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Leveraging Data-Driven Approaches for Performance-Based Management of Pump-and-Treat Remedies

May 21, 2024

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U.S. DEPARTMENT OF ENERGY BATTELLE

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Outline

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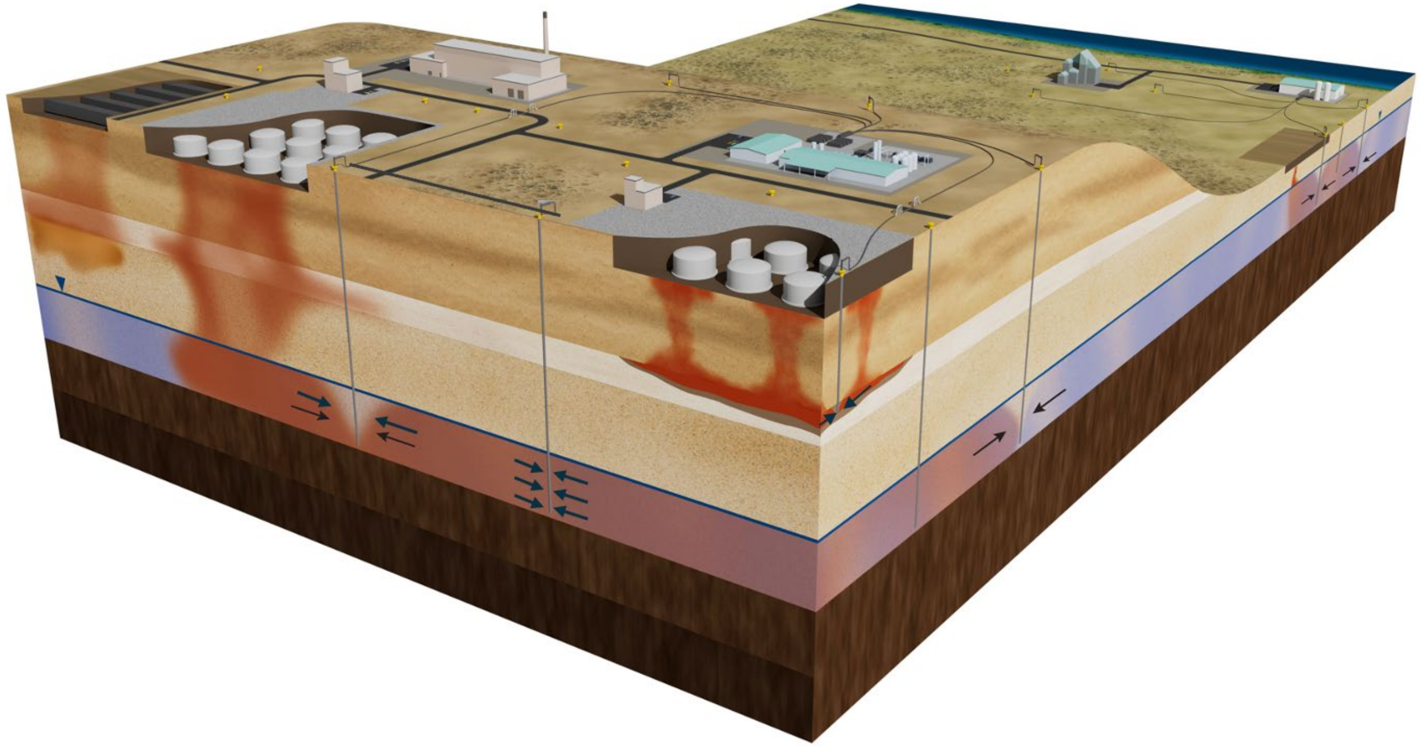
  - Computational approaches
  - Pre-screening tool framework
- Part 2: Pre-Screening Tool Demonstration
  - Hanford 200 West P&T
  - Scenario evaluation
- Part 3: Use of Deep-Learning Approaches
  - Well performance predictions
  - Increasing model efficiency

Part 1– Performance-Based Optimization of P&T



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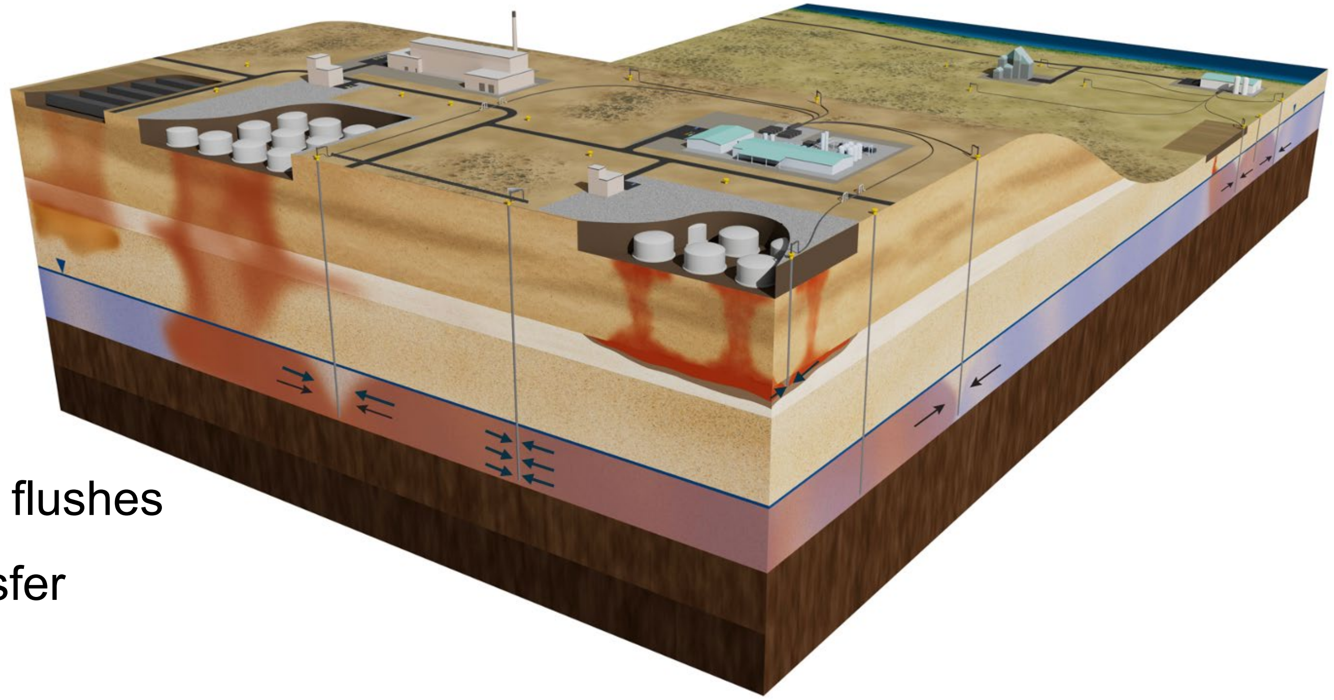
Pump-and-Treat (P&T) Systems

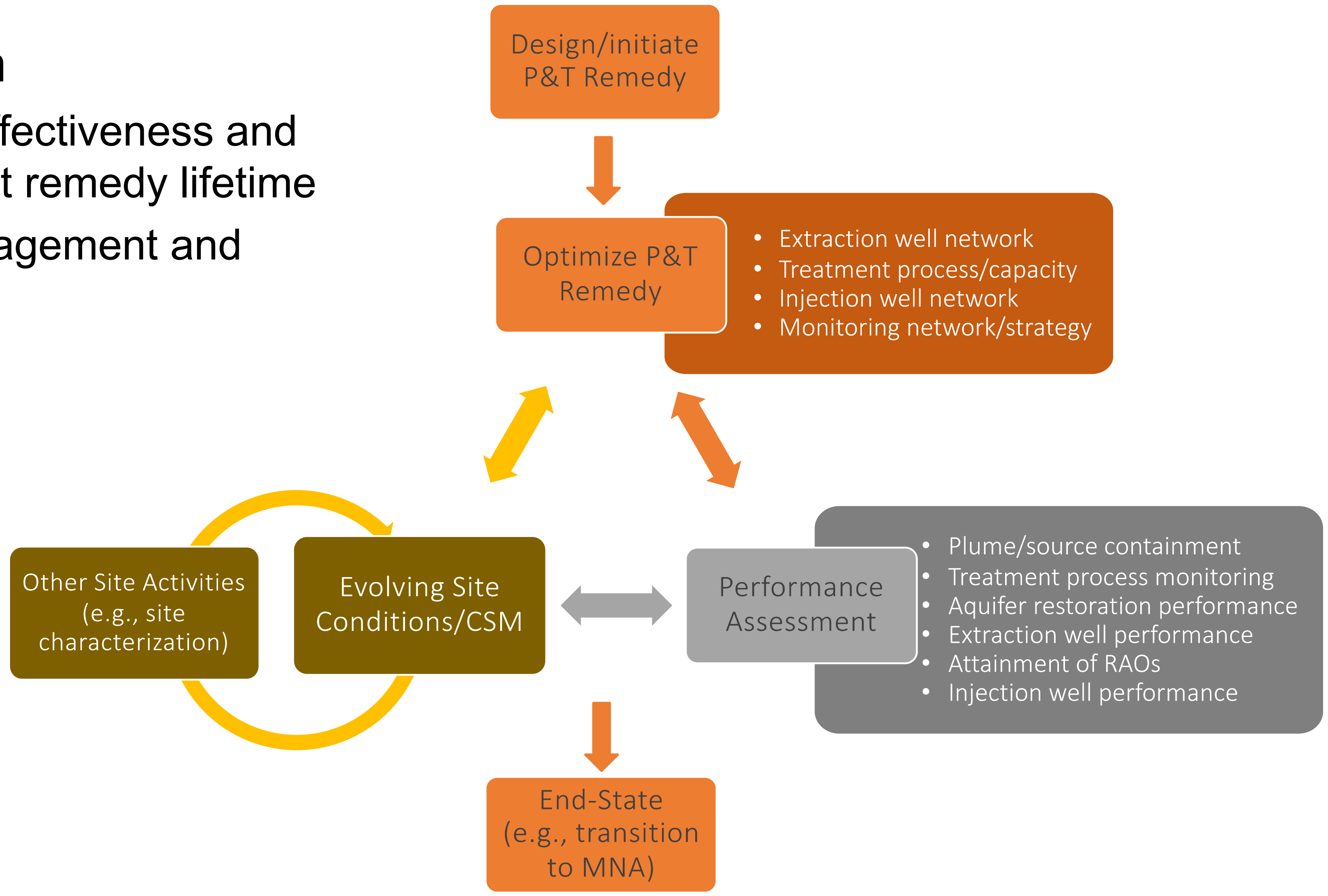
- Pump-and-treat (P&T) systems have been used for hydraulic containment and/or treatment of contaminated groundwater
  - A well network for groundwater extraction
  - Above-ground ex-situ treatment unit
  - Disposal system for the treated water
- Initial designs typically address large-scale containment and bulk treatment, and may not be an optimal design for mass removal and long-term effectiveness
  - Early goals focus on volumetric pumping
- Performance diminishes due to factors such as:
  - Heterogeneity
  - Large and dispersed plumes requiring multiple pore volume flushes
  - Presence of source zone and/or diffusion-limited mass transfer
  - Recalcitrant/competing contaminants

Pump-and-treat extraction well (adapted from PNNL-24741)



Performance-Based P&T Optimization

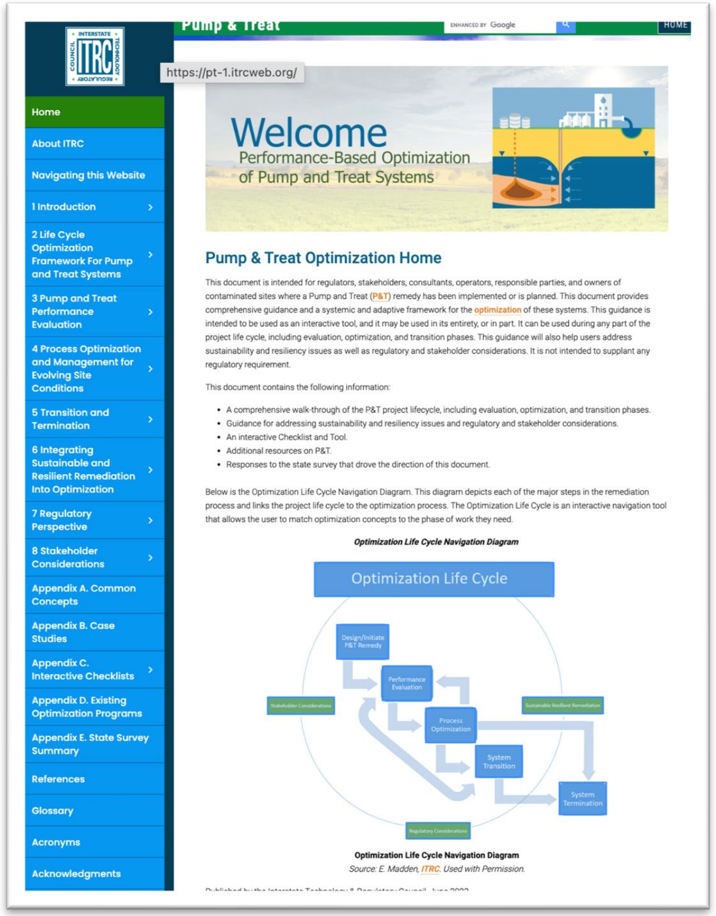
- Objective of periodic P&T optimization
  - Maintain/increase contaminant removal effectiveness and efficiency as much as possible throughout remedy lifetime
  - Well network and treatment capacity management and optimization
- Performance-based optimization approach relies on:
  - Continuous performance monitoring
  - Frequent updates to CSM based on the new data
  - Periodic evaluations of performance effectiveness and remedy lifetime
  - Computational optimization evaluations
    - Capacity & well network effectiveness



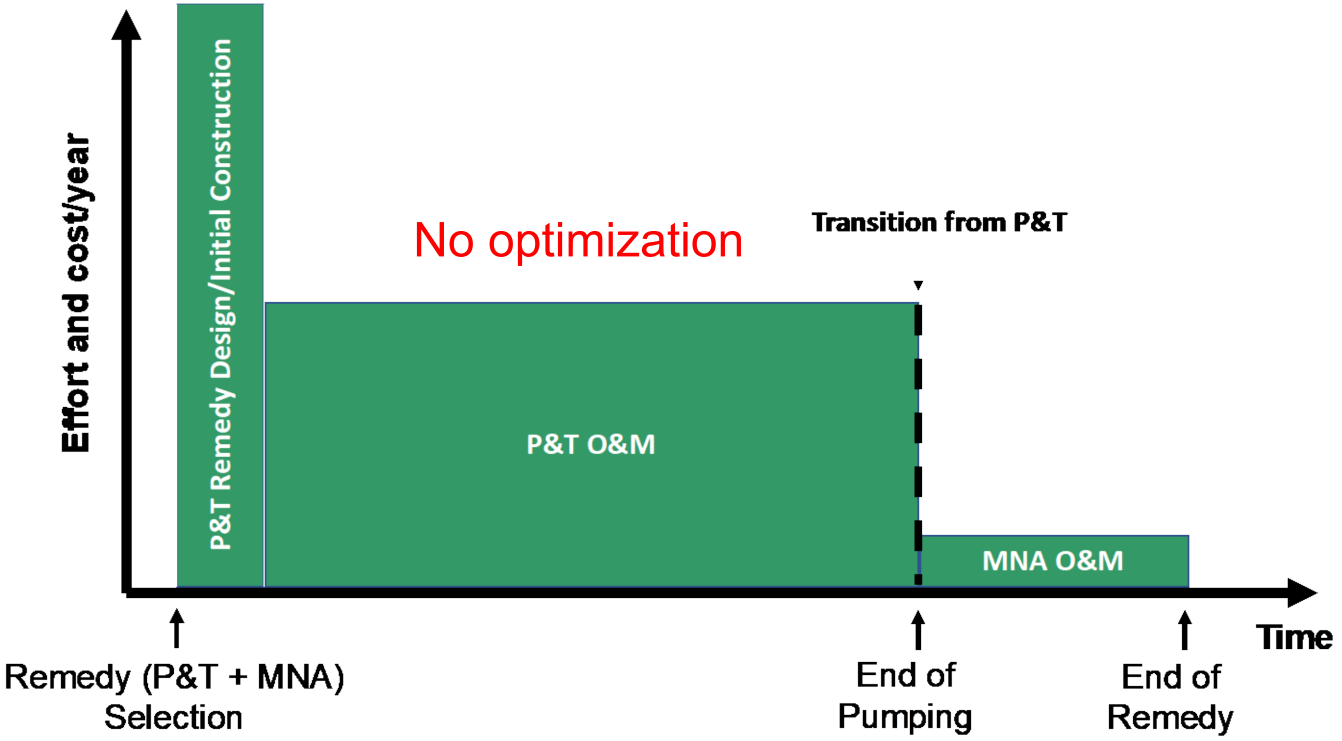
CSM = Conceptual Site Model
RAO = Remedial Action Objective

