Leveraging Data-Driven Approaches for Optimizing Pump-and-Treat Well Network Operations

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2023 RemPlex Global Summit

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Pump-and-Treat (P&T) Systems

- P&T remedies represent about 20% of the groundwater remedies under the Superfund program

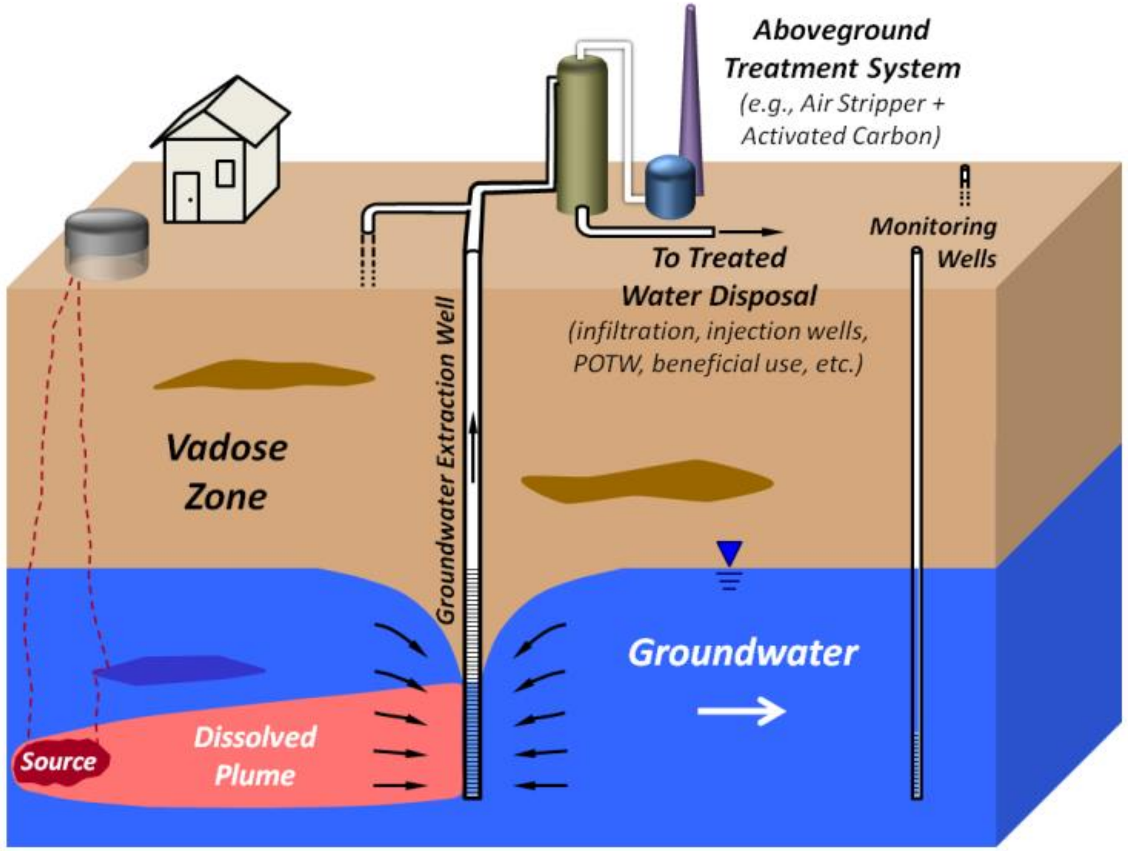


Diagram depicting a general pump-and-treat scenario
(*PNNL-24696*)

