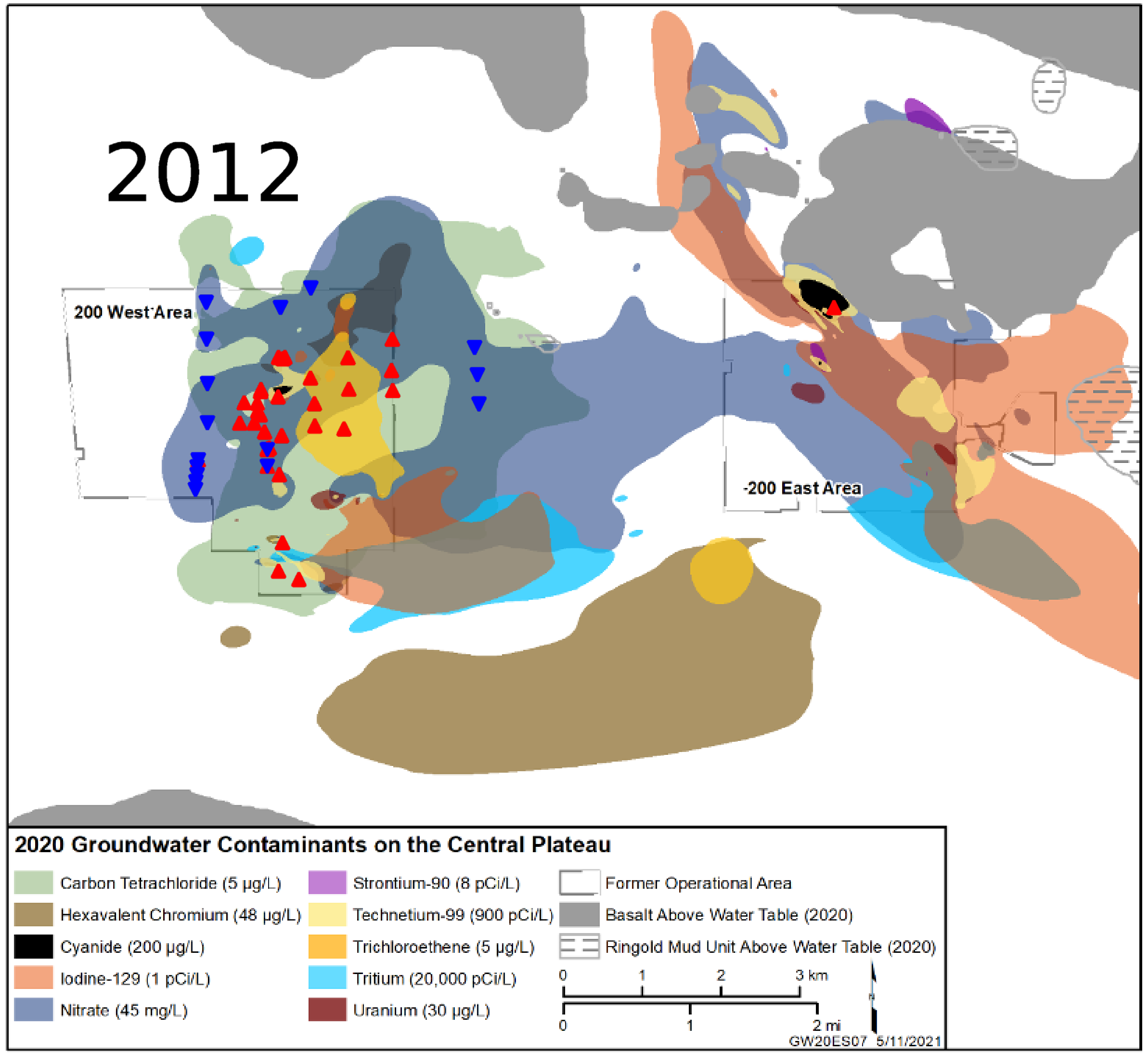
Multi-
- Objective
- Contaminant
- End-State Performance Criteria

The Hanford 200 West P&T System

- Contaminant Plumes
  - CCl_4, Tc-99, I-129, NO_3, etc., from plutonium separation and radioactive waste disposal (1943–1975).
- P&T Operations
  - Started in 2012, with ~70 extraction and injection wells currently in operation.
- Challenges
  - More CCl_4 plumes detected in the lower aquifer
  - longer-than-expected half-life (~630 years) than estimated when the RI/FS and ROD were completed.



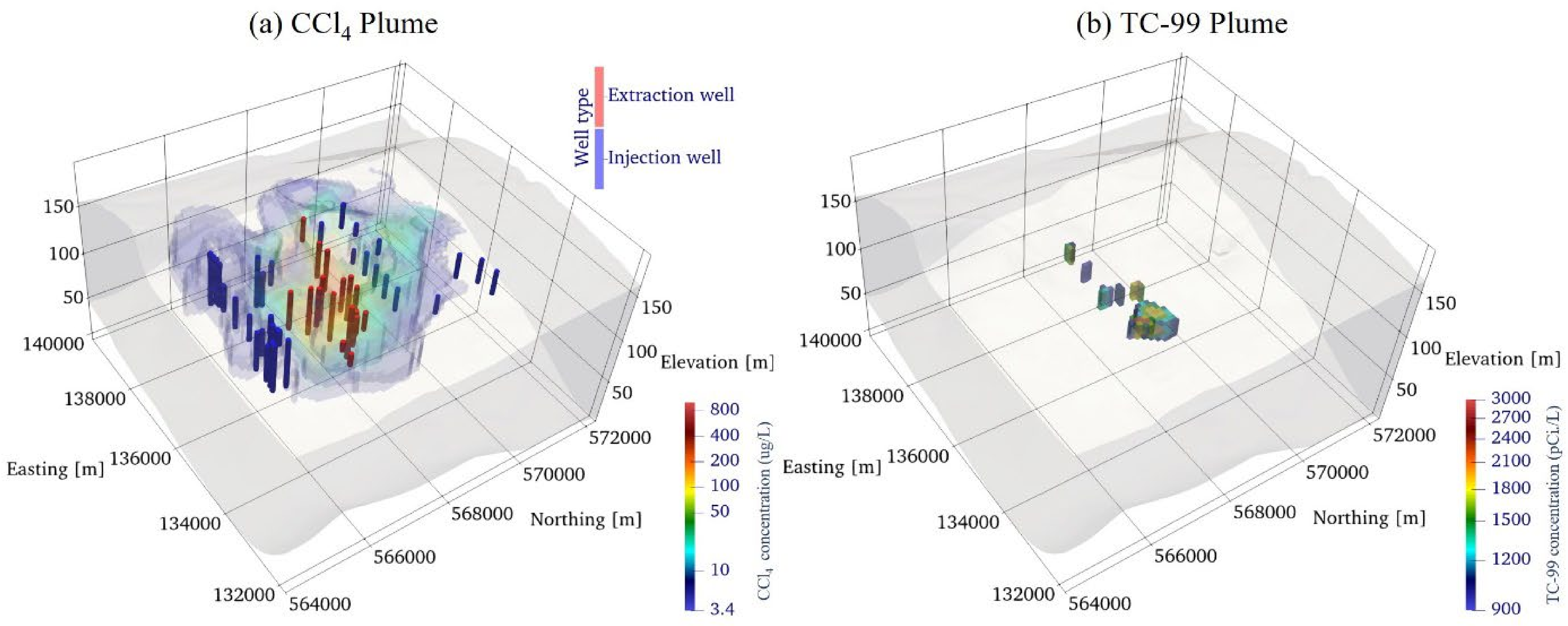
Groundwater contaminant plumes in the Central Plateau (DOE 2021)



- A systematic, performance-based approach is needed to evaluate alternative scenarios and determine the most effective well placement and pumping strategies

Numerical Model Serves as the High-Fidelity Basis for Training the Surrogate Model.