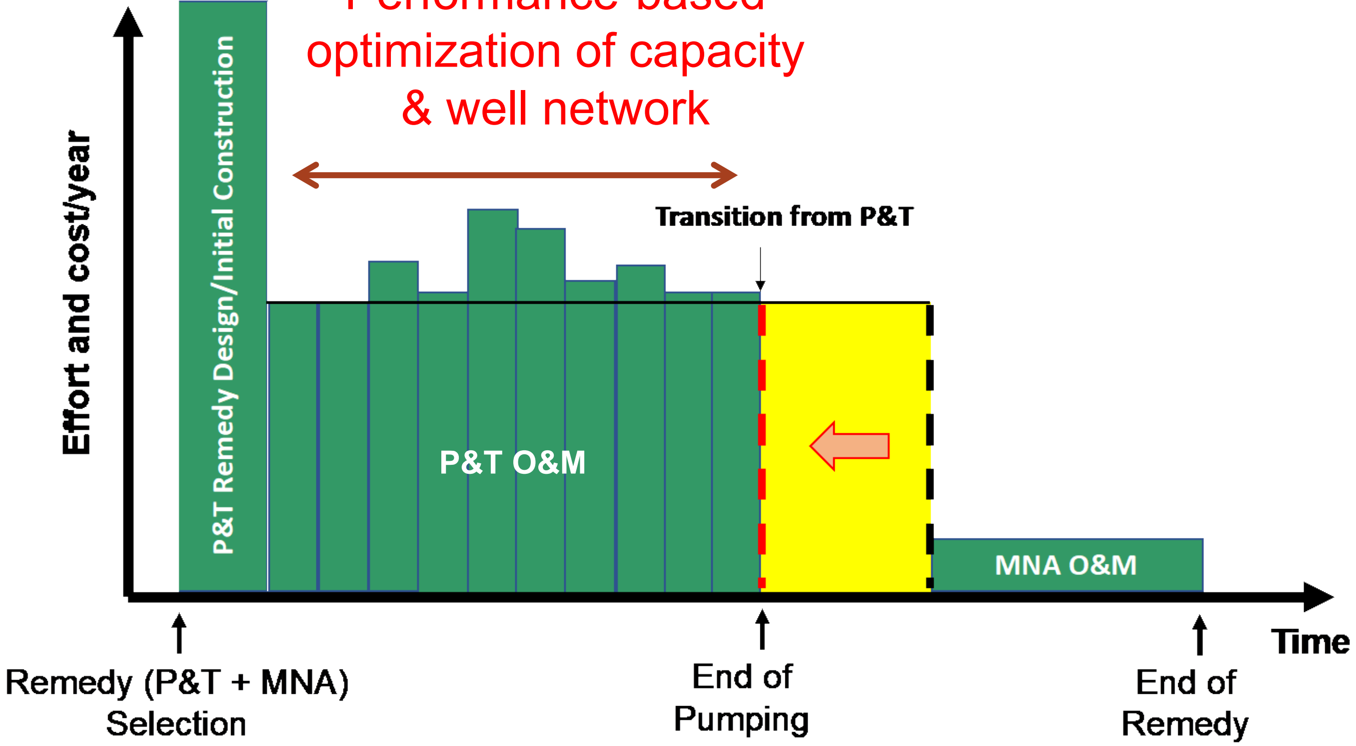
ITRC Guidance

- Interstate Technology Regulatory Council (ITRC)
- New performance-based P&T optimization guidance published in 2023



Adopted from the guidance

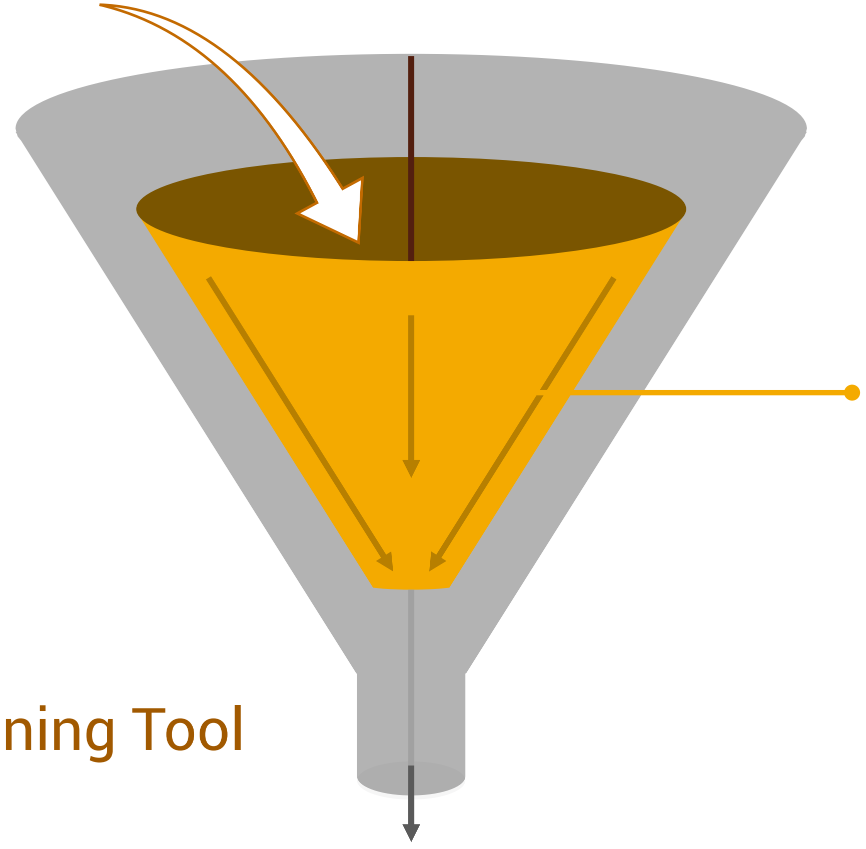




https://pt-1.itrcweb.org/

Computational Optimization and Pre-screening

- Formal optimization evaluations require:
  - Flow & transport (F&T) model of P&T system, coupled with optimization algorithms to run thousands of simulations
  - Resource intensive!
- Pre-screening (i.e., scoping) framework
  - Supports scenario evaluation to feed into decision tools
  - Reduced computational burden



- Comparative assessment of scenarios
- Narrower set of potentially successful optimization approaches
- Uncertainty evaluation

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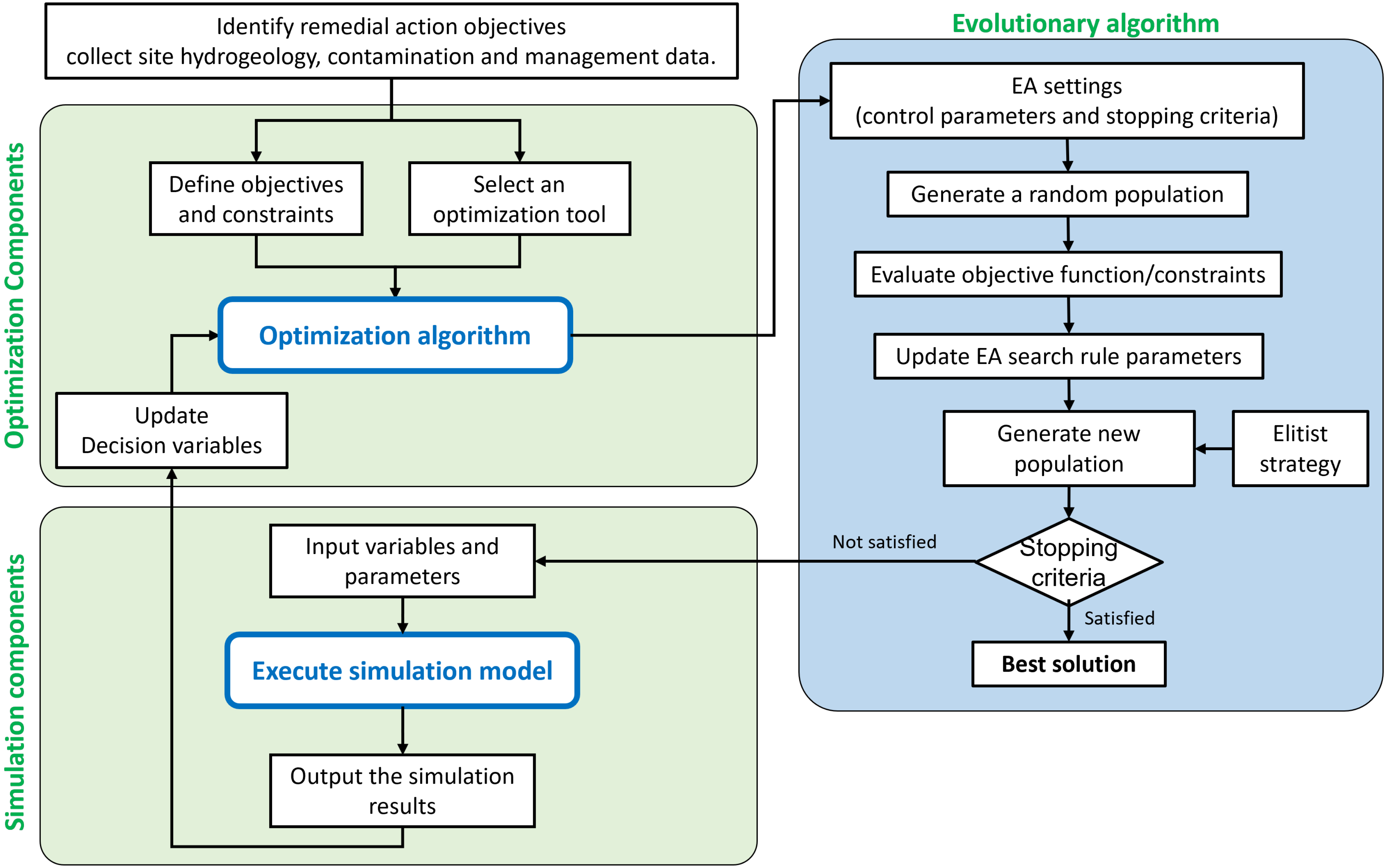
Pre-screening Tool Framework

- Effective optimization requires a well-crafted problem design, a rapid optimizer, and a fast-executing F&T model

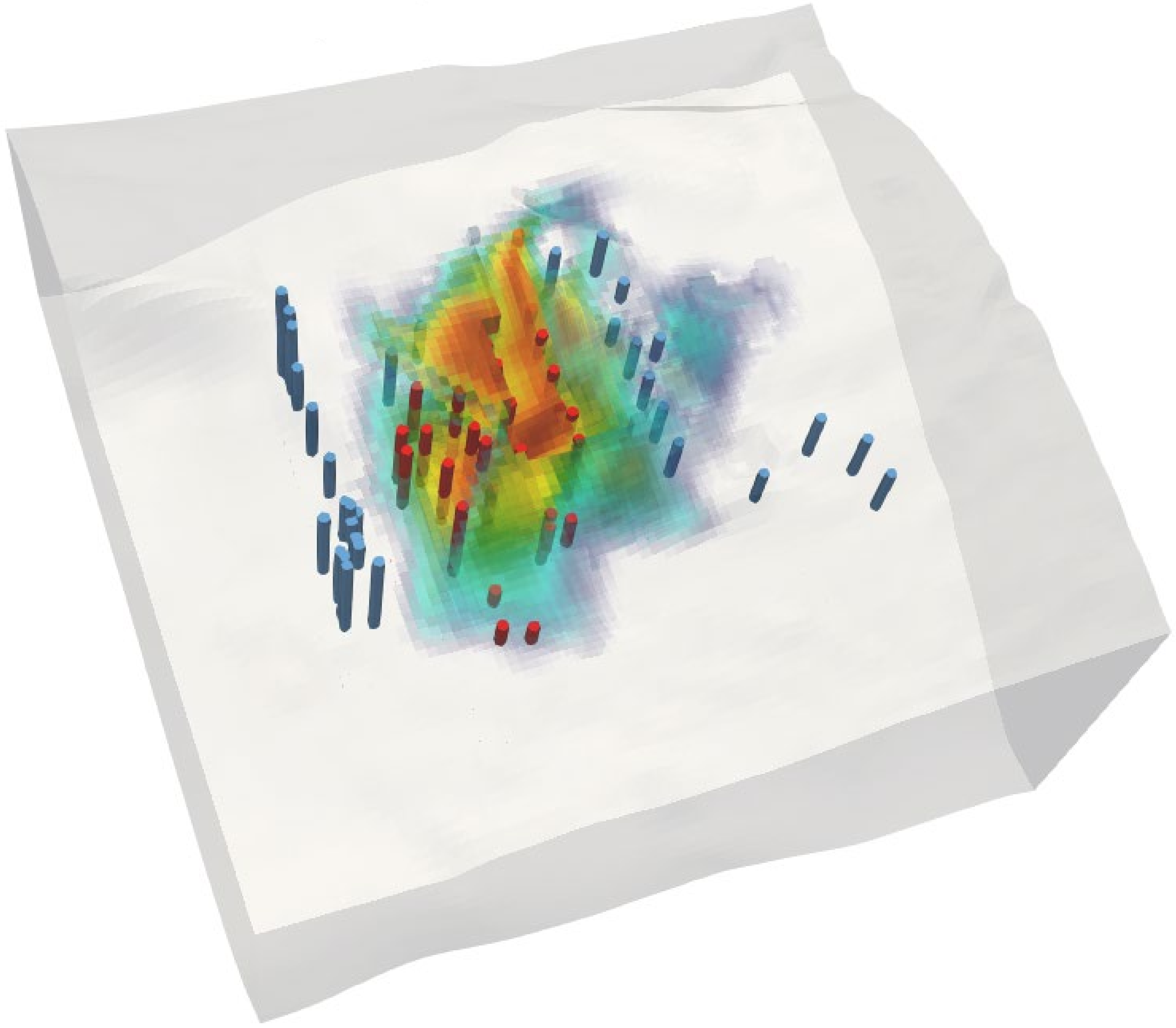
Formal optimization parameters

Reduced complexity fate and transport model



Stochastic approach for solving both single-objective and multi-objective problems

Part 2 – Pre-Screening Tool Demonstration



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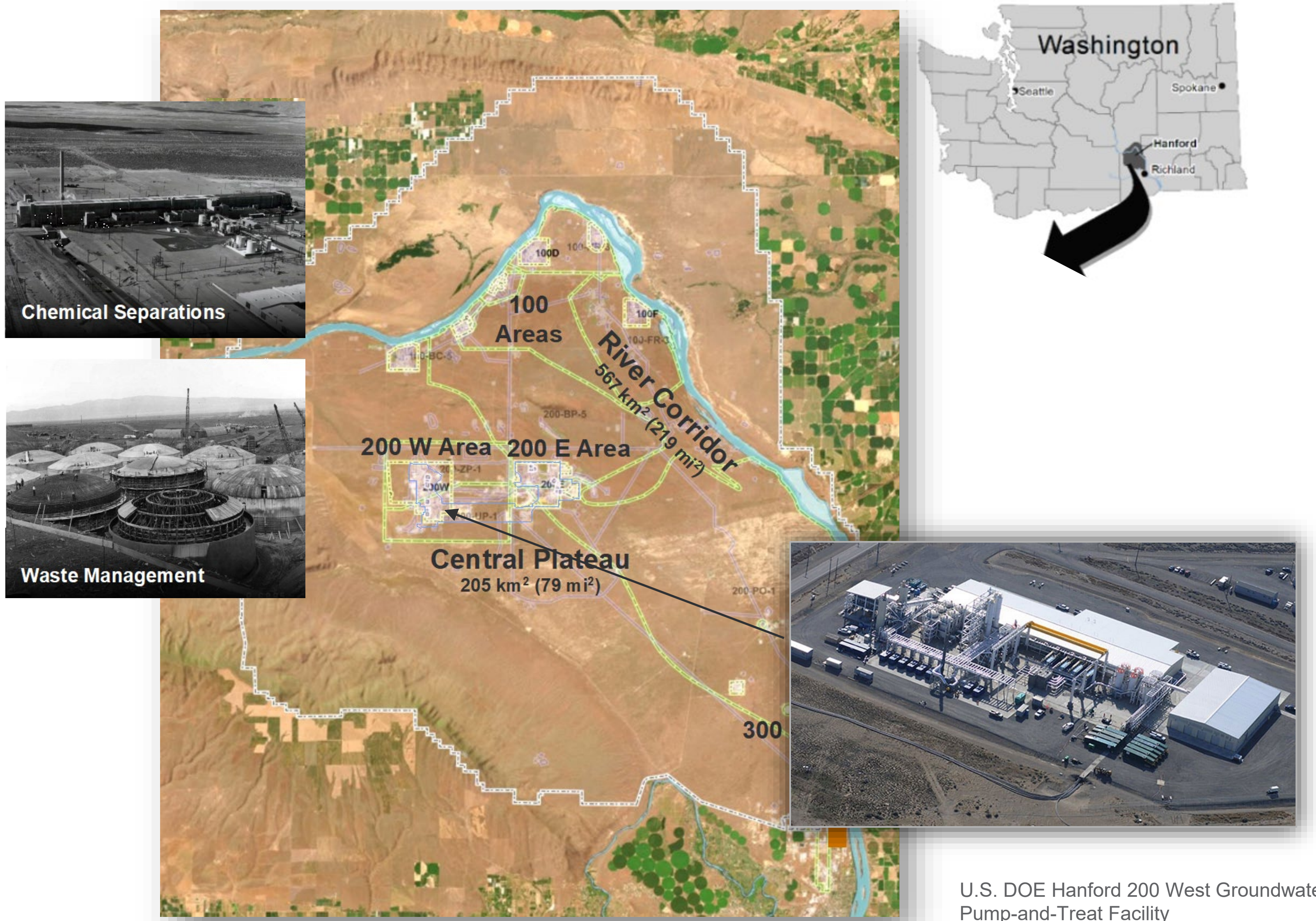
Hanford 200 West P&T

- Historical plutonium production for the Manhattan Project
- Operating since 2012 in the Central Plateau (CP) of the Hanford Site
  - Will be pumping for 25 years per 200-ZP-1 operable unit Record of Decision
- Addressing groundwater plumes:
  - Carbon tetrachloride (CTET)
  - Technetium
  - Uranium
  - Chromium
  - Nitrate*
- Current treatment capacity is 2500 gpm
  - 38 existing extraction wells
  - 30 existing injection wells