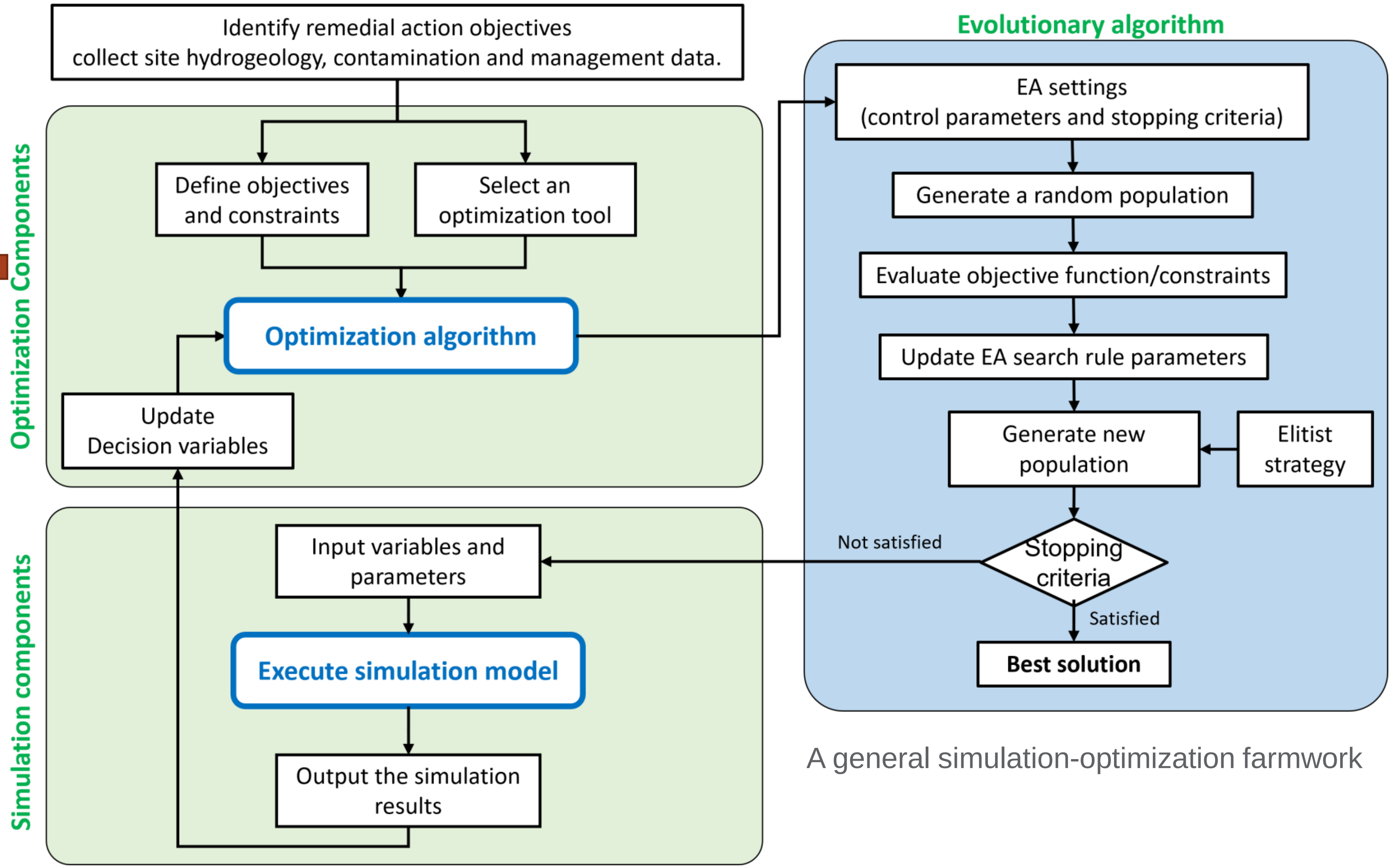
U.S. DOE Hanford 200 West Groundwater Pump-and-Treat Facility
(*https://www.usa.skanska.com/what-we-deliver/projects/57299/*)

- Initial designs typically address large-scale containment and bulk treatment, and may not be an optimal design for mass removal and long-term effectiveness
- Performance-based optimization can maintain the effectiveness and efficiency of these remedies

Directly Appling Formal Simulation-Optimization Framework to Complex Sites is Challenging

Complex interactions between optimization constraints, objectives, and site conditions