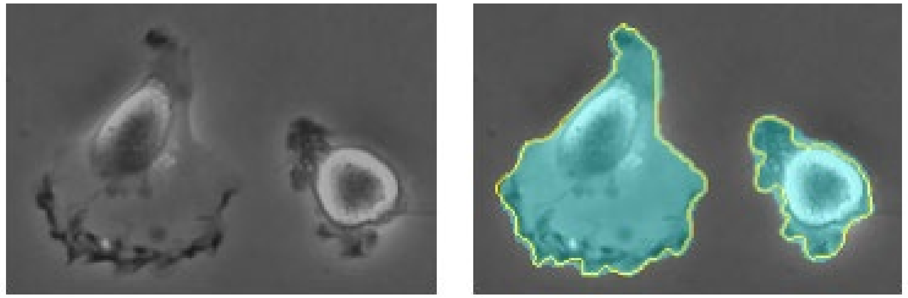
► Model Domain of the 200 West Area



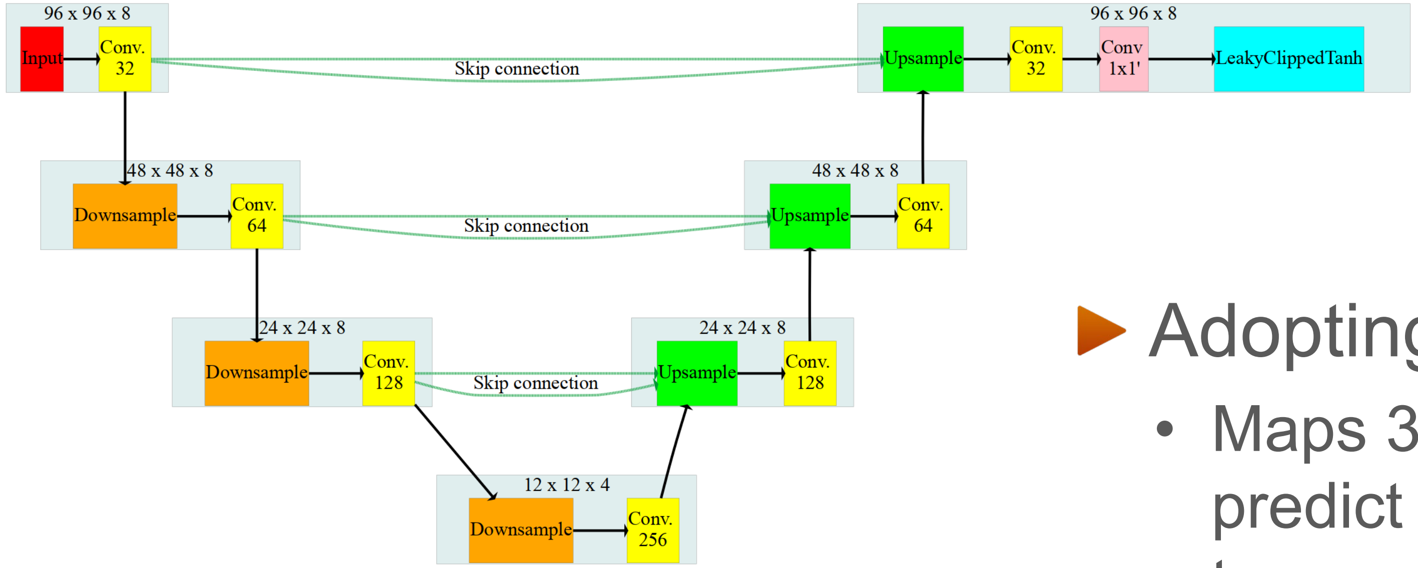
- Seven hydrostratigraphic layers with varying hydraulic properties.
- 83×80 grid model (100-m resolution) capturing plume distribution and flow pathways.

From Medical Image Segmentation to 3D Groundwater Contaminant Plume Prediction

- U-Net was originally developed as a powerful tool for biomedical image segmentation.



(Ronneberger et al., 2015)



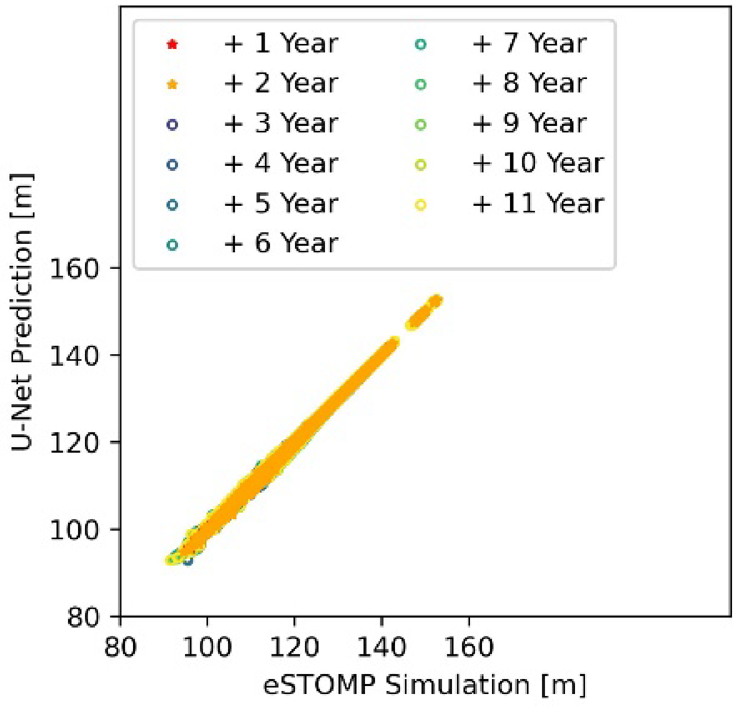
U-Net uses an encoder-decoder architecture with skip connections to extract features and generate high-resolution predictions.

- Adopting U-Net for Groundwater/Plume Prediction
  - Maps 3D hydraulic head and concentration images to predict future groundwater flow and contaminant transport.
  - An analytical solution enforces physical consistency, enhancing accuracy and realism.

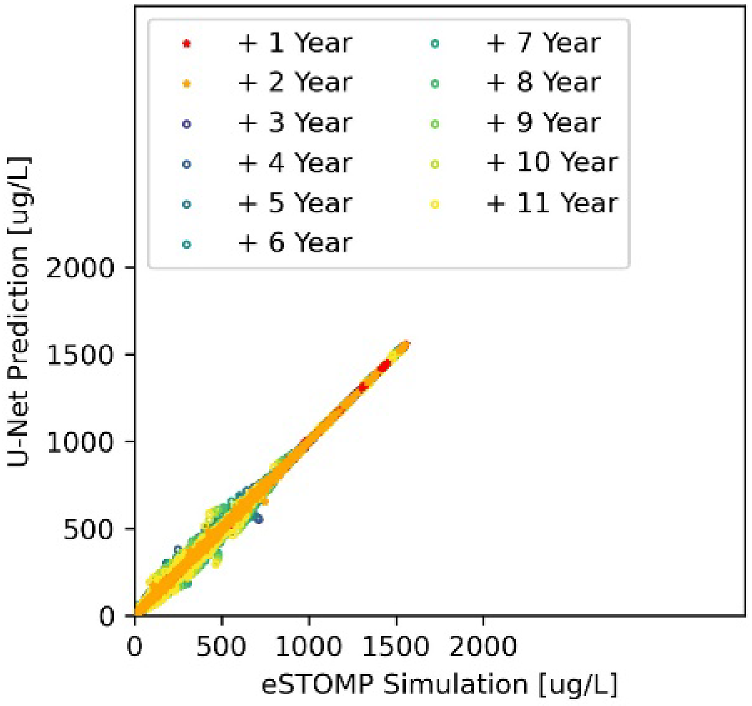
Surrogate Model Performance – Accuracy and Computational Efficiency