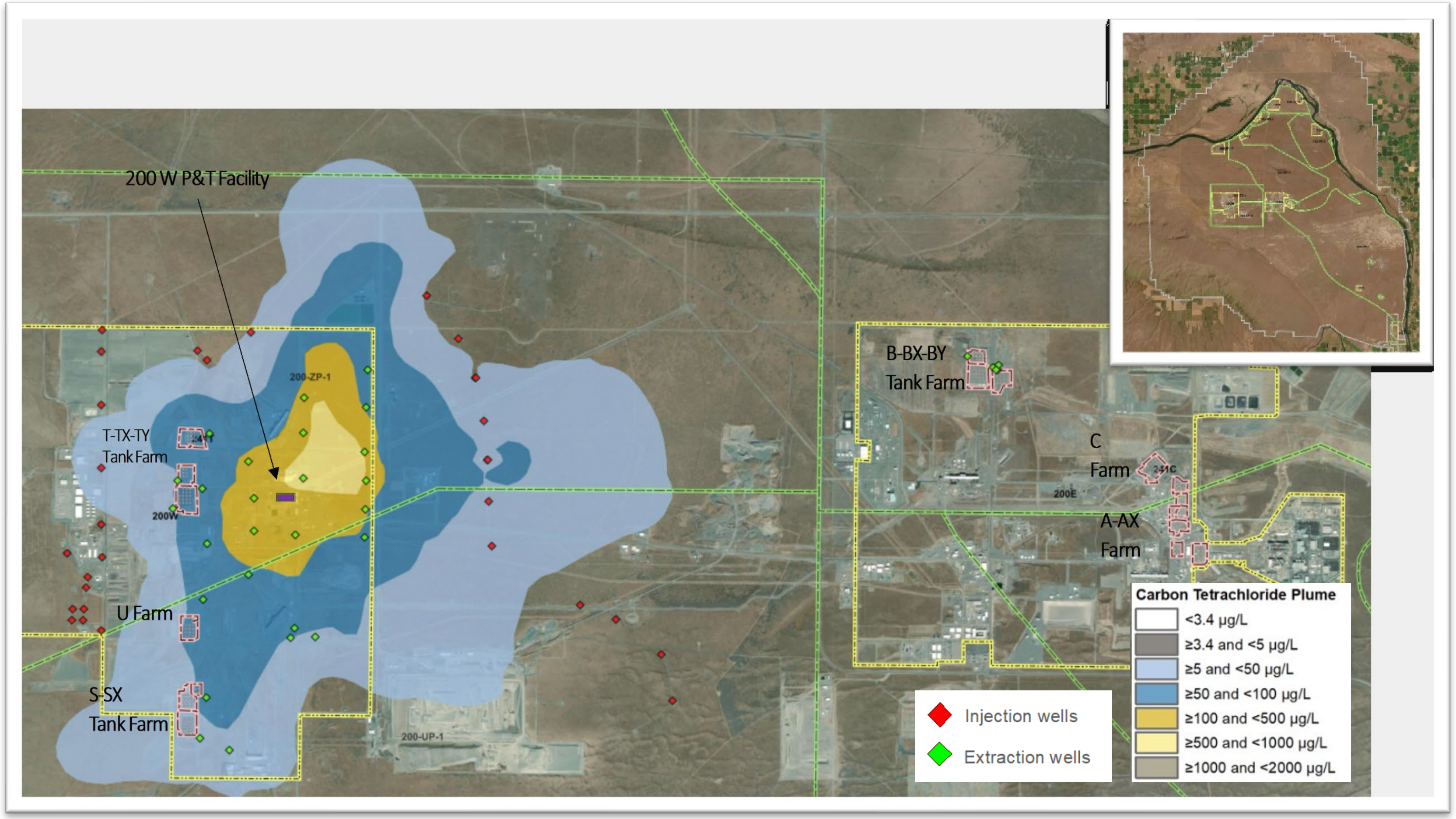


U.S. DOE Hanford 200 West Groundwater Pump-and-Treat Facility (https://www.usa.skanska.com/what-we-deliver/projects/57299/)

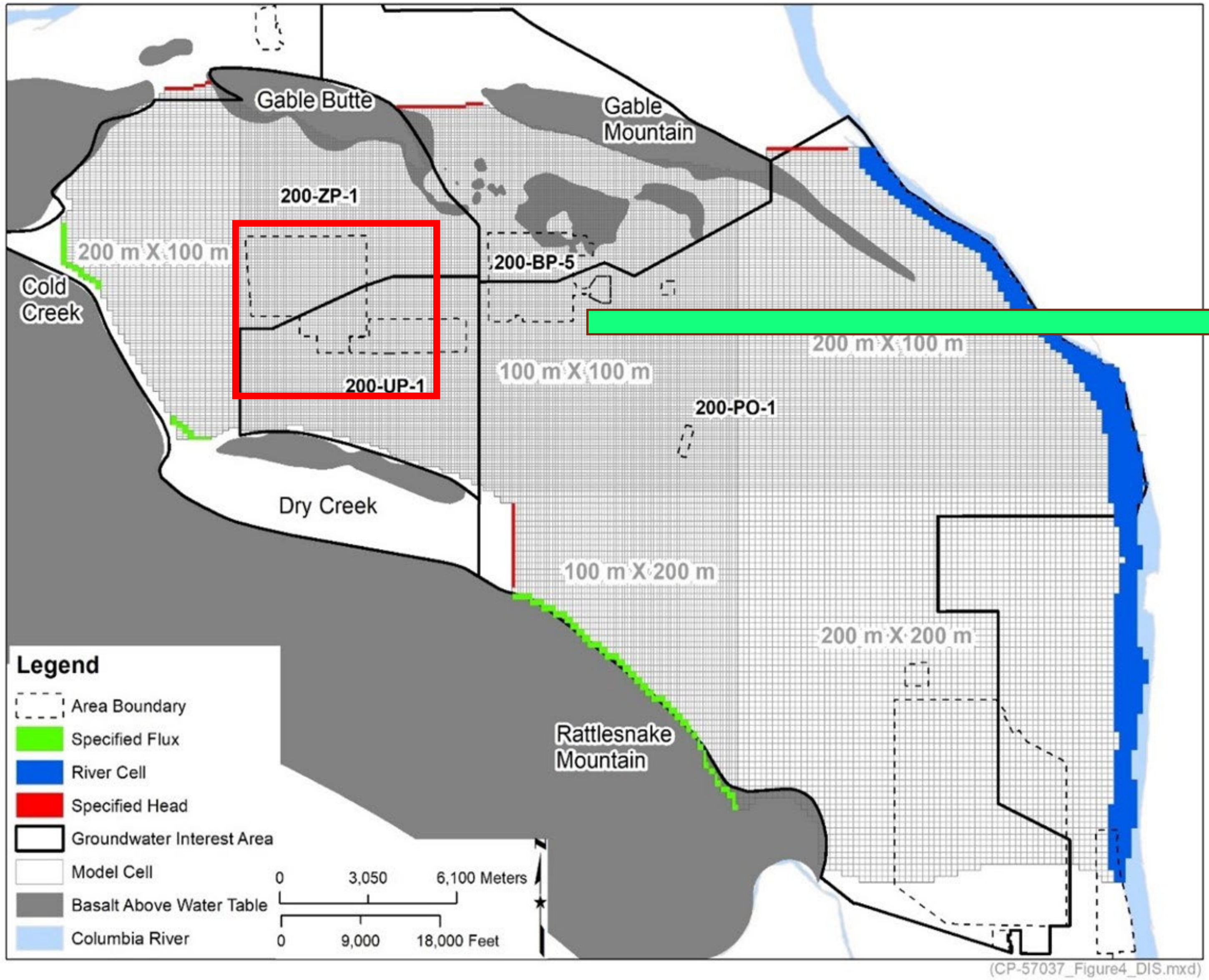
* Nitrate treatment is currently suspended under an optimization study

200 West P&T: Optimization Study

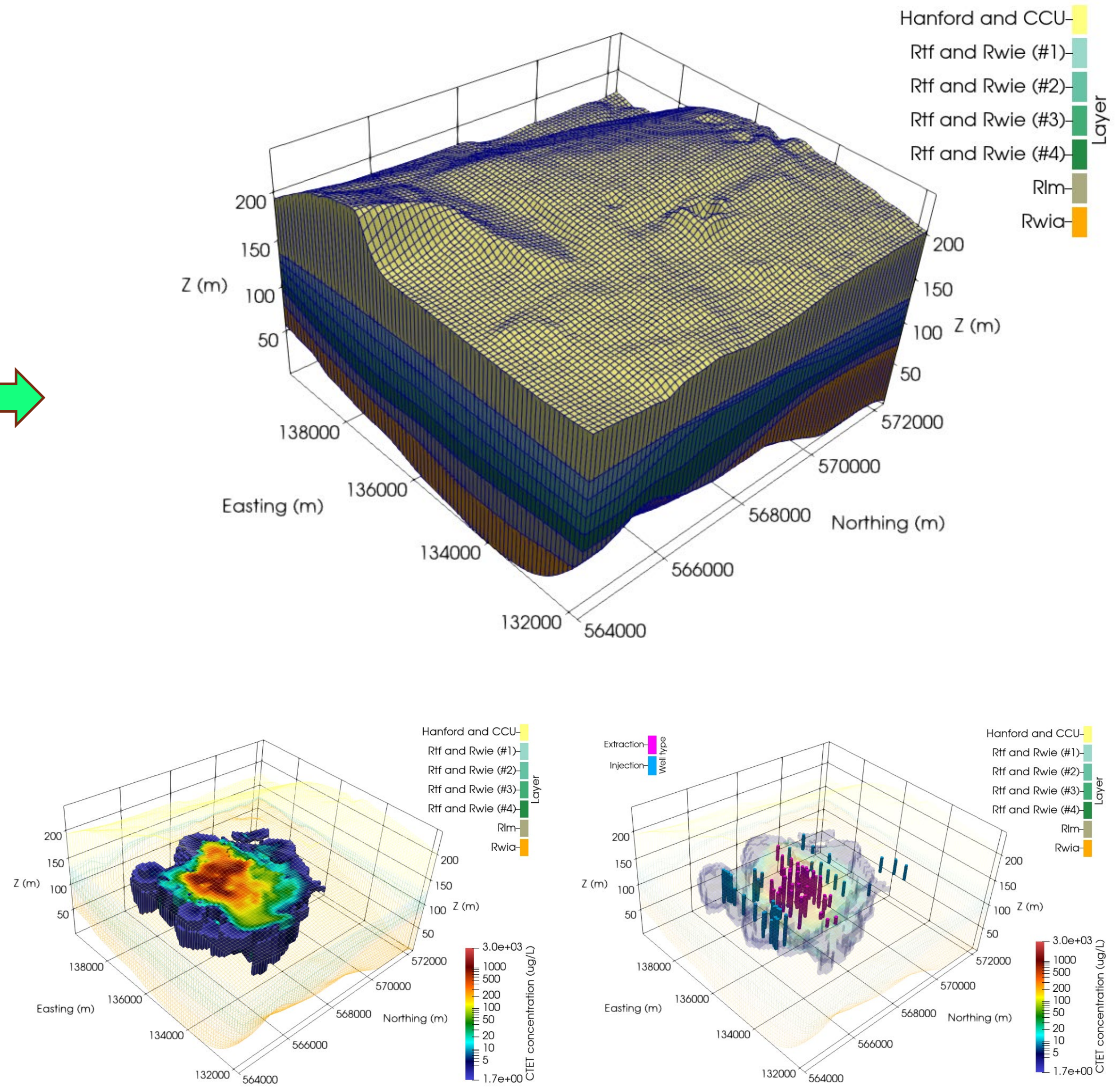
- Large carbon tetrachloride plume in the 200-ZP-1 Operable Unit (OU)
  - Slower CTET degradation rate
  - More contaminant mass in the aquifer
  - Diminishing performance at some wells
- 200-ZP-1 OU Optimization Study Plan to evaluate
  - Increasing carbon tetrachloride removal and treatment
  - Evaluating the transition to monitored natural attenuation (MNA) for nitrate, consistent with RAOs



Reduced Complexity Model Setup



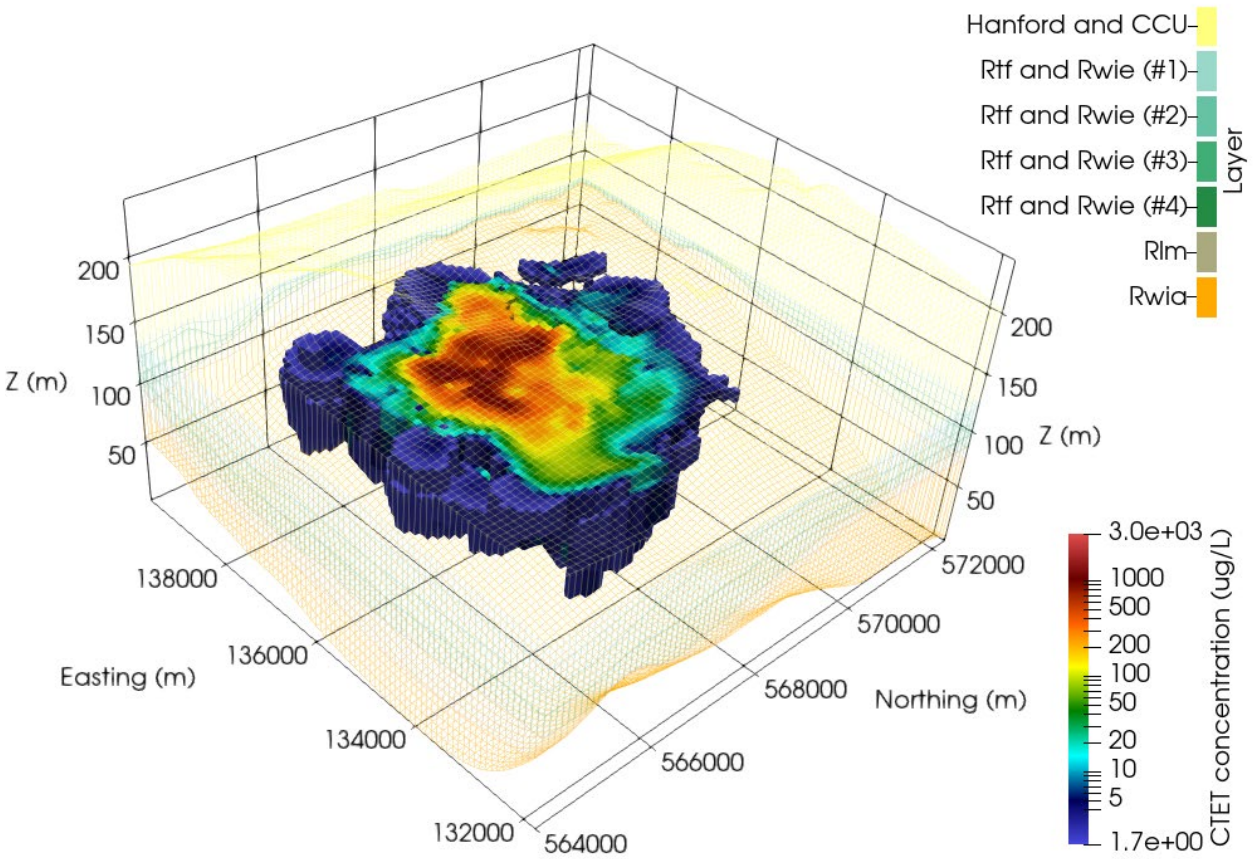
Plateau to River (P2R) Version 8.3 Model Extent and Groundwater Flow Boundary Conditions (source: ECF-HANFORD-22-0114-REV.0)



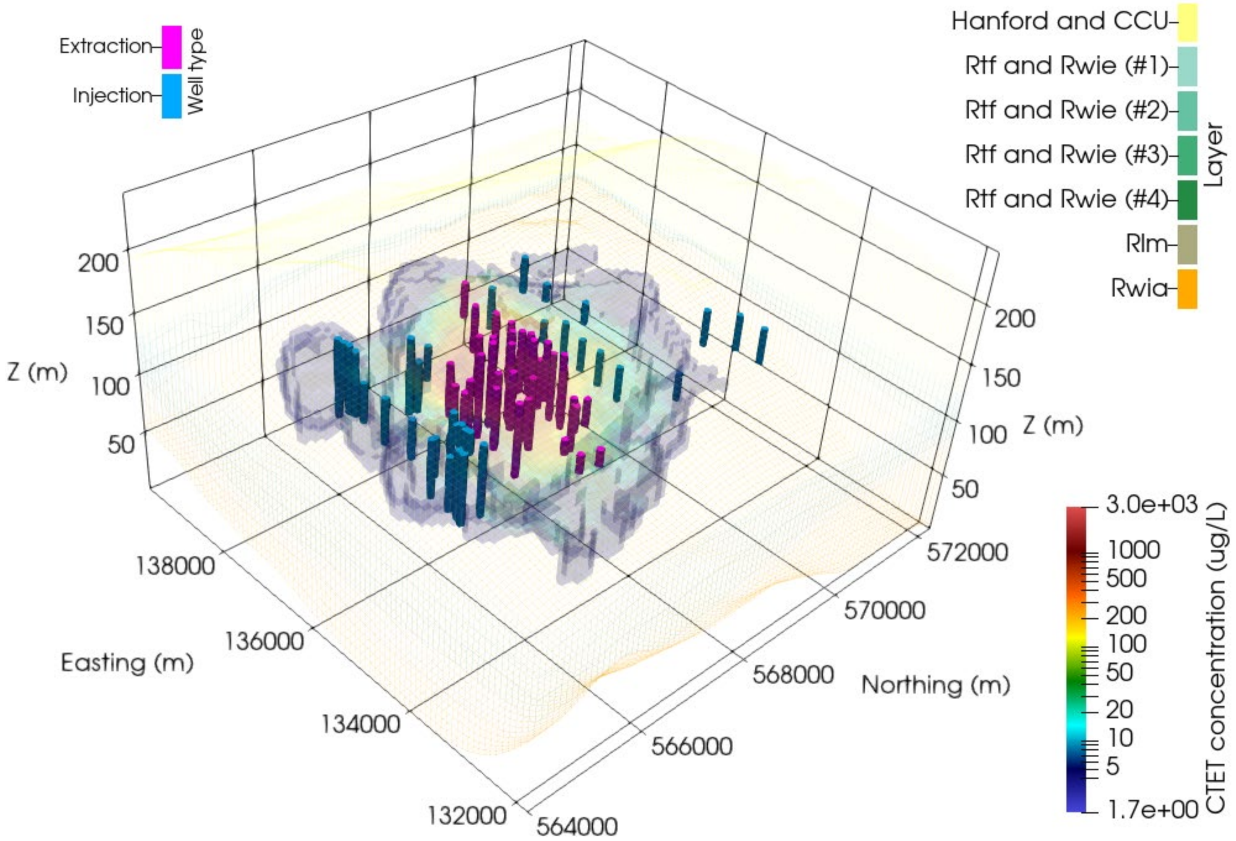
Reduced Complexity Model Domain
(eSTOMP model domain)

Reduced Complexity Model Setup

- Initial CTET plume (2015)