Extensive compute time for simulating complex sites



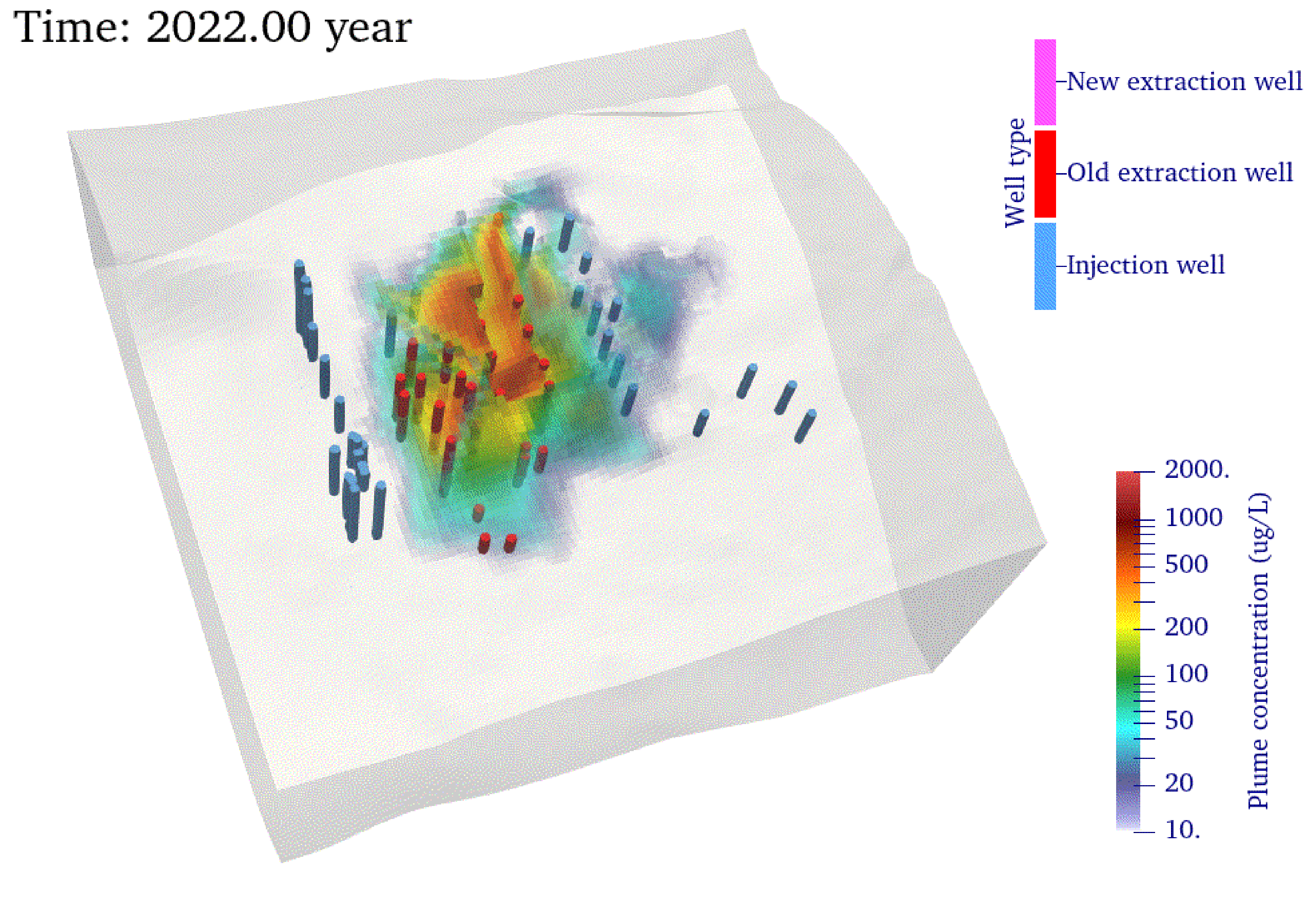
A general simulation-optimization farmwork