- Prediction Accuracy and Stability Over 12 Years

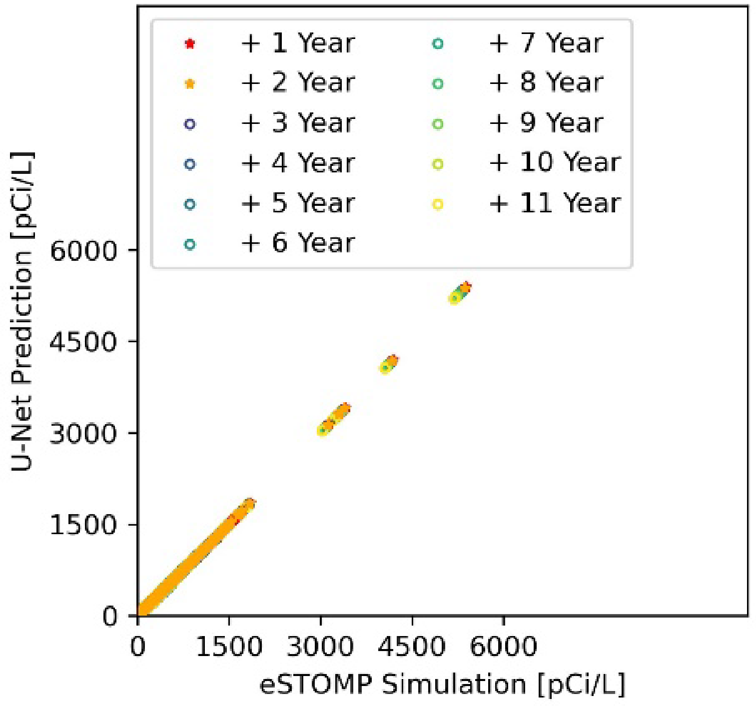
Groundwater level
RMSE 0.02 m → 0.07 m



CCl_4 (cleanup criterion: 3.4 ug/L)
RMSE 0.28 μg/L → 1.61 μg/L



Tc-99 (cleanup criterion: 900 pCi/L)
RMSE 0.17 → 0.76 pCi/L



- U-Net predictions run in approximately 600 milliseconds per step on a single CPU core, compared to 3–5 minutes per eSTOMP simulation on eight cores, achieving a speedup of over 1,000 times.

Optimization: Scenario Setup for Comparative Evaluation

Current Time 2024 — 2026 — End of Pumping 2038

Scenarios

Baseline

No Optimization (static well network)
P&T Capacity (gpm)
3400

Scenario-1

Well Network Optimization
P&T Capacity (gpm)
3400

Scenario-2

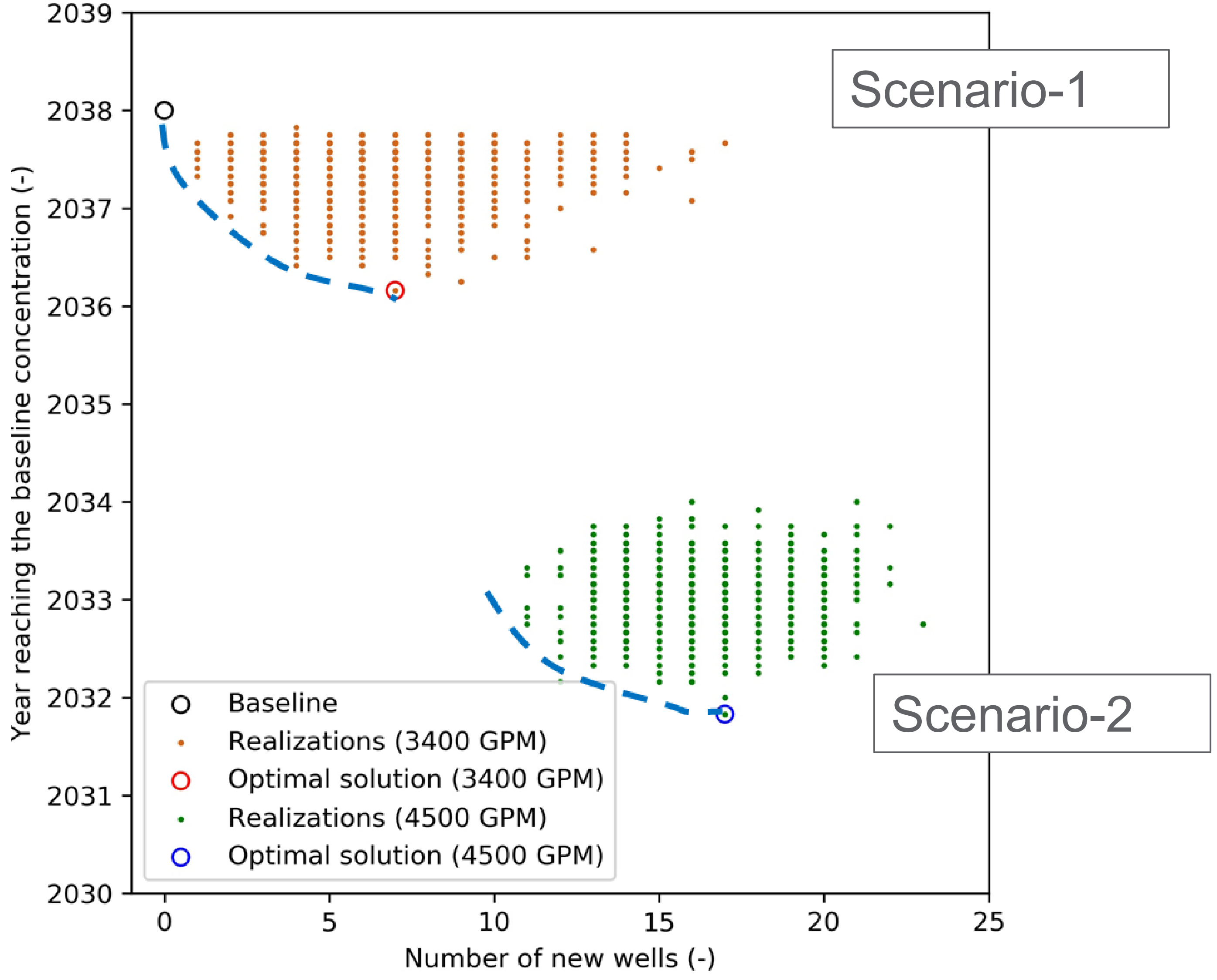
Well Network Optimization	
P&T Capacity (gpm)	
3400	4500

End-state Performance Criteria:
Baseline 95th percentile concentration level in 2038

Opt. Goal #1	Opt. Goal #2
Minimize active cleanup timeframe	Maximize total CTET mass recovery

Results for Goal #1 (Minimizing active pumping timeframe)