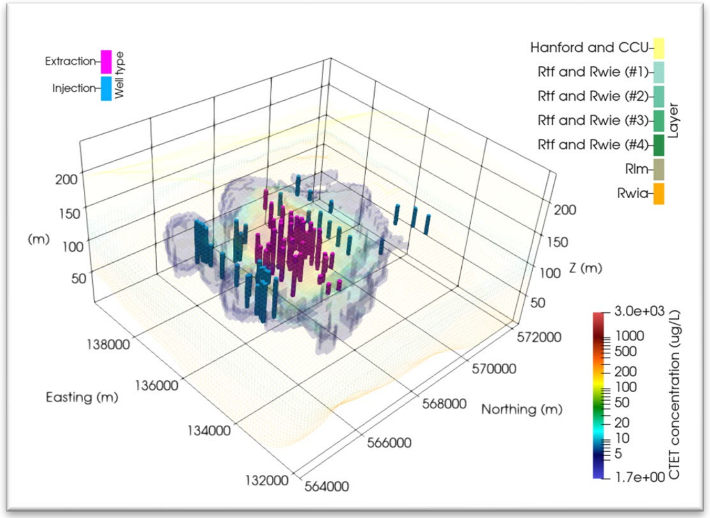


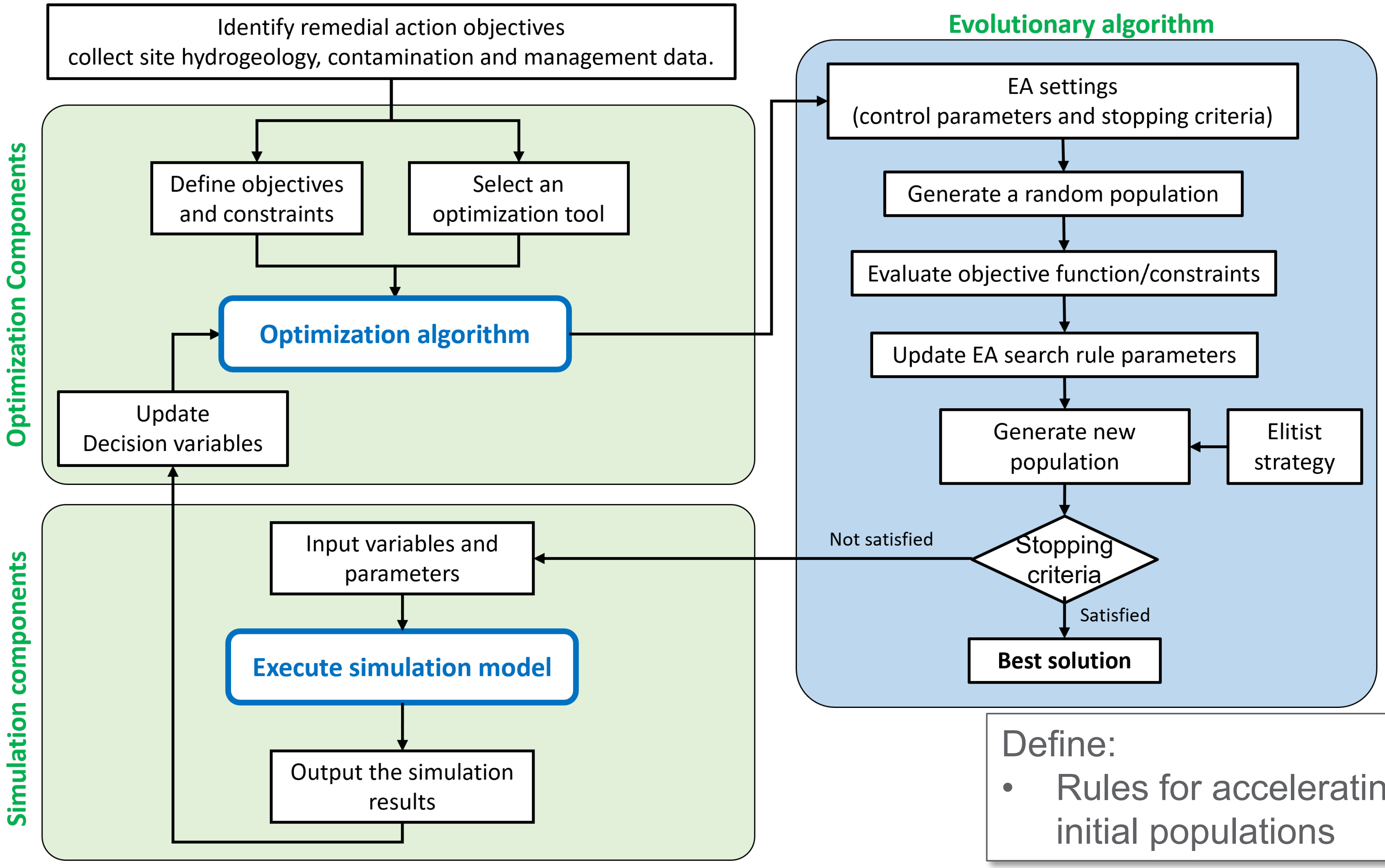
- Existing extraction and injection wells



Pre-Screening Tool Optimization Setup

Define:
- Optimization goal (e.g., mass recovery, pumping timeframe minimization, etc.)
- Constraints
  - Treatment capacity
  - Well installation rules





Define:
- Rules for accelerating initial populations

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

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

Scenario-1

Well Network Optimization
P&T Capacity (gpm)
3400

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

Scenario-2

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

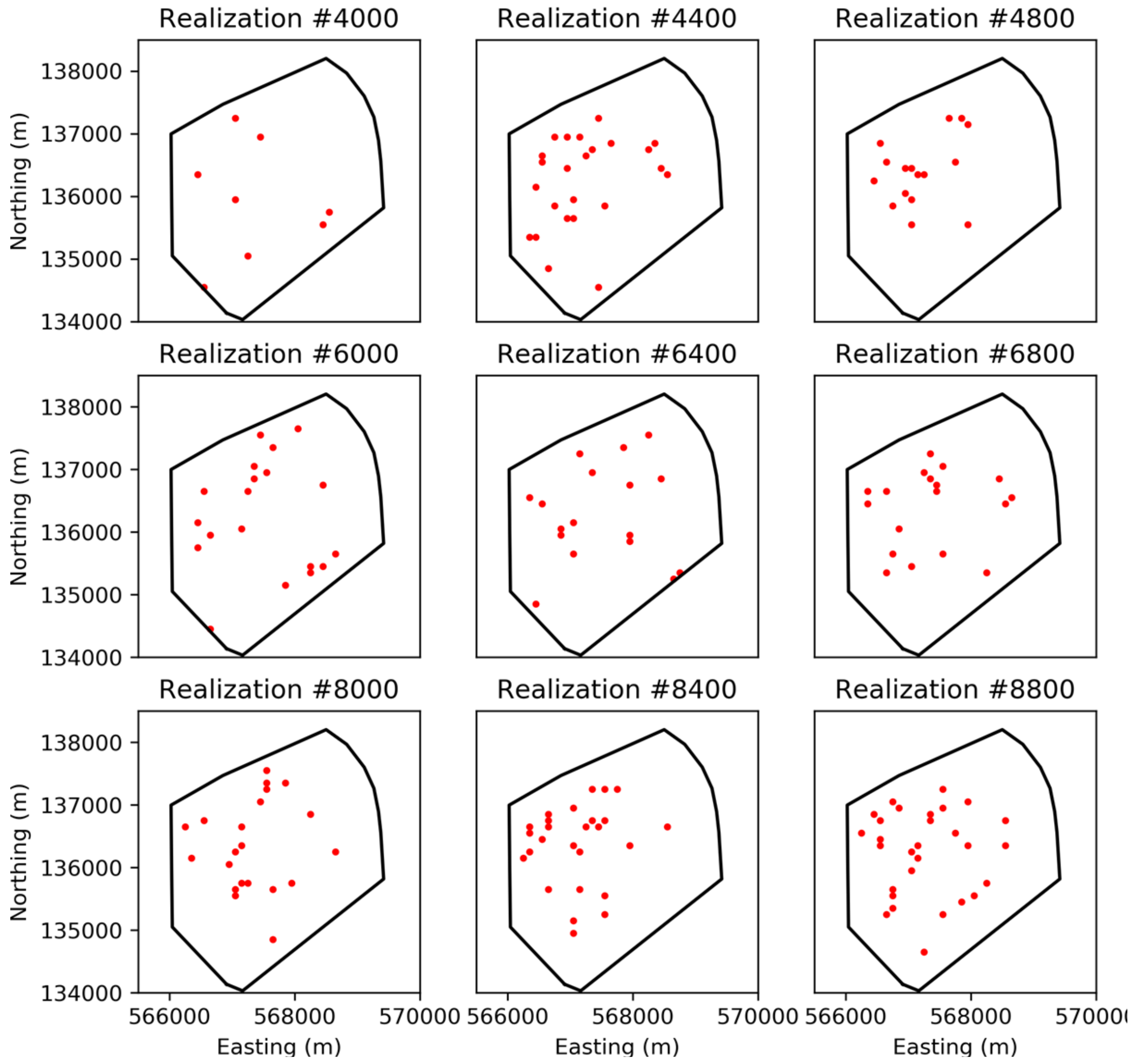
Optimization Constraints: Well Installation

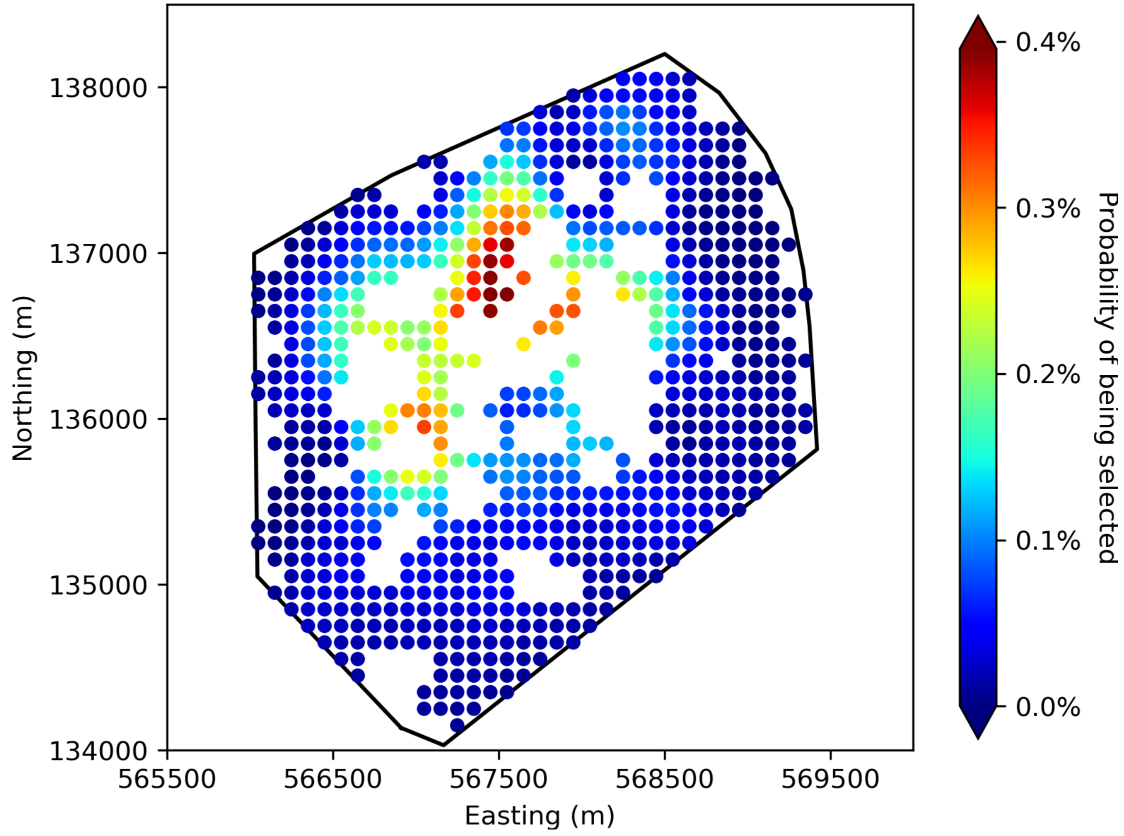
- Parameterization rules:
  - **Rule 1**: One-to-one well replacement with a maximum number of active wells (based on the total capacity of the treatment plant)
  - **Rule 2**: Each well only has one operation period
  - **Rule 3**: Each well has a fixed pumping rate
  - **Rule 4**: When a new well replaces an old well, the new well inherits the pumping rates of the old one

Example Realizations from the Evolutionary Algorithm

Optimization Setup: Well Locations

- Concentration-weighted sampling to create the initial population for the optimization simulation

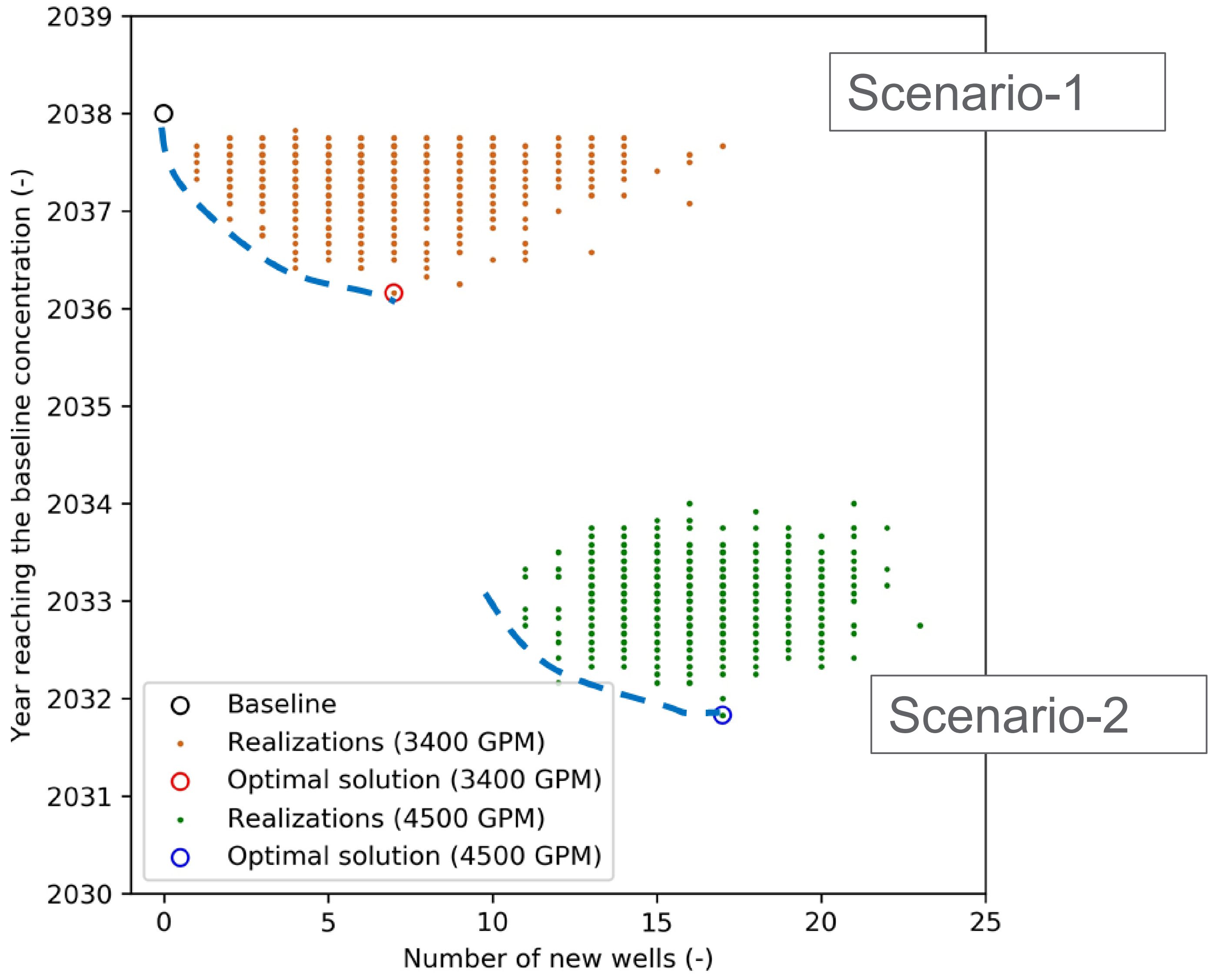




- High concentration locations are more likely to be chosen for installing new wells in initial realizations

Results for Goal #1 (Minimizing active pumping timeframe)

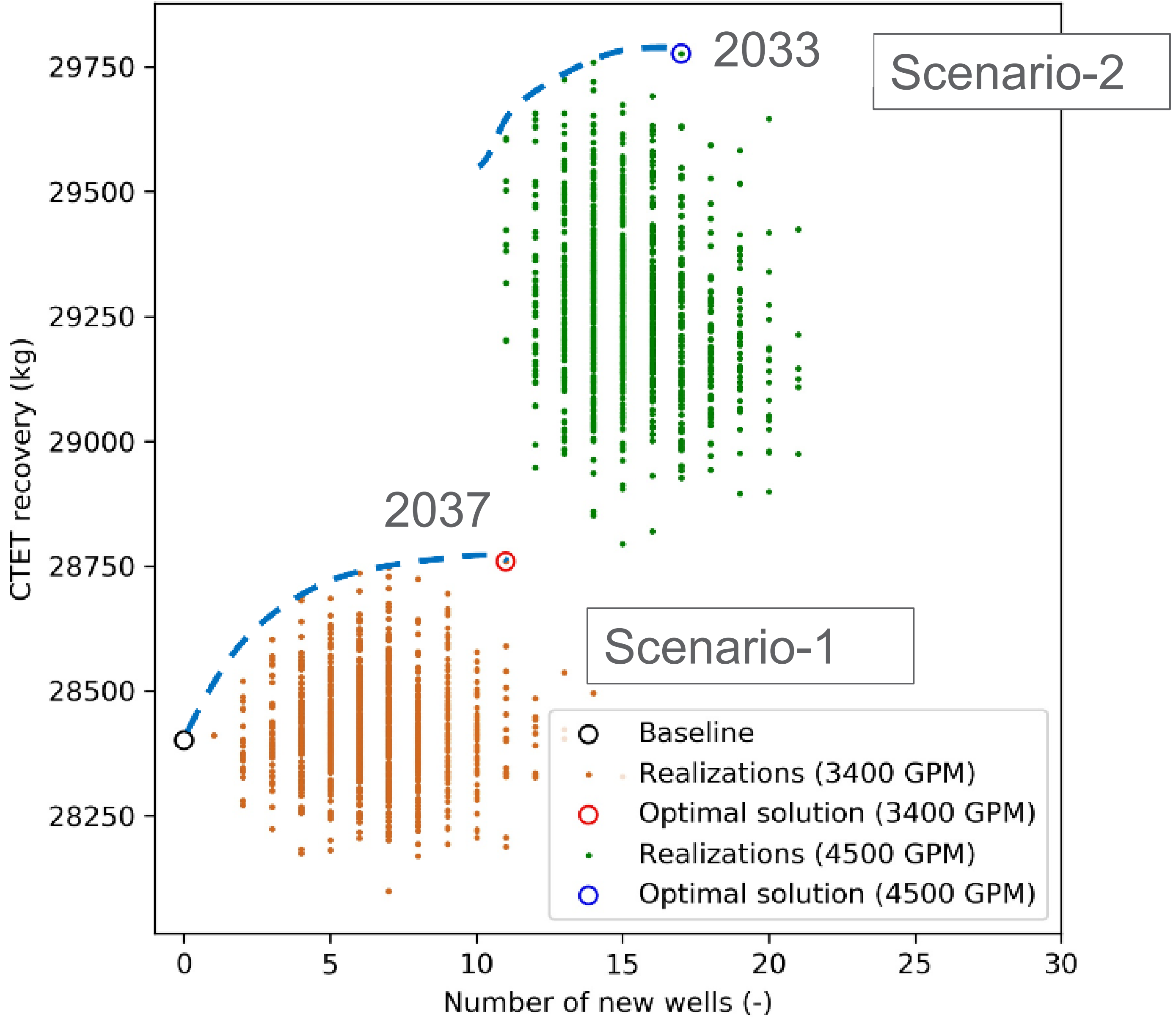
- Scenario-1 with well network optimization only (i.e., constant P&T capacity at 3400 gpm) achieves ~ 8% reductions in active remediation timeframe
  - Total of 7 new wells are added to the network
  - Achieves the same 95th percentile concentration level as the baseline with 2 fewer years of pumping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