Tens of thousands of model runs to find optimal solution

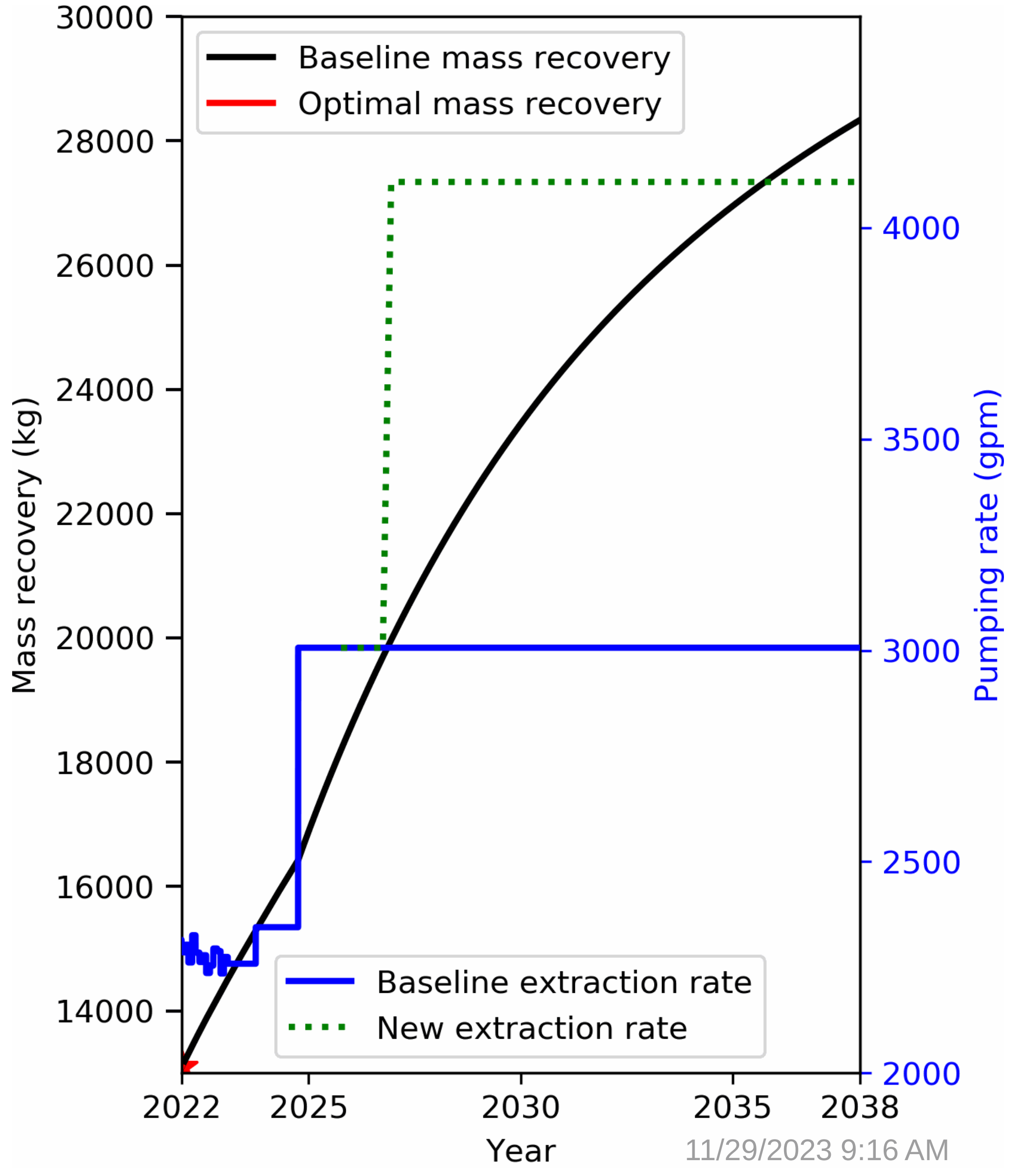
- Effective optimization requires a well-crafted problem design, a rapid optimizer, and a swift flow and transport model