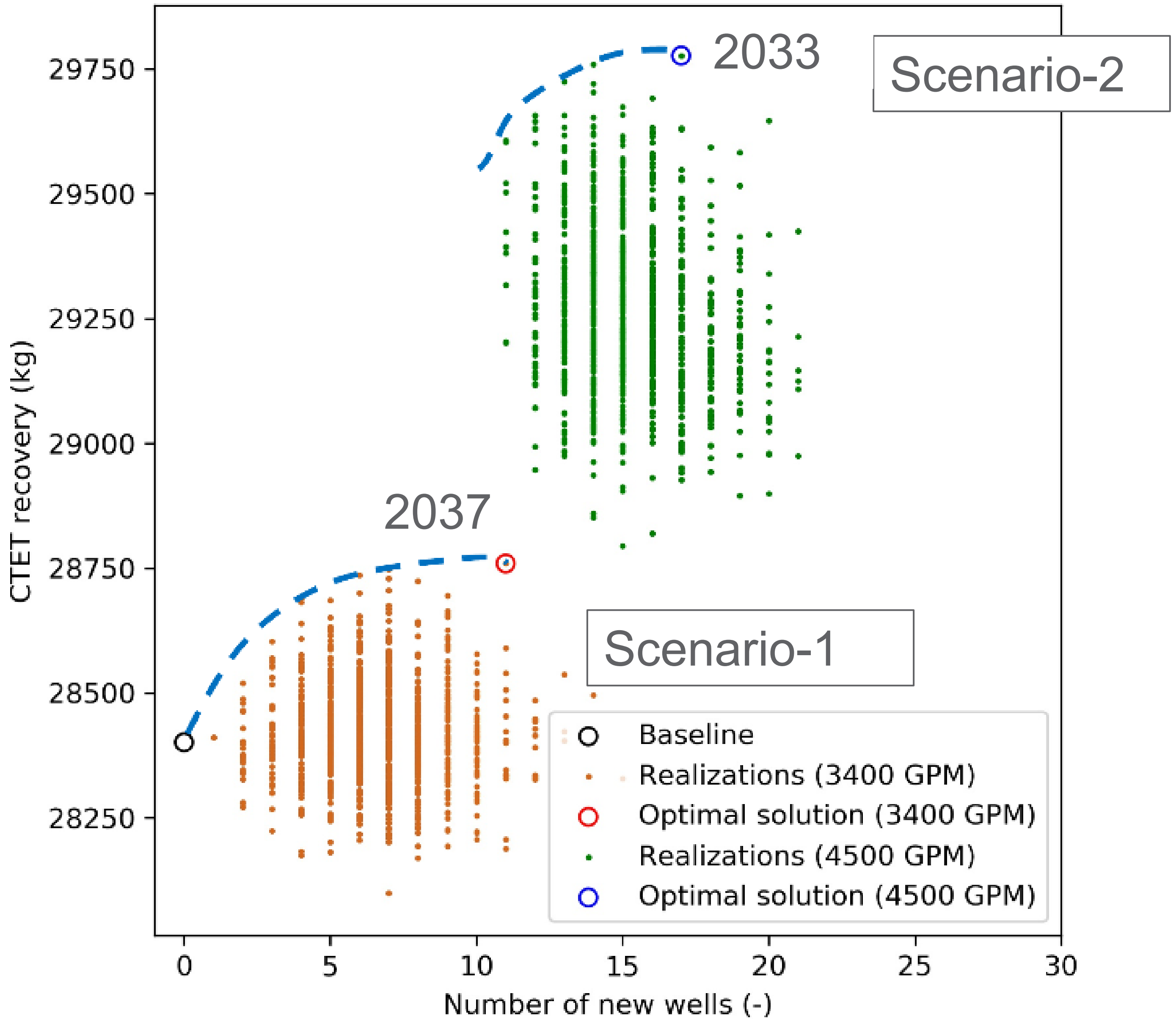
- Scenario-1 with well network optimization only (i.e., constant P&T capacity at 3400 gpm) achieves ~ 8% reductions in active remediation timeframe
  - Total of 7 new wells are added to the network
  - Achieves the same 95th percentile concentration level as the baseline with 2 fewer years of pumping
- Scenario-2 with well network optimization and increasing P&T capacity is found to have relatively more reduction in remedy lifetime, ~24%
  - Total of 17 new wells added to the network
  - Achieves the same 95th percentile concentration level as the baseline with 6 fewer years of pumping



Relation between # new wells added versus pumping timeframe

Results for Goal #2 (Maximizing CCl_4 Mass Recovery)

- Scenario-1 provides about ~ 4% reduction in pumping timeframe
  - A total of 11 wells added to the network
  - Achieves the same 95th percentile concentration level as the baseline with 1 year less pumping
- Scenario-2 provides about ~20% reduction in pumping timeframe
  - A total of 13 wells added to the network
  - Achieves the same 95th percentile concentration level as the baseline with 5 fewer years of pumping

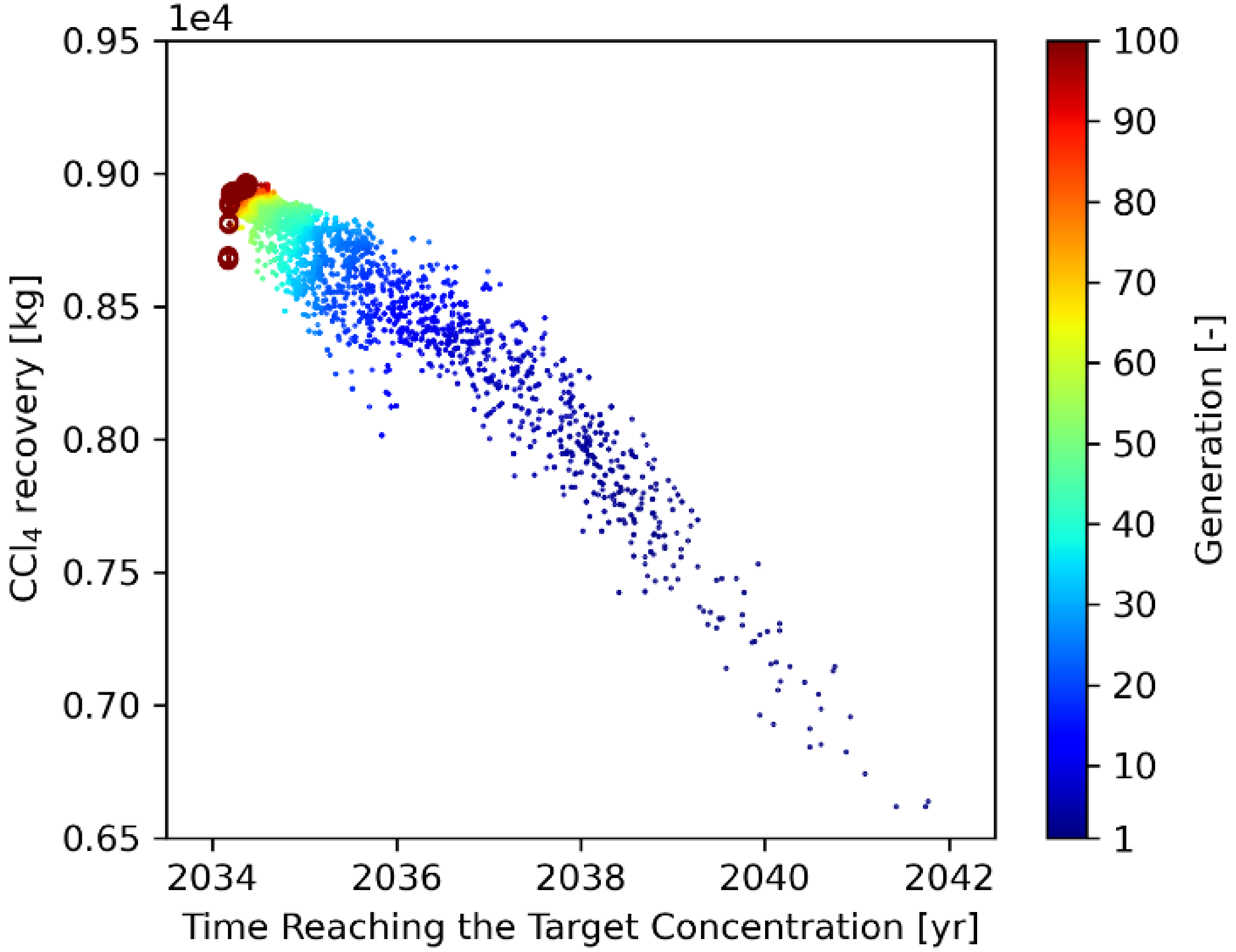


Relation between simulated total CTET mass recovery and the number of new wells added