Results for Goal #2 (Maximizing CTET 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

Scenario1: Optimal Solution at 3400 GPM

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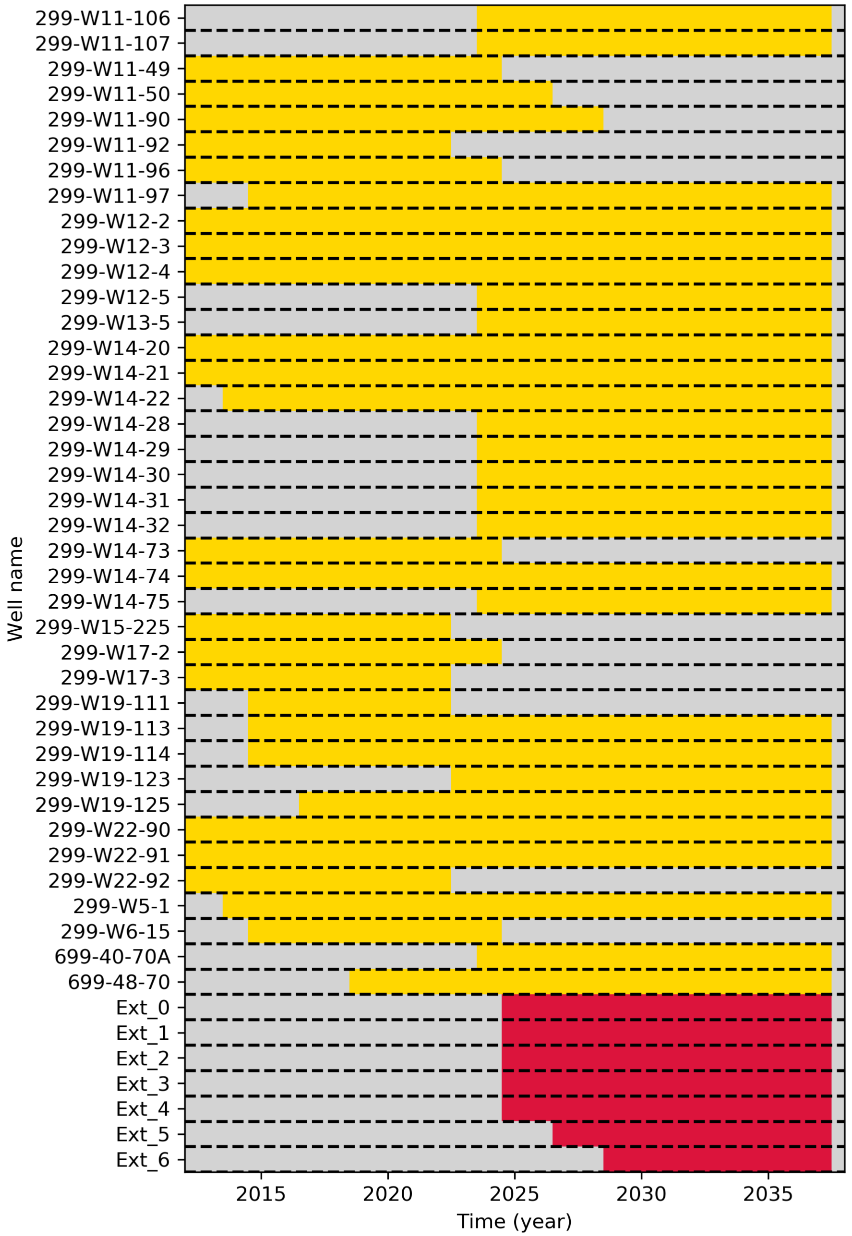
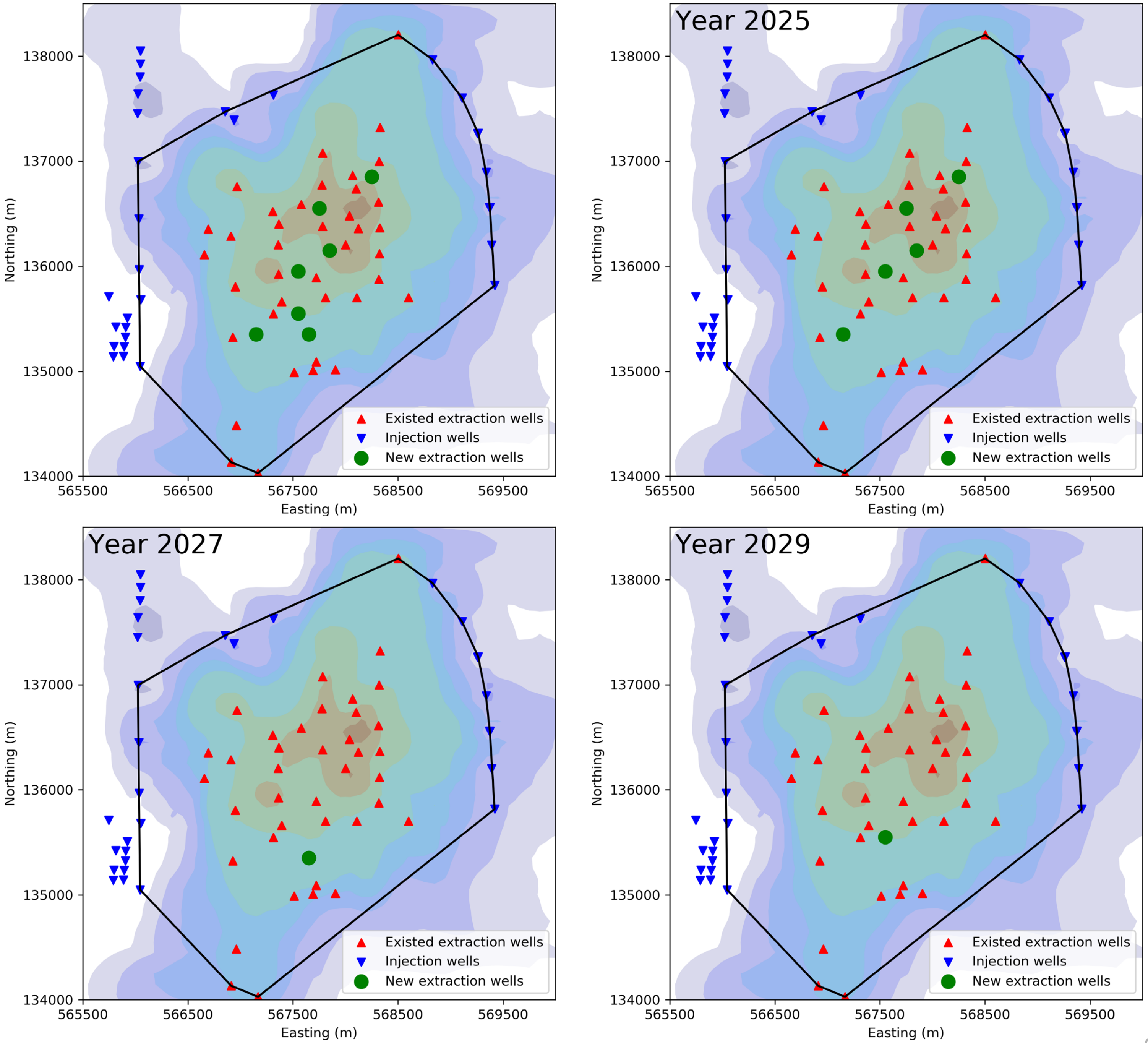
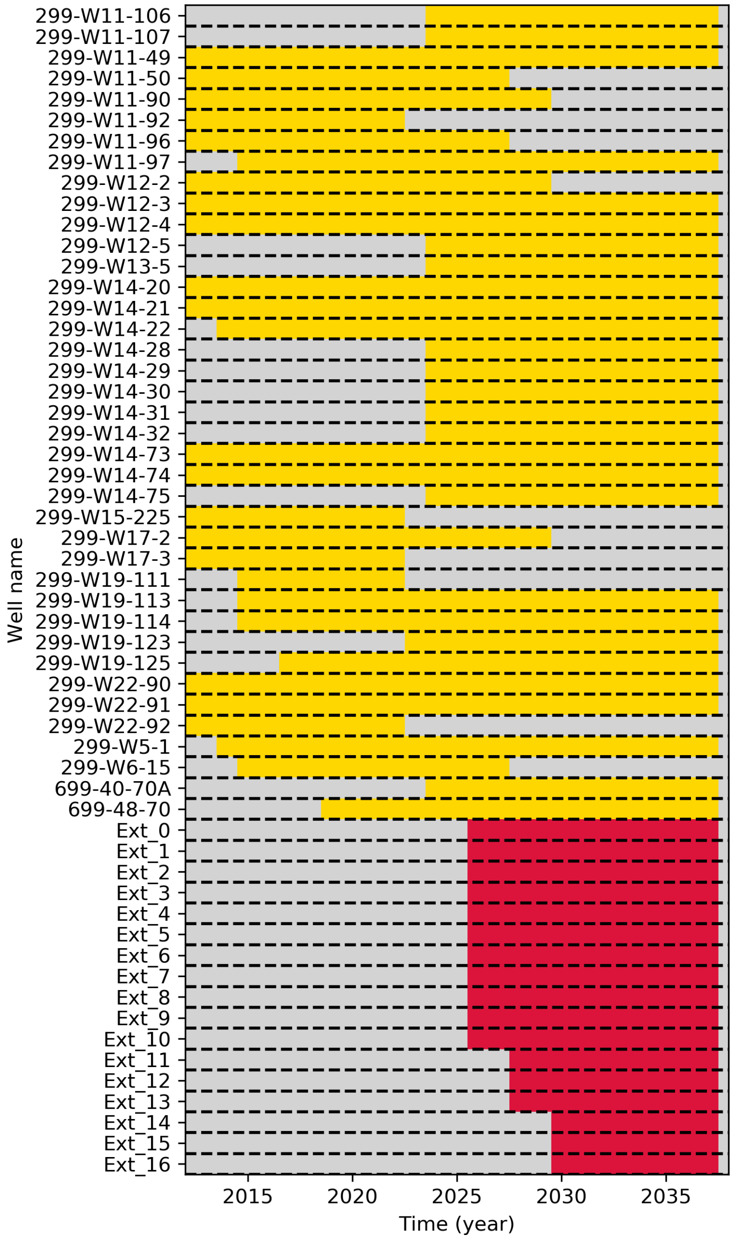
- Installation schedule and new well locations

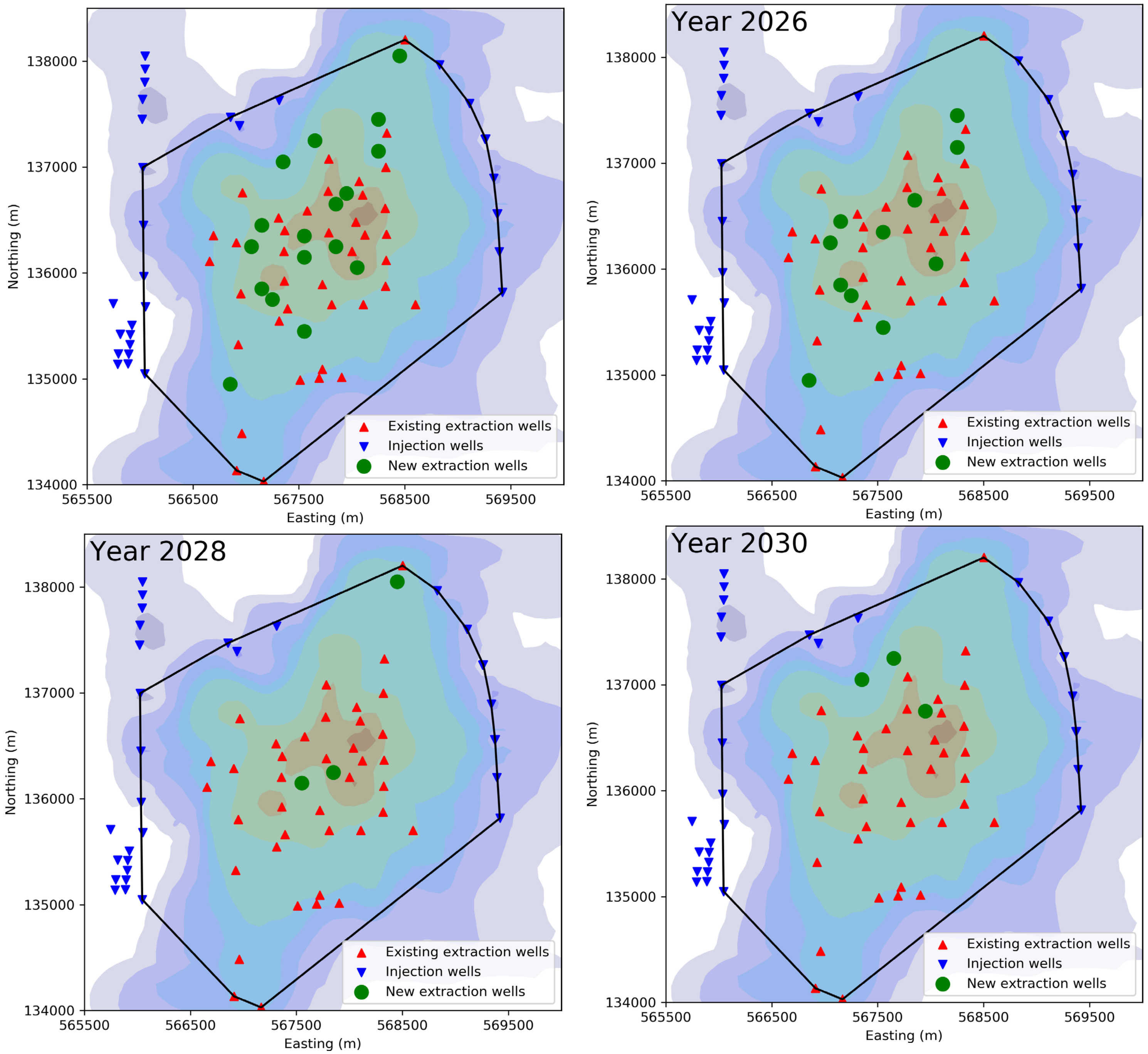




Scenario2: Optimal Solution at 4500 GPM

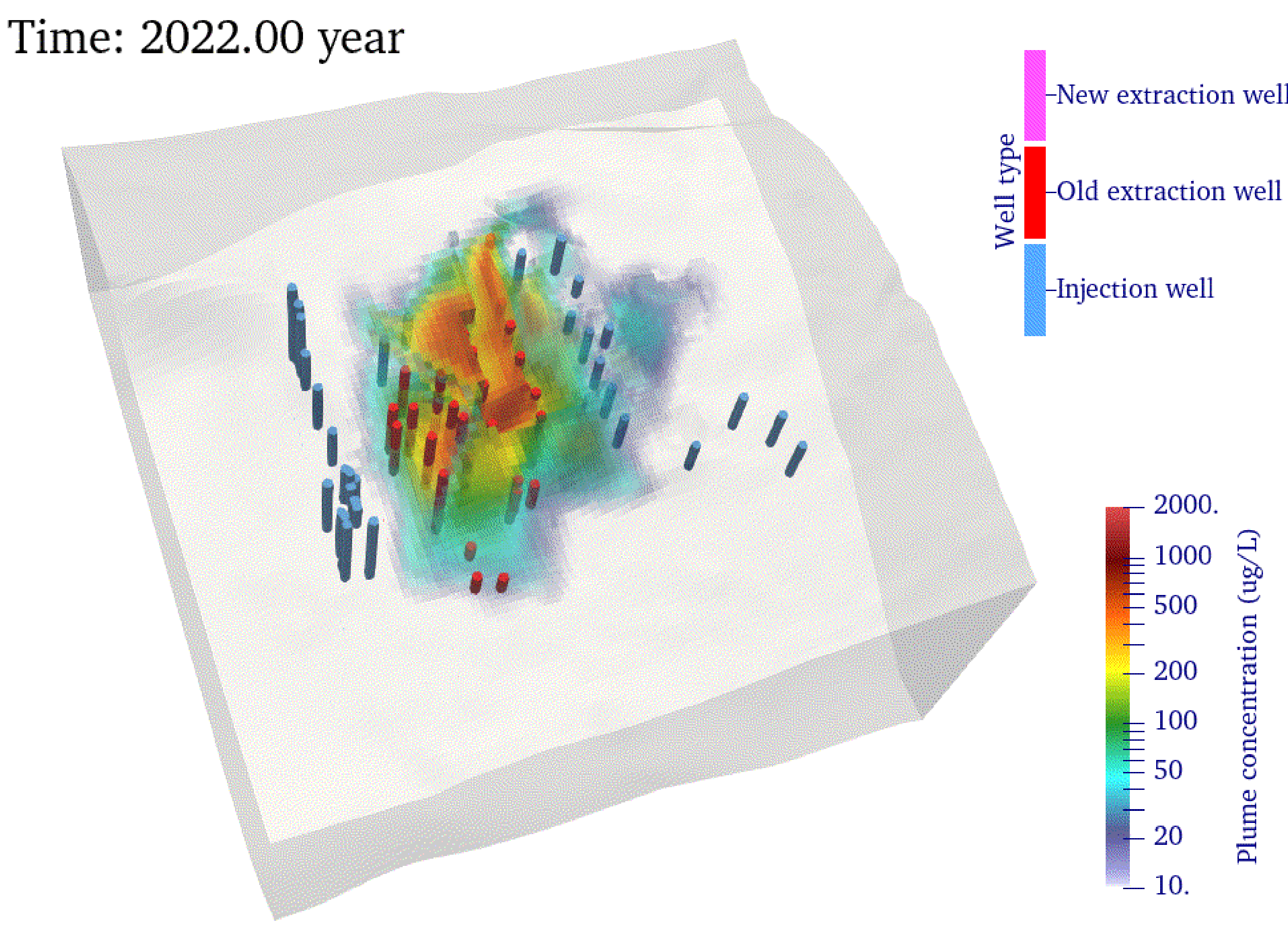
- Installation schedule and new well locations