Multi-objective Optimization: Balancing CCl_4 Cleanup Time and Mass Recovery

- Optimization Objectives
  - Minimizing CCl_4 Cleanup Time
  - Maximizing CCl_4 Mass Recovery

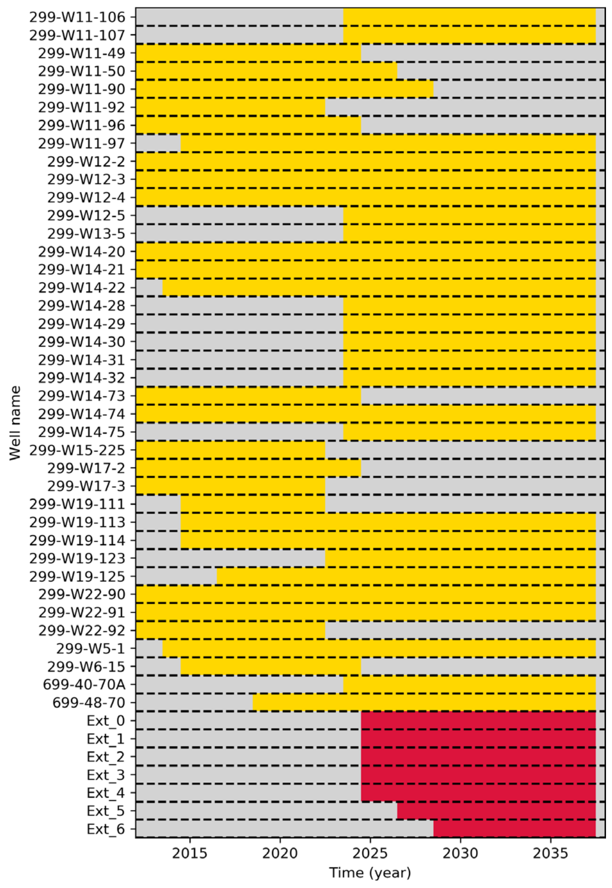
- Key Findings
  - The Pareto front shows a strong correlation—greater mass recovery generally accelerates cleanup.
  - Variability exists—some well network designs achieve similar mass recovery but differ in cleanup time.
  - The final Pareto front highlights trade-offs, where improving one objective (e.g., cleanup time) comes at the expense of the other (e.g., mass recovery).

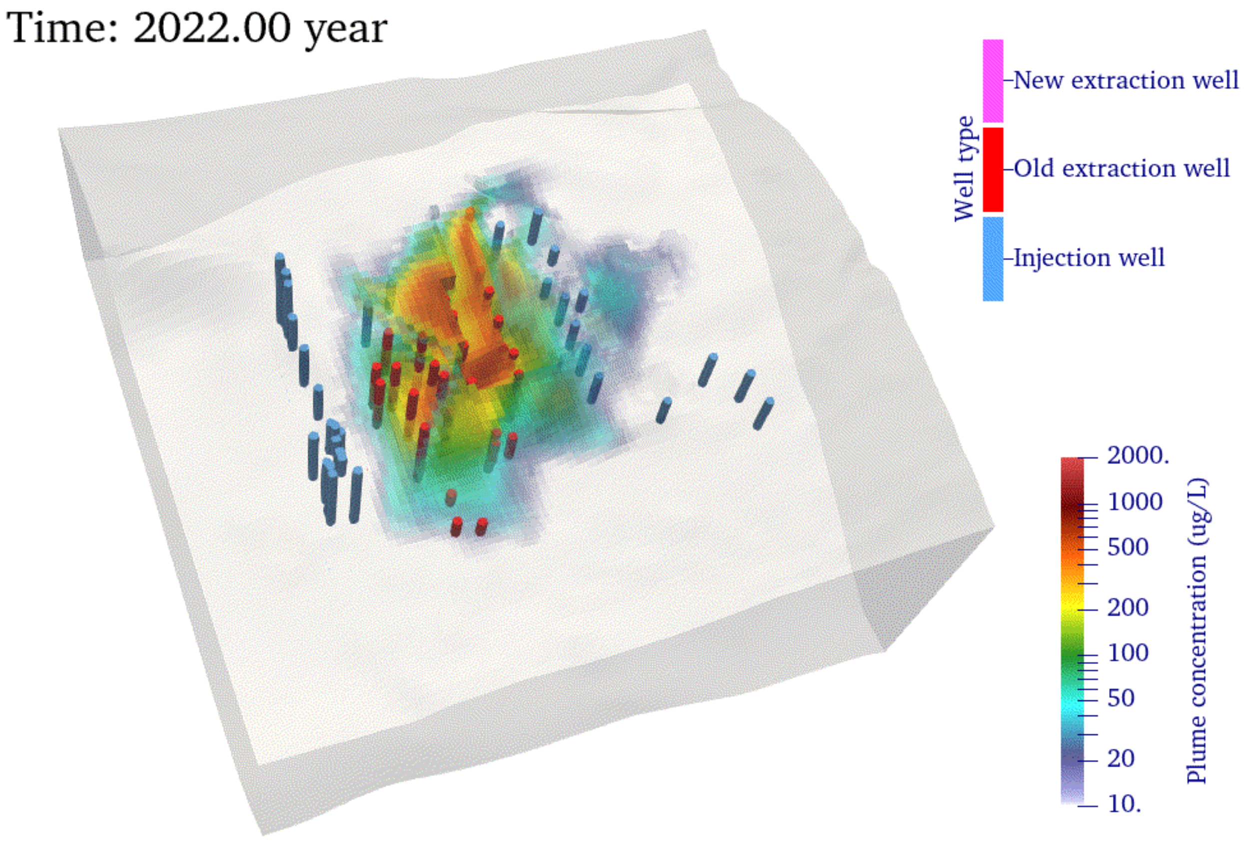


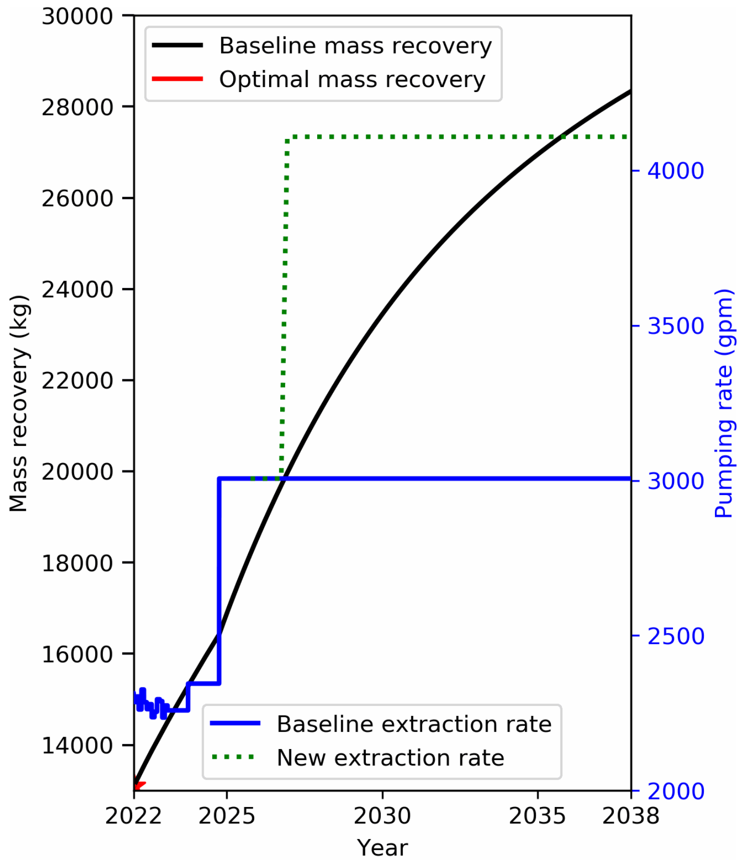
Pareto front showing trade-offs between CCl_4 cleanup time and mass recovery, with solutions evolving over generations (blue → early, red → optimized).