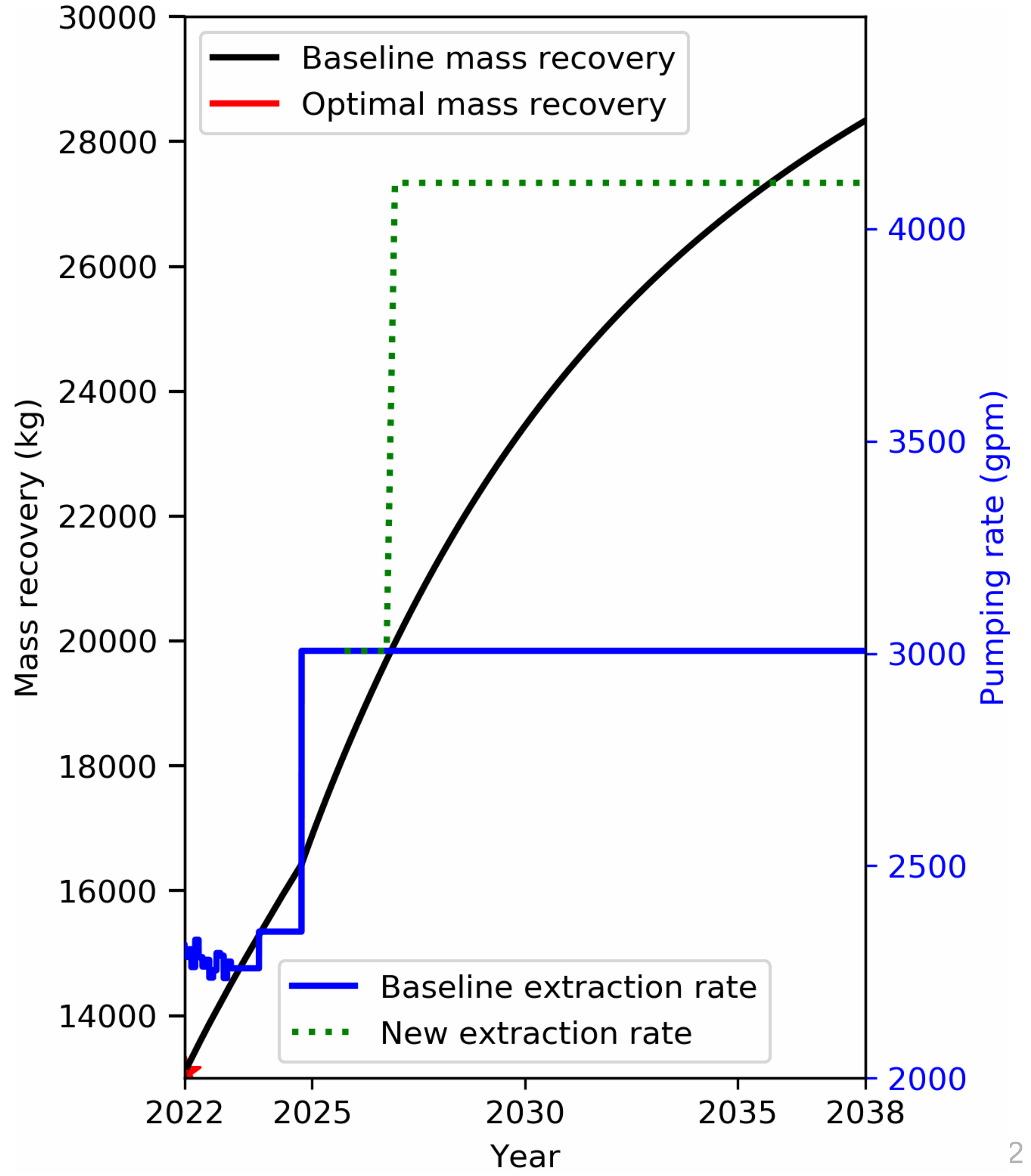


3D Animation of the Optimal Case

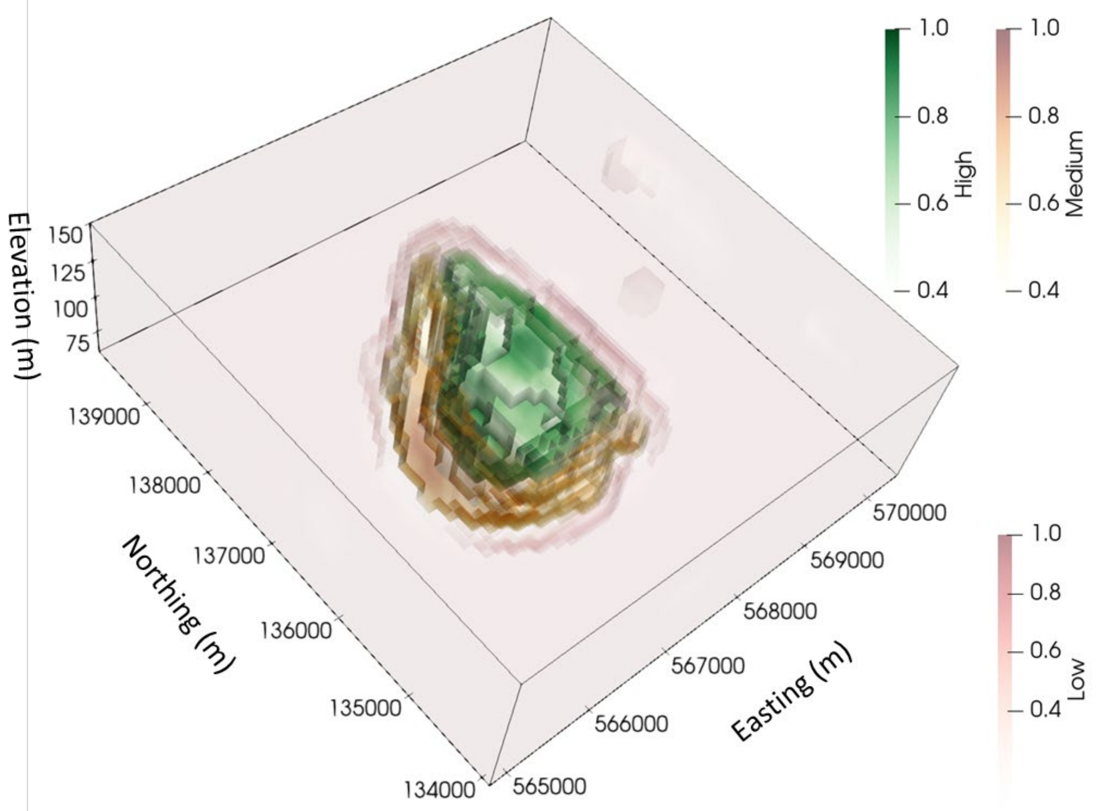
Predicted plume dynamics



Predicted mass recovery



Part 3 –
Use of Deep-Learning Approaches in the Pre-Screening Tool Framework



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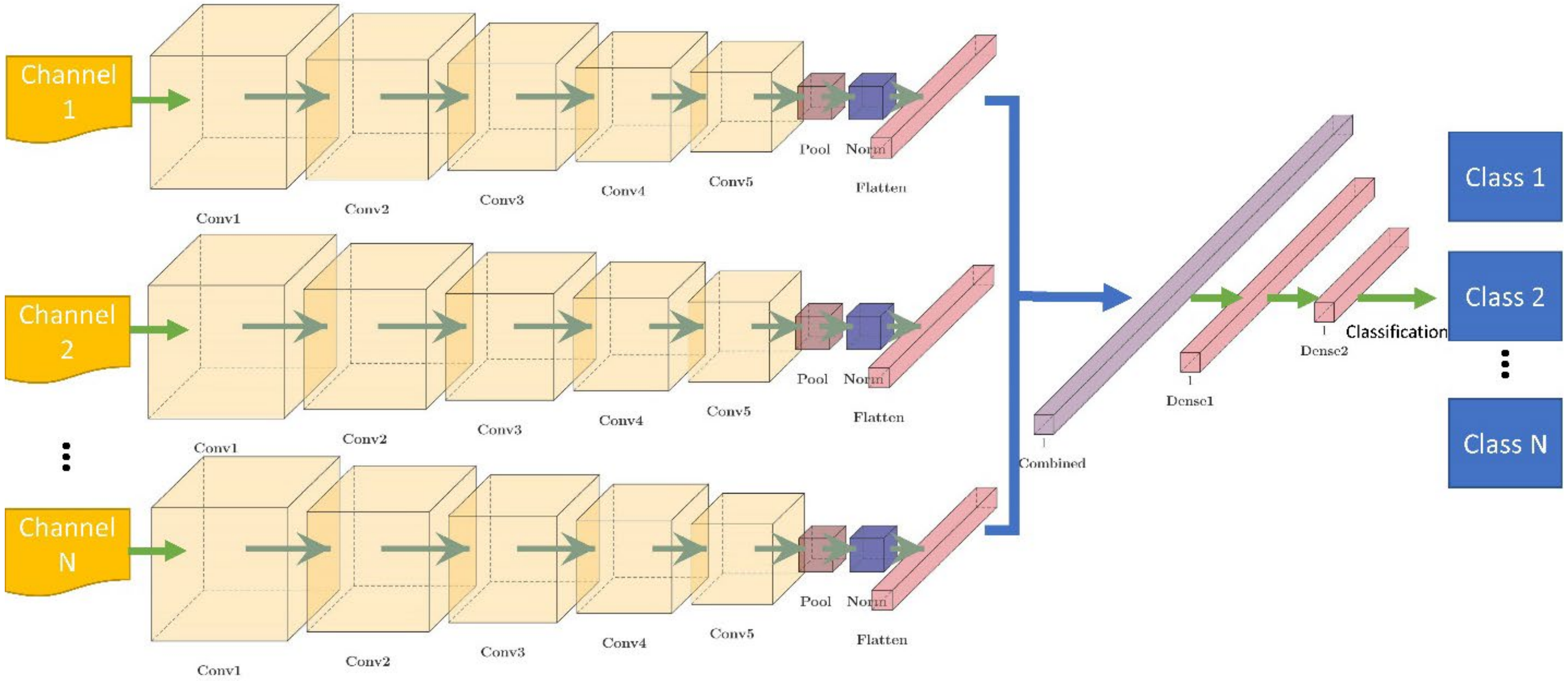
Alternative Approach: Well Location Selection

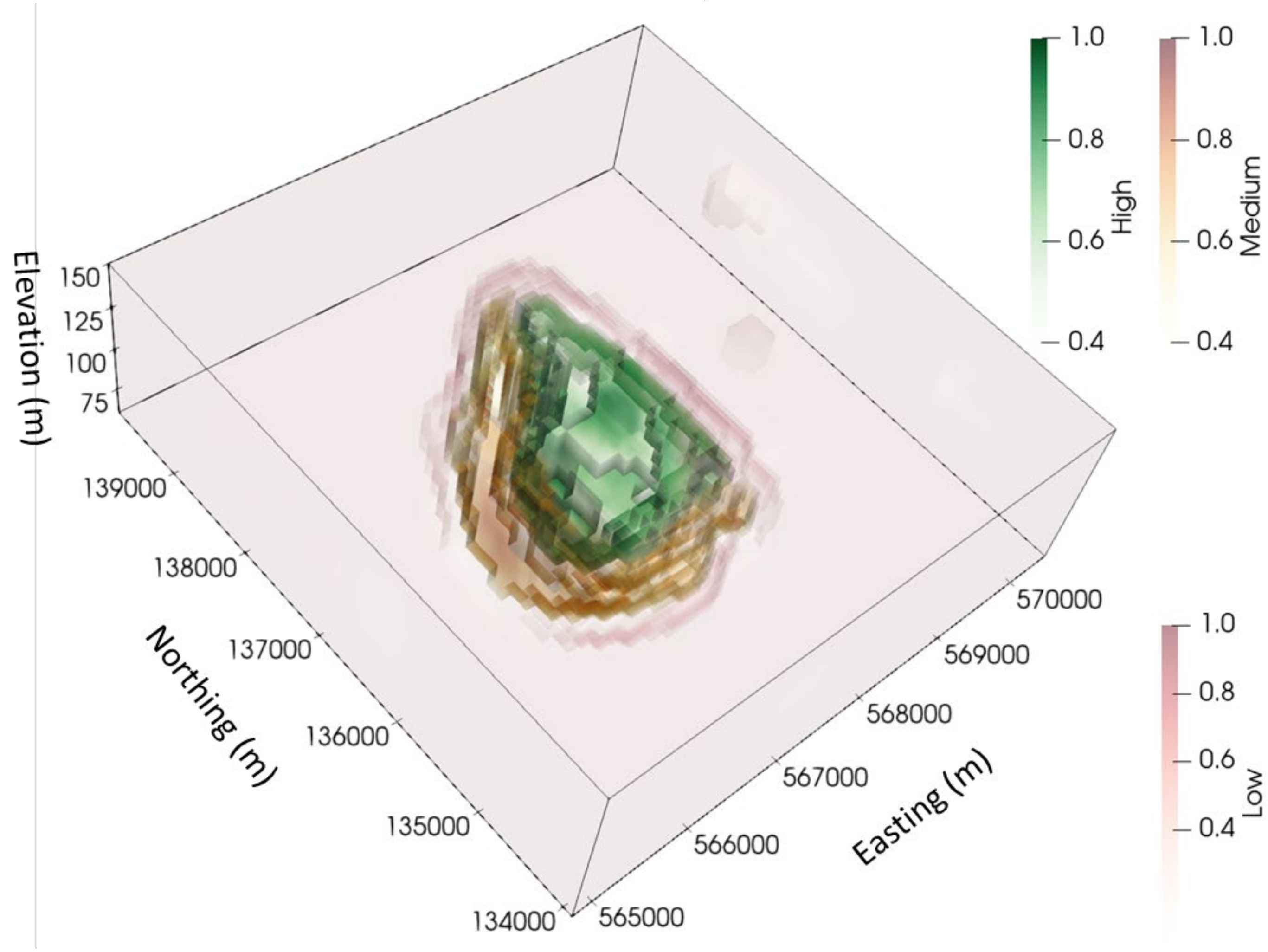
- A deep-learning model was developed for predicting extraction well performance for a given location in the model domain
  - Model relies on existing well performance data (2012-2023) and the data on site geology



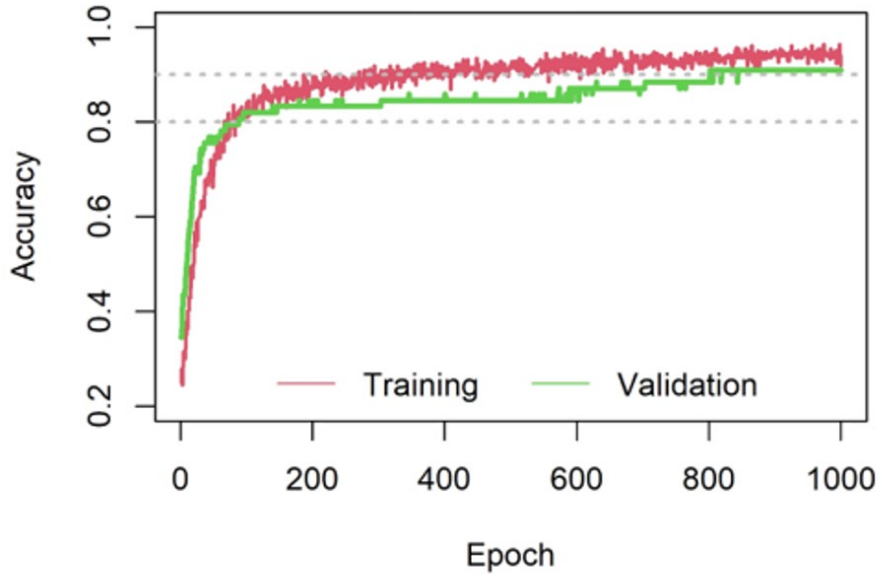
Multi-Channel Three-Dimensional Convolutional Neural Network (MC3D-CNN) framework

Deep Learning Model: A MC3D-CNN Framework for Well Performance Prediction

- The trained deep learning (DL) model was used to predict future well performance ranking on each 100×100×5 m pixel for entire model domain.

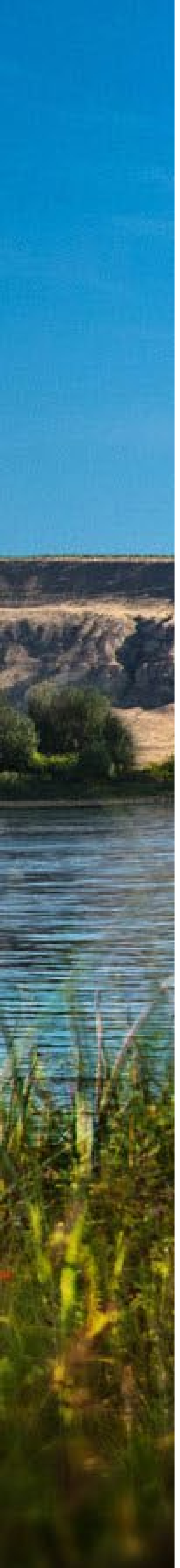


3D performance ranking map. Green, orange, and red colors indicate high, medium, and low performance rankings.