Example of Optimized P&T Well installation Plan

- Pumping strategy of the optimal solution
- Predicted plume dynamics
- Predicted mass recovery

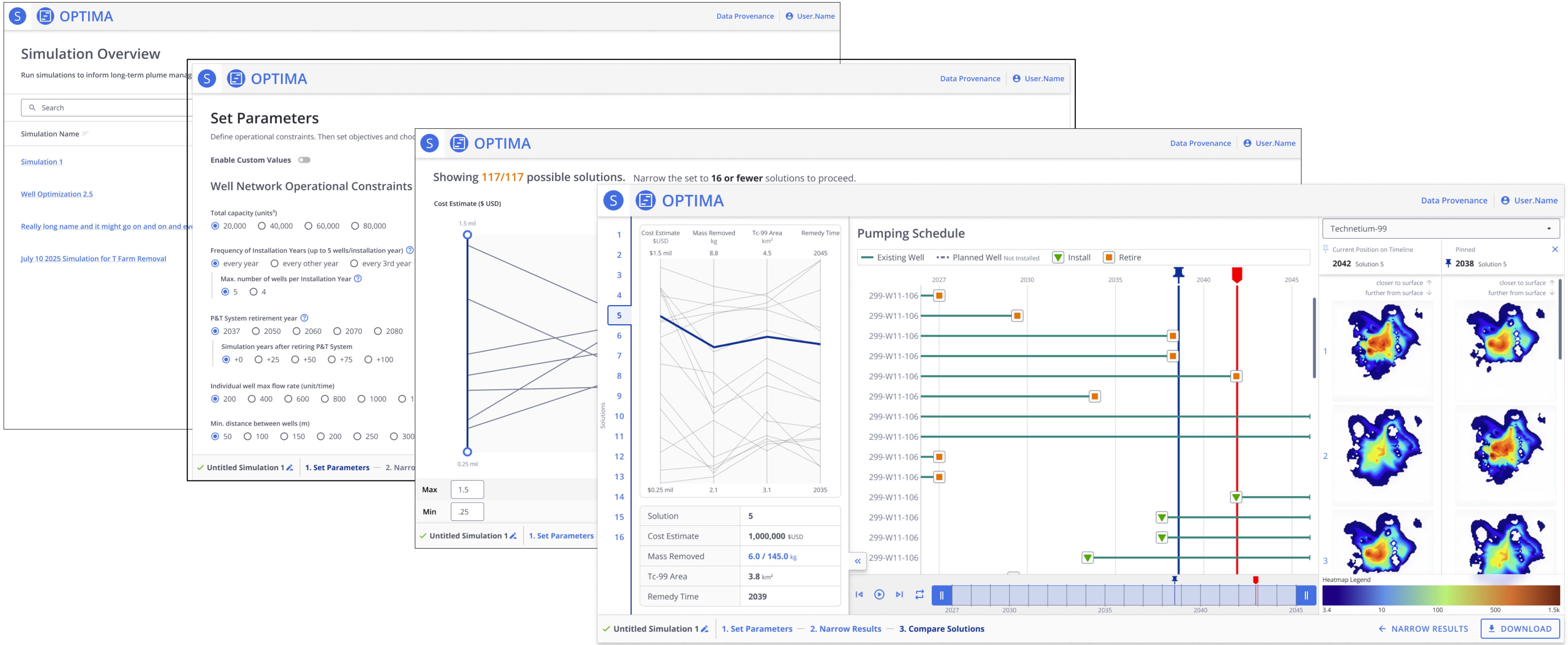






▶ Integrated optimization identifies efficient well configurations that achieve faster/higher mass recovery

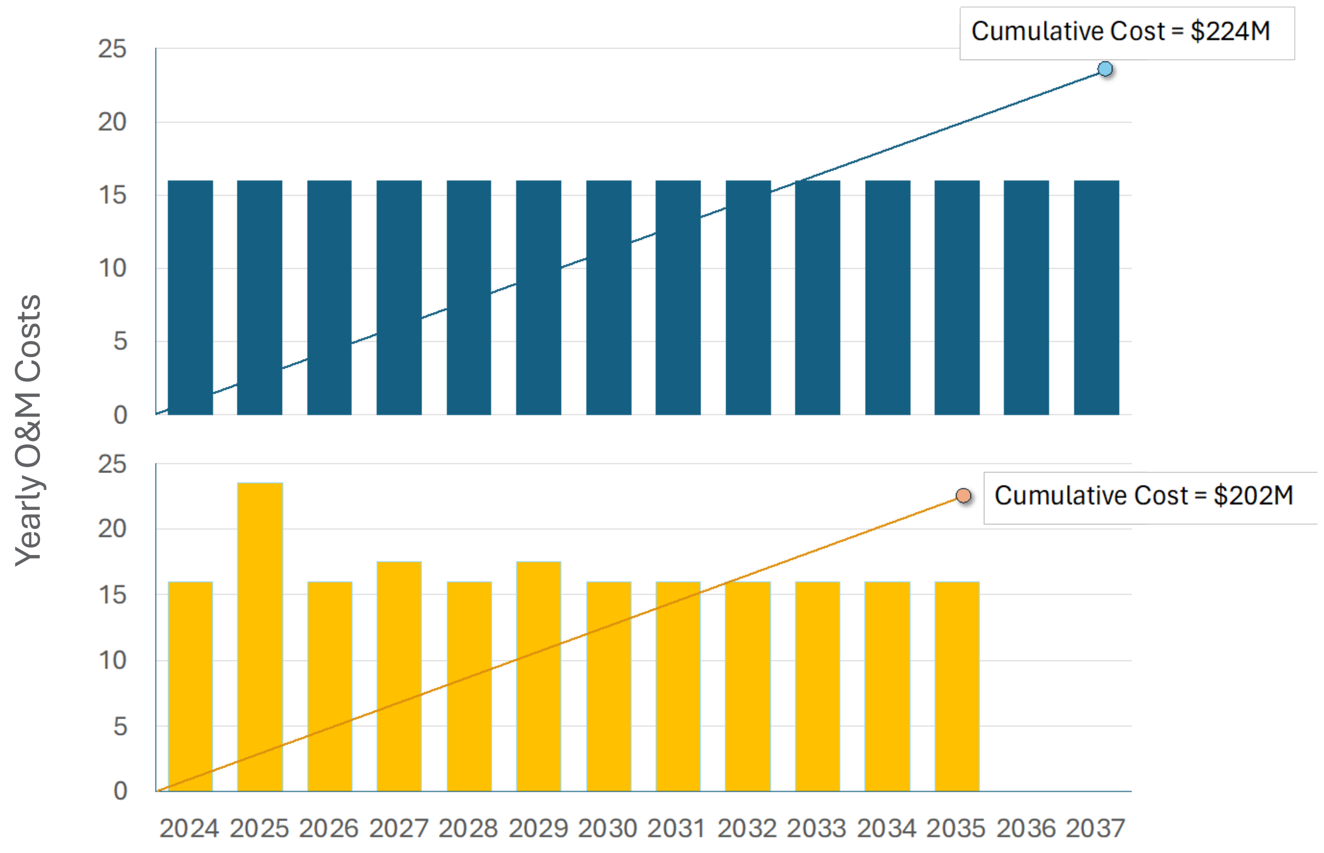
OPTIMA Web-Based Tool



▶ Integrated, web-based interface to set operational constraints, launch and manage optimization runs, and review multi-objective trade-offs with interactive visualizations.

Key Takeaways

- OPTIMA supports rapid scenario evaluation and transparent trade-off analysis, informing end-state–driven strategies for P&T capacity and well configuration.
- Results demonstrate shorter cleanup timelines and reduced lifecycle effort, while maintaining performance and compliance requirements.
- Deep-learning surrogates provide the speed needed to apply this framework routinely across scenarios.



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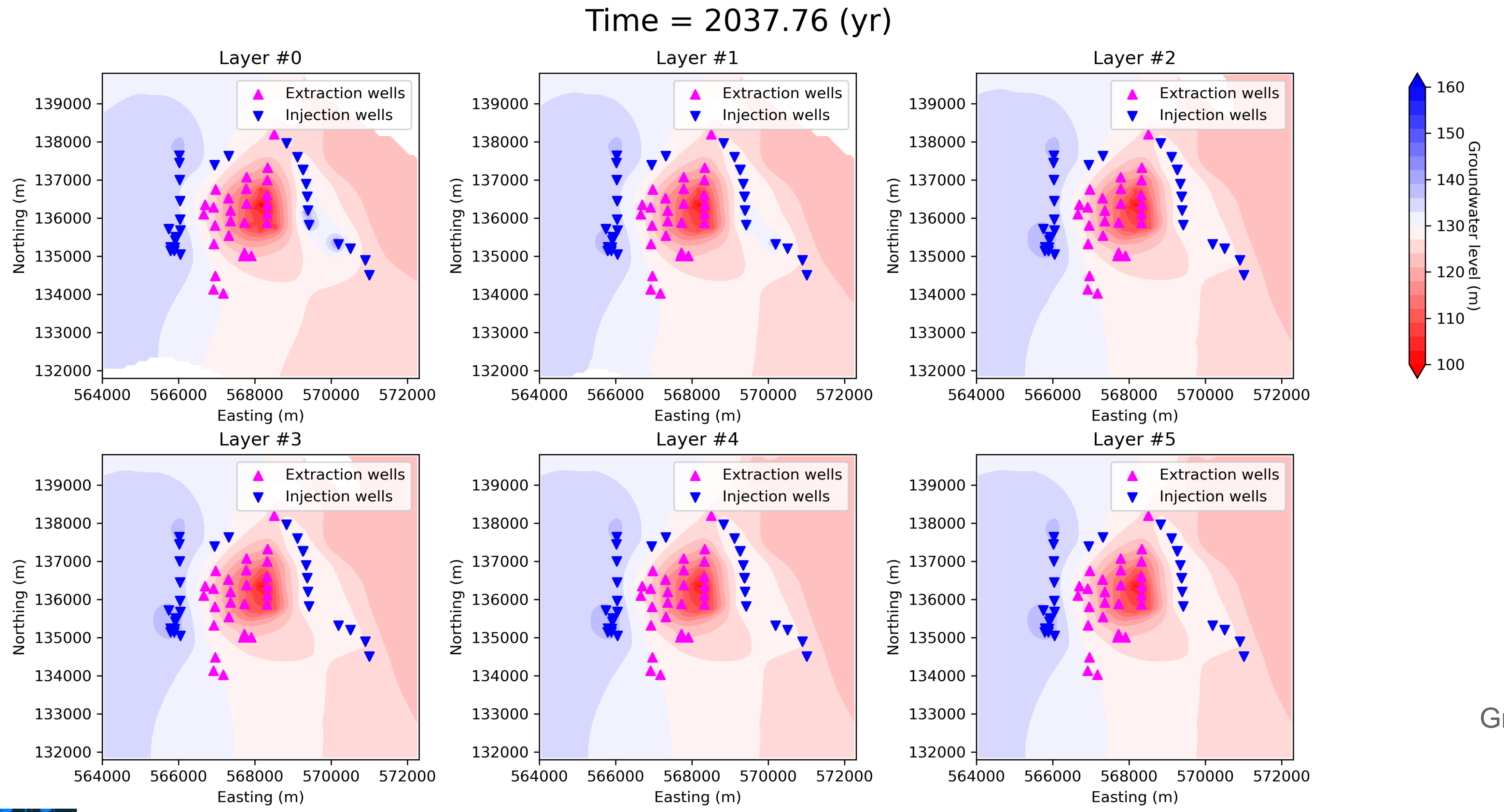
Funding for this work was provided by the U.S. Department of Energy Hanford Field Office under the Deep Vadose Zone – Applied Field Research Initiative. Pacific Northwest National Laboratory is operated by Battelle Memorial Institute for the Department of Energy under Contract DE-AC05-76RL01830.