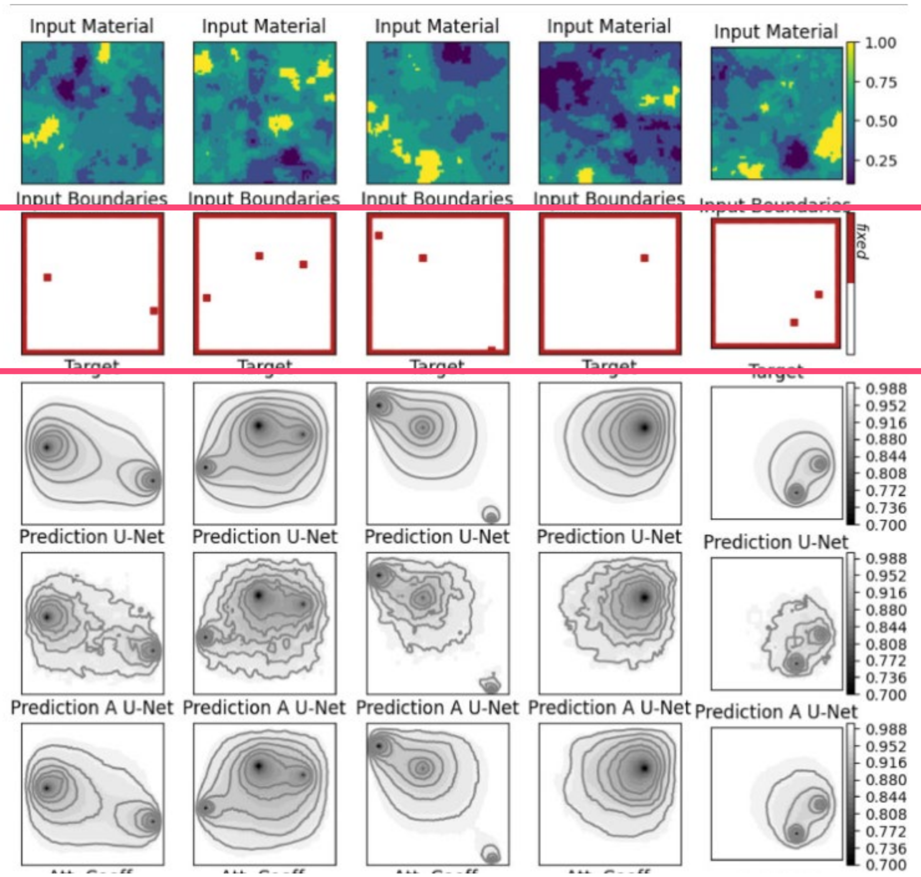
MC3D-CNN model accuracy during model training

- Application of the MC3D-CNN DL model
  - Rebalance pumping rate of existing wells
  - Reduce number of candidate well locations for P&T optimization simulation
  - Integrate into flow and transport models to provide on-the-fly optimization of pumping rate



Alternative Approach: 3-D Plume Model

- An alternative deep-learning model, U-NET application, is currently being developed to replace parts of the F&T model role in the pre-screening tool framework as surrogate model



Input #1:hydraulic conductivity

Input #2:well location

Target: Groundwater Level (GWL)

Prediction: GWL (method #1):

Prediction: GWL (method #2)

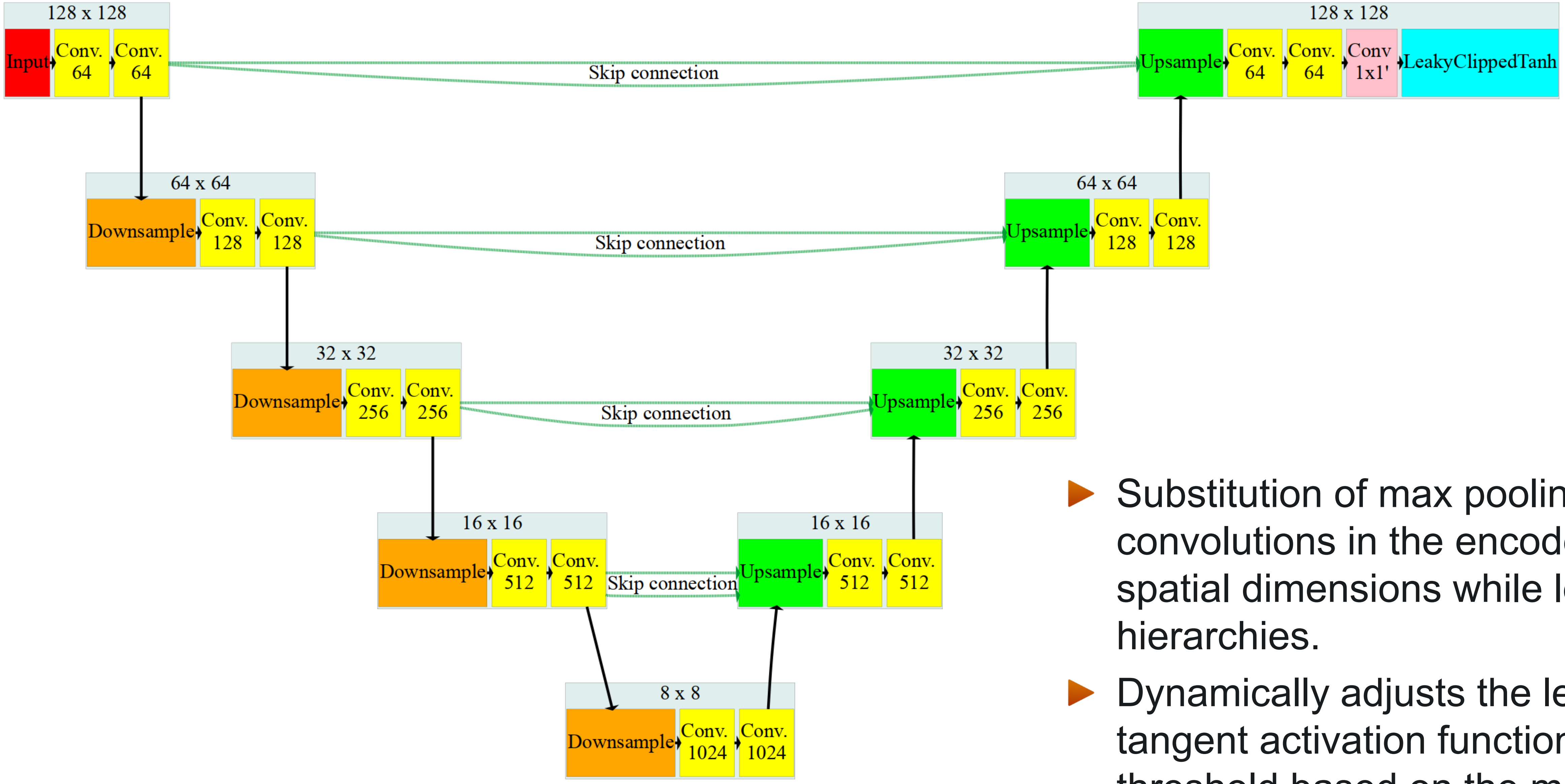
Our approach: incorporating analytical solutions as predictors in U-Net models

$$h = h_0 - \frac{Q}{2\pi T} \ln\left(\frac{r}{r_0}\right)$$

Explicit physical constraints/regularization?

Taccari, Maria Luisa, Jonathan Nuttall, Xiaohui Chen, He Wang, Bennie Minnema, and Peter K. Jimack. “Attention U-Net as a Surrogate Model for Groundwater Prediction.” *Advances in Water Resources* 163 (May 1, 2022): 104169.

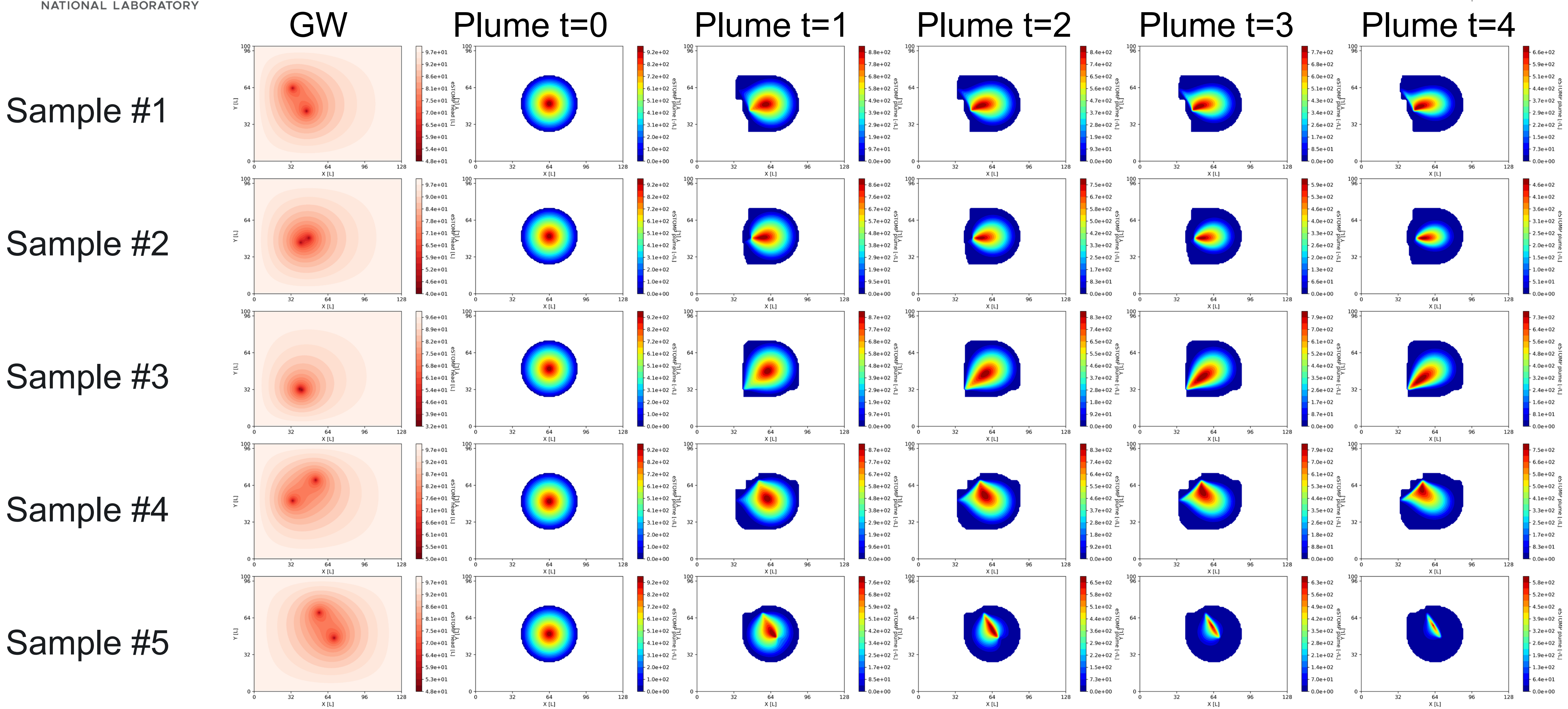
U-Net Architecture for 2-D Plume Prediction



Modified U-Net Architecture for groundwater plume prediction

- Substitution of max pooling with strided convolutions in the encoder blocks to reduce spatial dimensions while learning spatial hierarchies.
- Dynamically adjusts the leaky hyperbolic tangent activation function's clipping threshold based on the maximum concentration.

U-Net Architecture for 2-D Plume Prediction

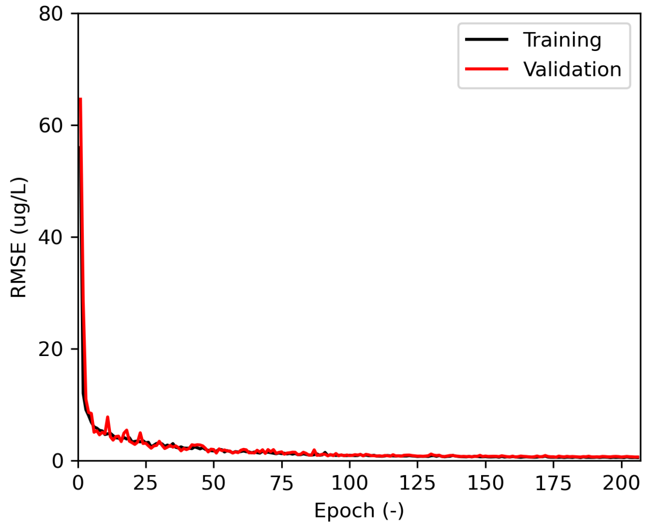


Samples of training data images

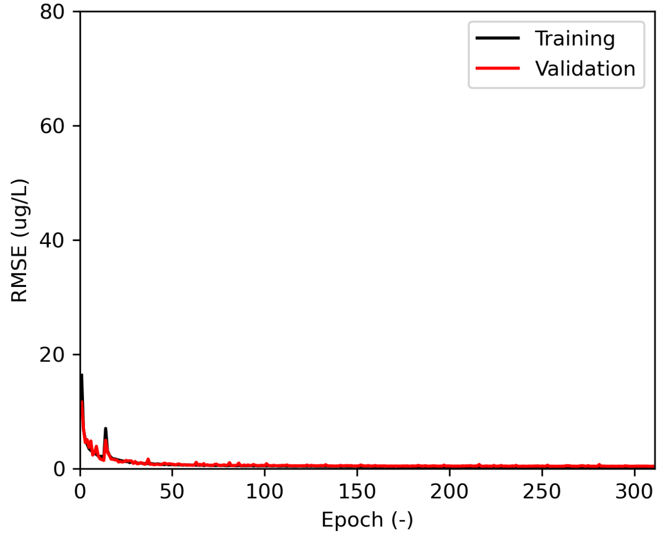
- Case #1: Input - Groundwater level; Output - Predicted plume state at t=4.
- Case #2: Input - Groundwater level and plume data at t=n-1; Output - Plume state at t=n.

2-D Mode Training and Testing Results

Model training results

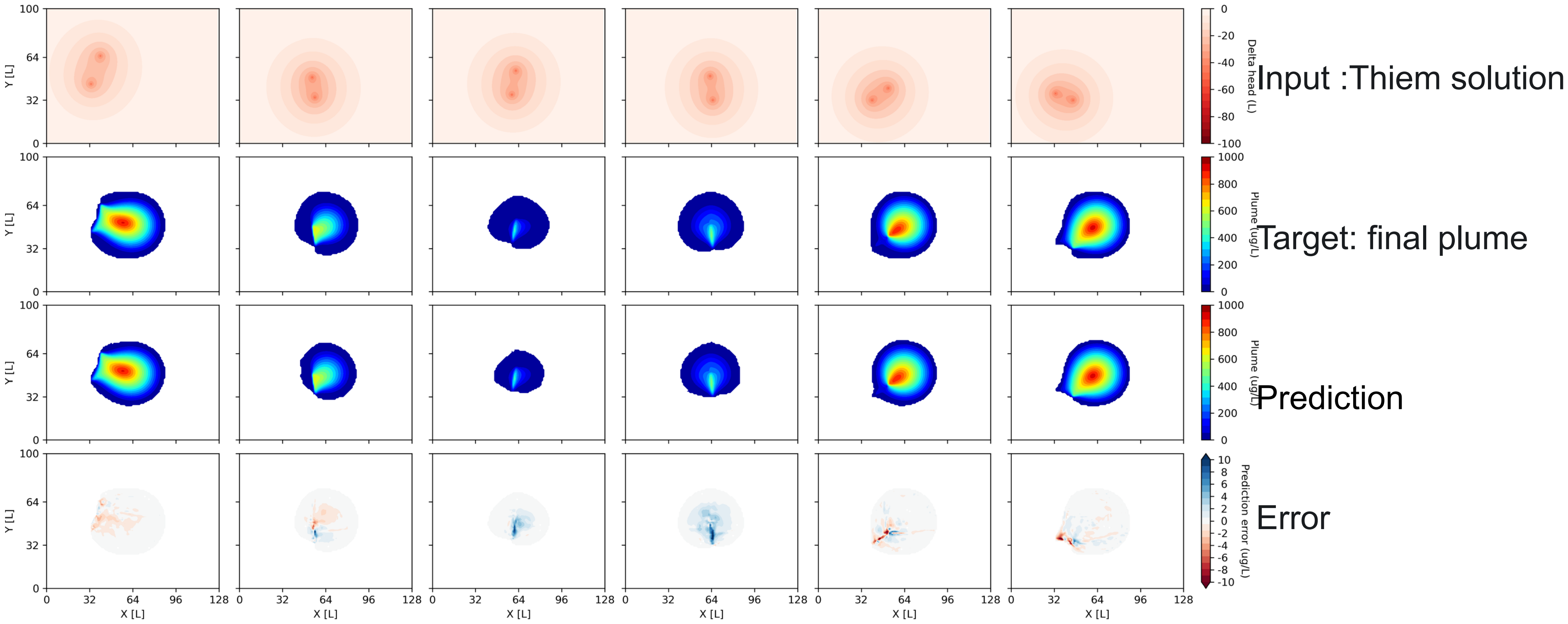


Model training results of case #1 (RMSE 0.62)



Model training results of case #2 (0.41)

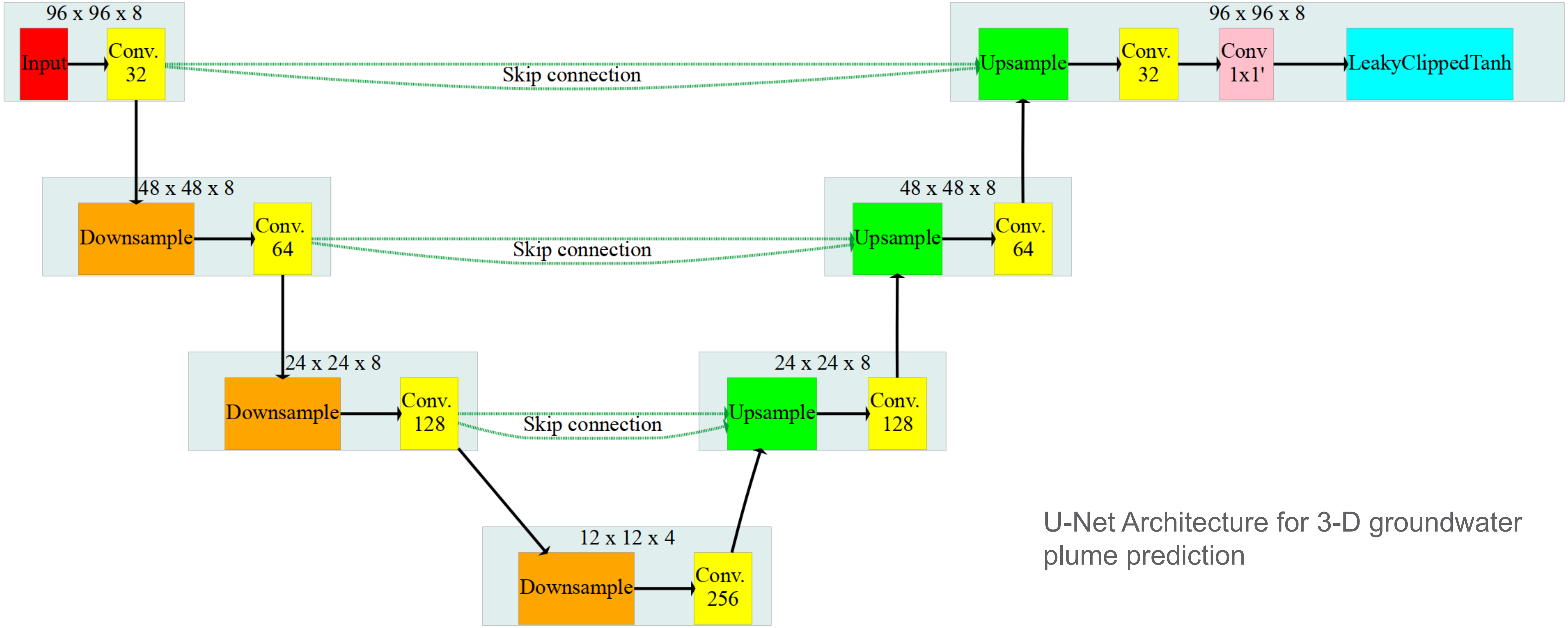
Model predictions



Case #1 testing RMSE: 0.78; Case #2 testing RMSE: 0.44

- Training data size: 7000; validation data: 1500; testing data: 1500.
- Both cases exhibit strong performance.
- As expected, case #2 begins with a smaller initial training and validation error and ends with a lower final error.

U-Net Architecture for 3-D Plume Prediction

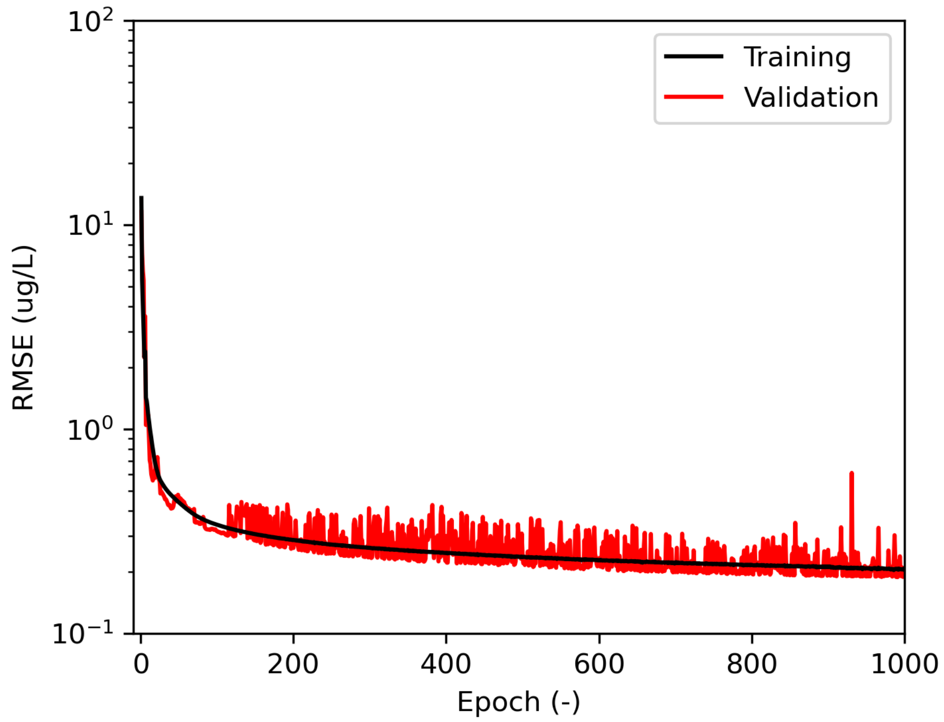


U-Net Architecture for 3-D groundwater plume prediction

- Reduced number of convolutional layers
  - Enhanced memory efficiency by cutting parameters from ~32M down to ~1.7M
- Switch to plume change predictions

3-D Model Training and Testing Results

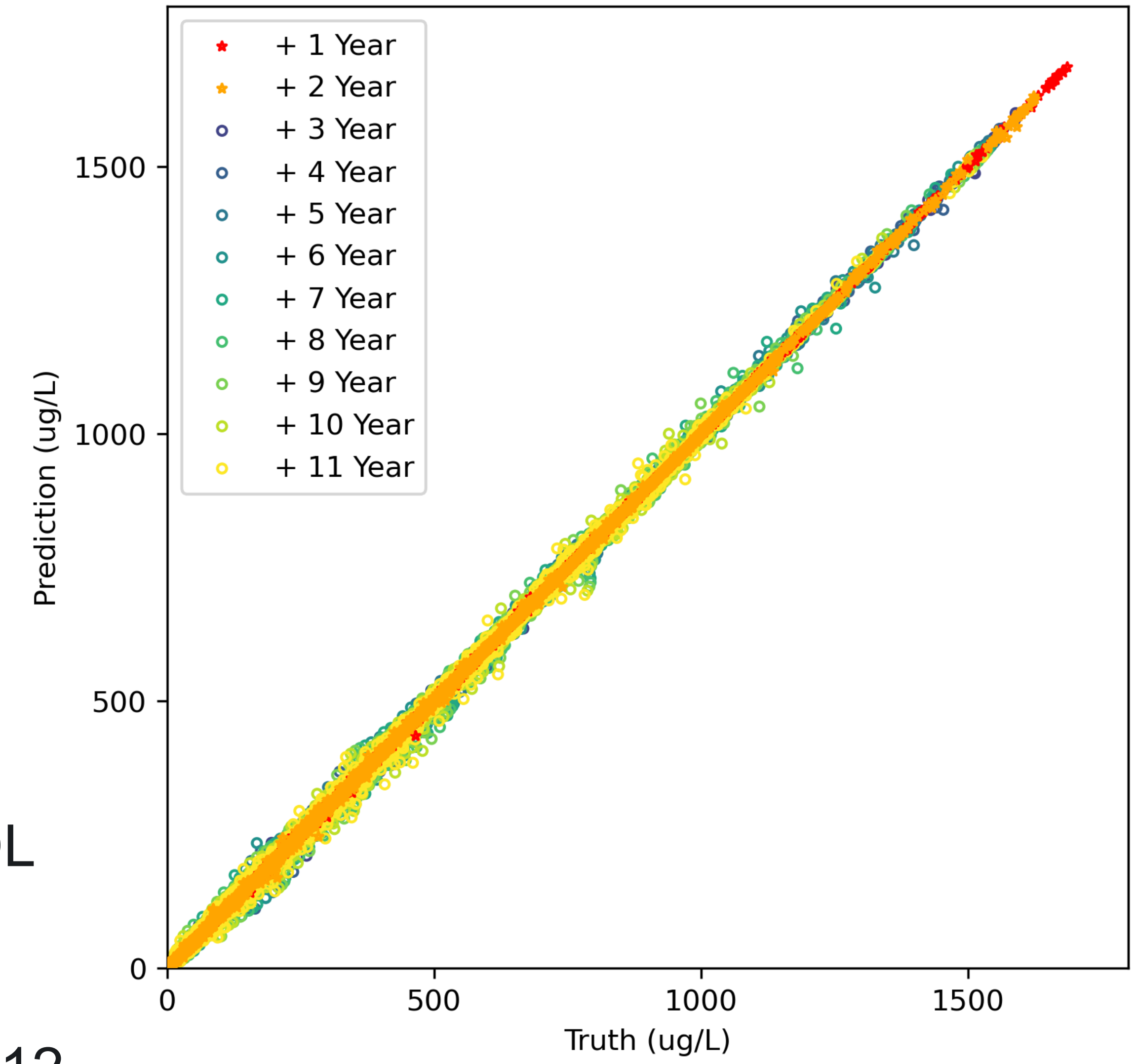
- Model training results



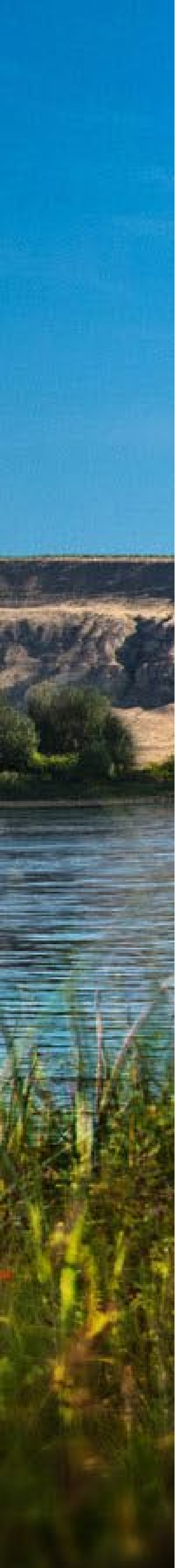
Model training results (0.19 μg/L)

- After hyperparameter tuning, the best-trained DL model achieved 0.19 μg/L testing accuracy (the clean-up level is 3.4 μg/L).
- The prediction error increased to 1.8 μg/L after 12 years of forecasting.

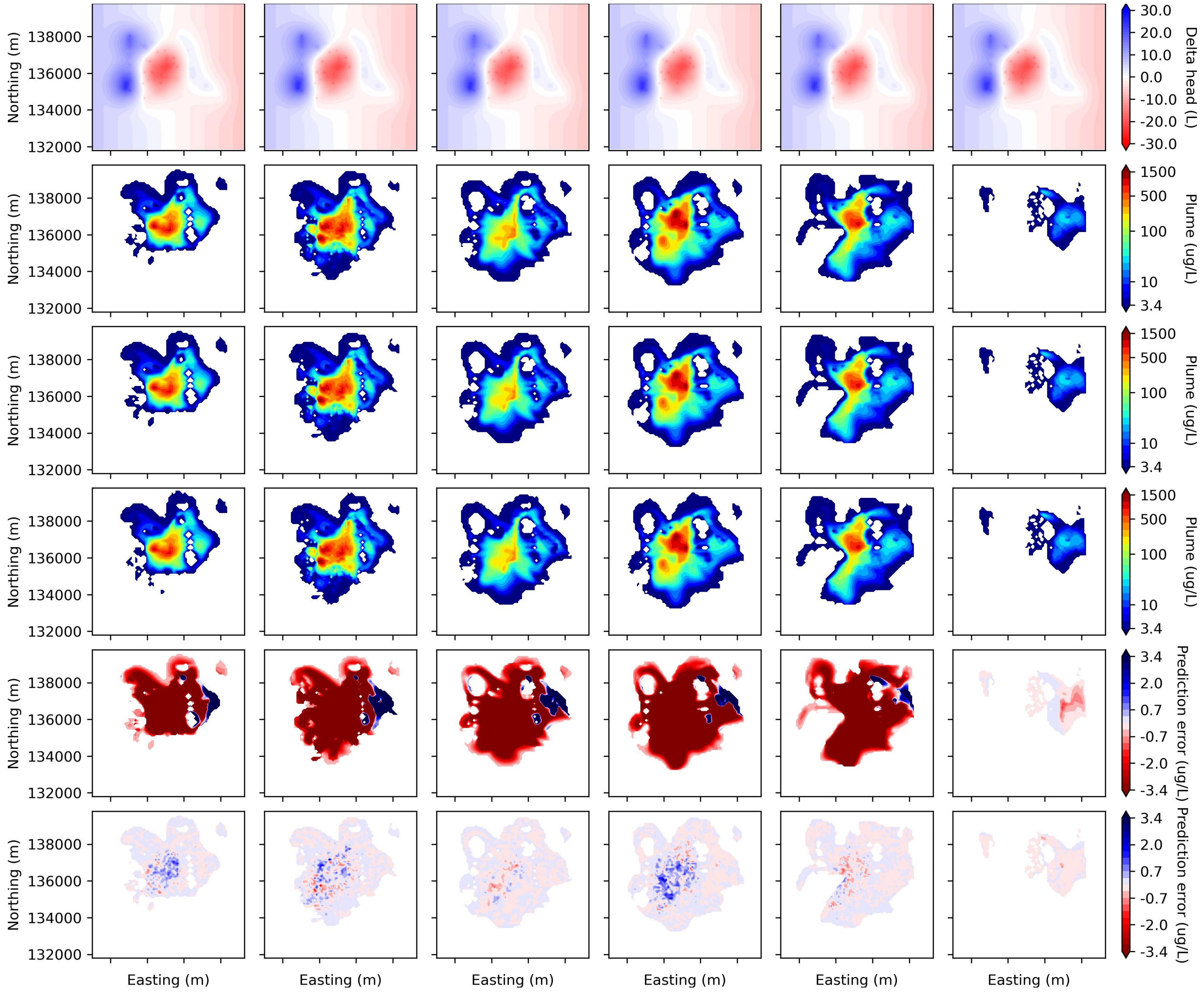
- Model predictions



One-to-one comparison in multi-year forecasting



Model Predictions: Example #1



Input #1:thiem solution

Input #2:plume at year N

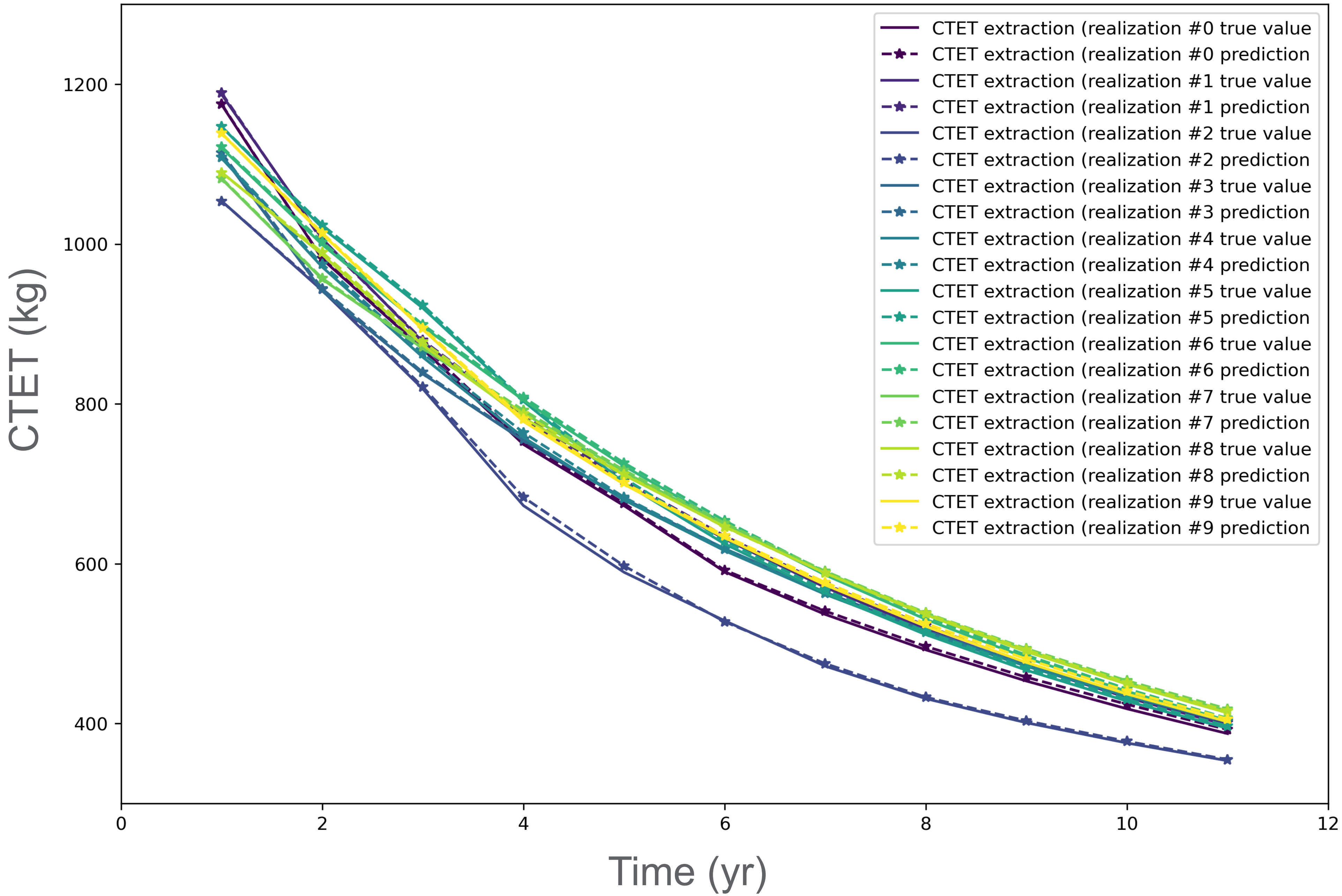
Target: plume at year N+1

Prediction: plume at year N+1

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

Prediction error (row 4-row2)

Multi-year Mass Recovery Prediction from the U-Net Surrogate Model



Conclusions

- P&T optimization pre-screening tool
  - Readily allows evaluation of system behavior for multiple scenarios
  - Leads to proposed active management strategies to achieve the defined optimization goals
- Formal optimization of a P&T well network was demonstrated
  - Well network size, well locations, and pumping operational strategy to meet optimization goals
  - Can include treatment capacity considerations
  - Results show potentially to reduce cleanup timeframe and increase mass recovery
- Optimal outcomes vary with optimization objectives and constraints
  - Maximum mass recovery selected as the optimization goal may not provide the shortest cleanup timeframe
- Deep-learning approaches can significantly improve computational application of the framework

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Questions?