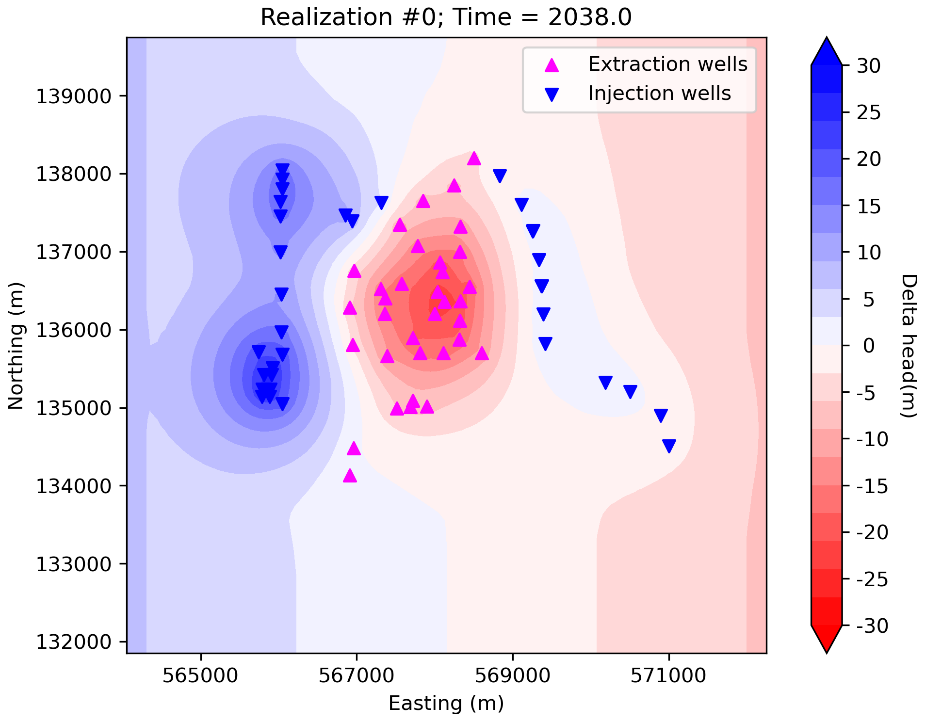
Thank you

Supporting information

Thiem Estimation vs. Numerical Model Simulation



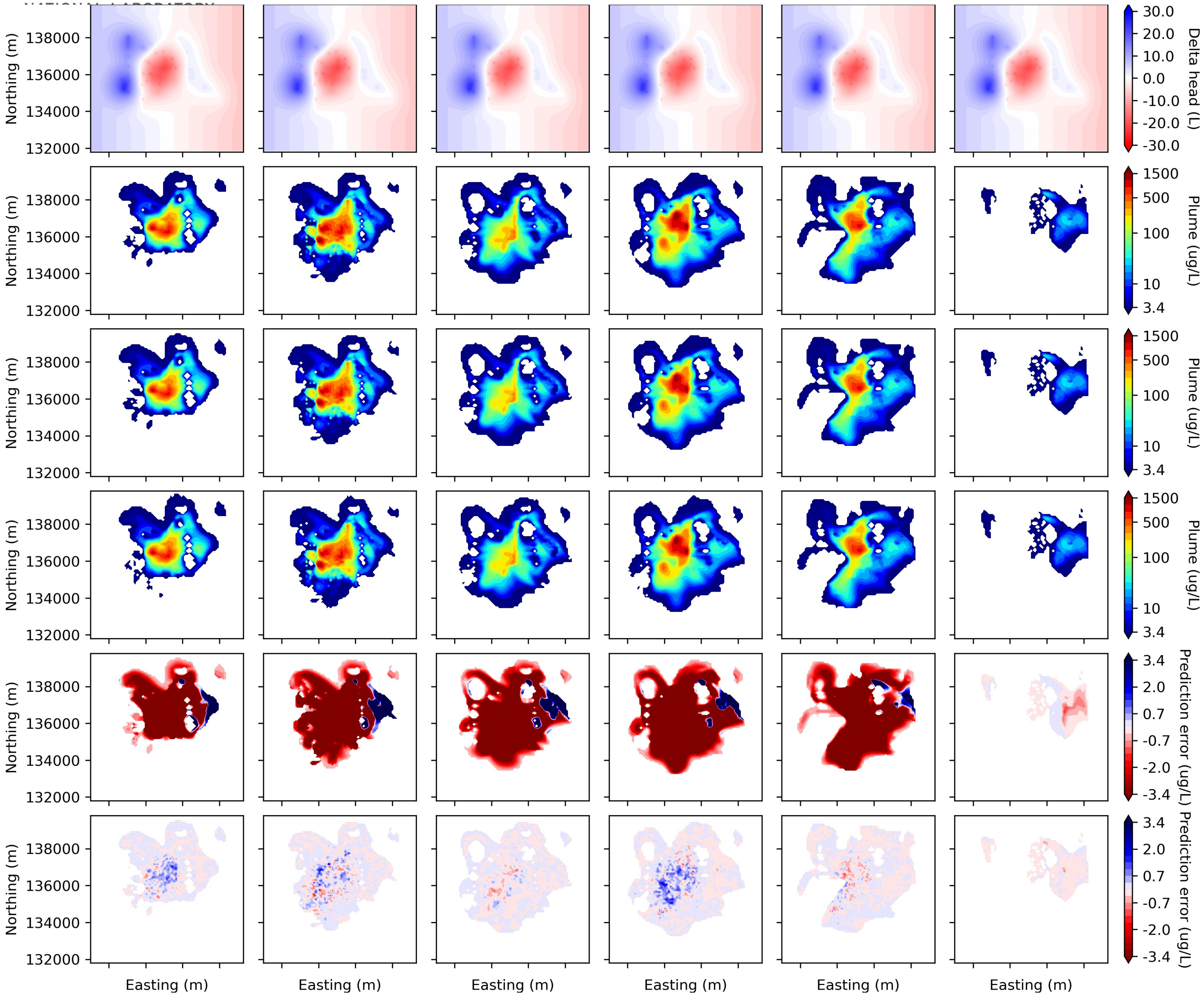
Groundwater level simulation results from P2R MODFLOW model



Groundwater level simulation results from Thiem estimation

- Discrepancy due to oversimplified assumptions in Thiem solution regarding aquifer thickness, hydraulic conductivity, and baseflow gradient

Model Testing



Input #1:thiem solution

Input #2:plume at year N

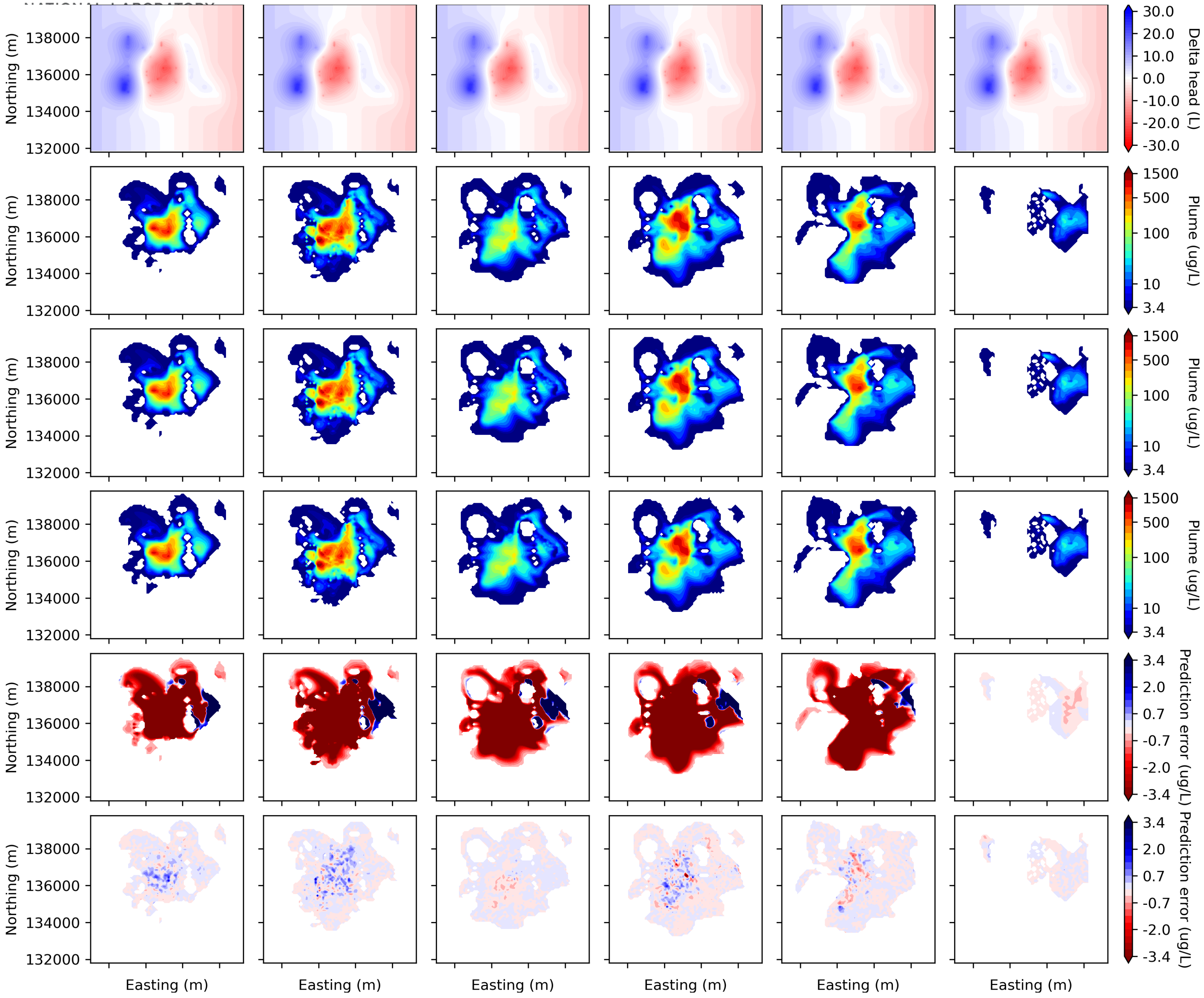
Target: plume at year N+1

Prediction: plume at year N+1

Plume change over year N (row 3-row 2)

Prediction error (row 4-row3)

Model Testing



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