Example of Optimized P&T Well installation Plan

- Predicted plume dynamics



- Predicted mass recovery



Example of optimized modeling results for the Central Plateau area at Hanford

U-Net: A Popular Framework for Image-to-image Translation Tasks

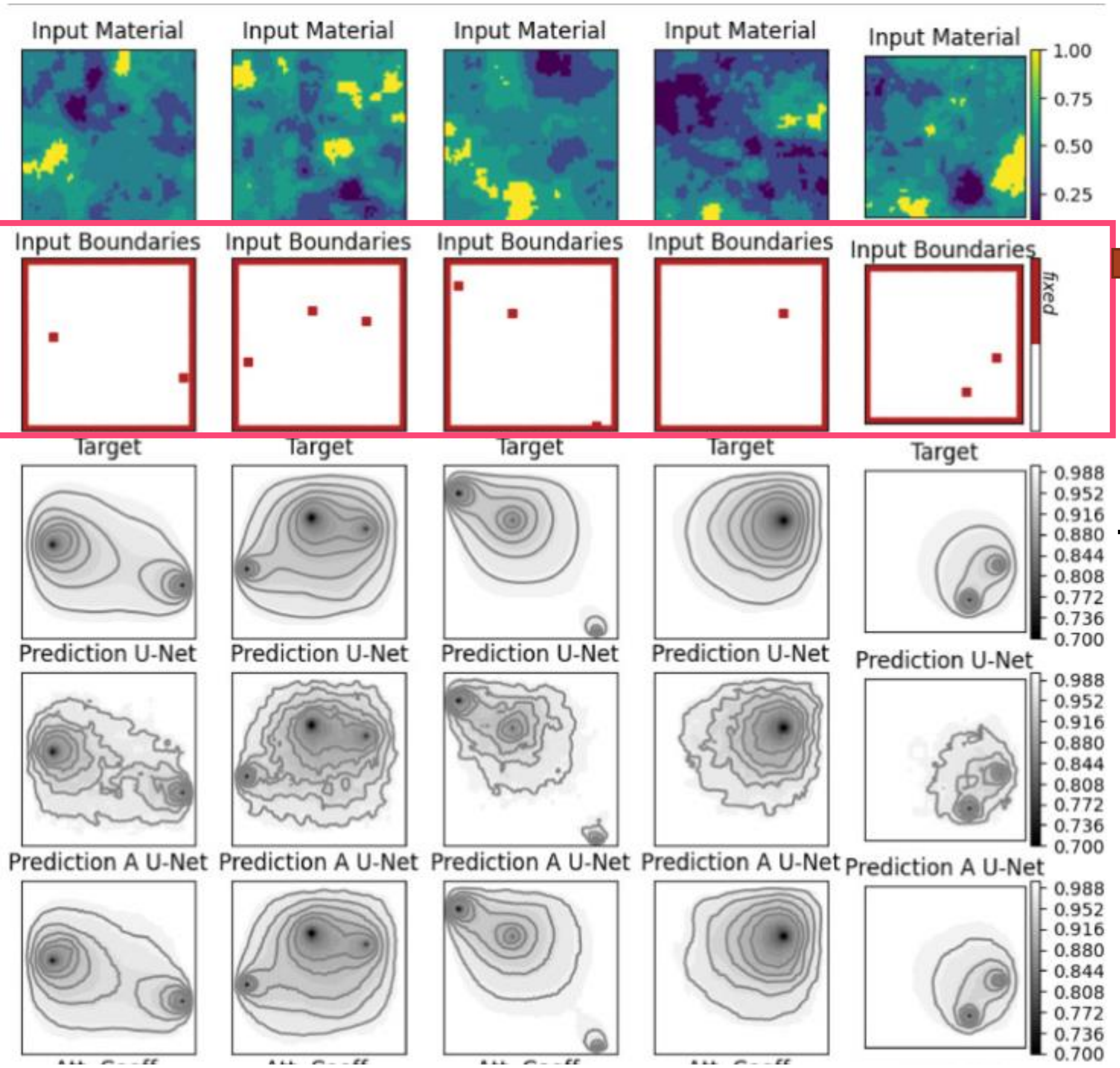
- U-Net originated in biomedical segmentation (Ronneberger et al., 2015); subsequently leveraged in earth science as a powerful autoregression tool
  - Turbulence modeling: Fonda et al. (2019), Wang et al. (2019).
  - Subsurface fluid dynamics: Santos et al.(2020), Tang et al. (2020), Sun (2020), Wen et al. (2022).
  - Meteorological data downscaling: Sha et al. (2020).
  - Extended use in land cover classification, hydrometeorology, and many others

- The bulk of these studies remain within the realm of academic research; field applications of subsurface-related studies have yet to be reported, especially for P&T systems.

- Challenges in applying U-Net to P&T systems:
  - Adaptability: Changing well positions affects system dynamics, challenging model reusability.
  - Complexity: Modeling solute transport is inherently more complex than groundwater level prediction.

U-Net: A Popular Framework for Image-to-image Translation Tasks

- A typical U-Net application in subsurface surrogate model



Input #1:hydraulic conductivity

Input #2:well location

Target: Groundwater Level (GWL)

Prediction: GWL (method #1):

Prediction: GWL (method #2)

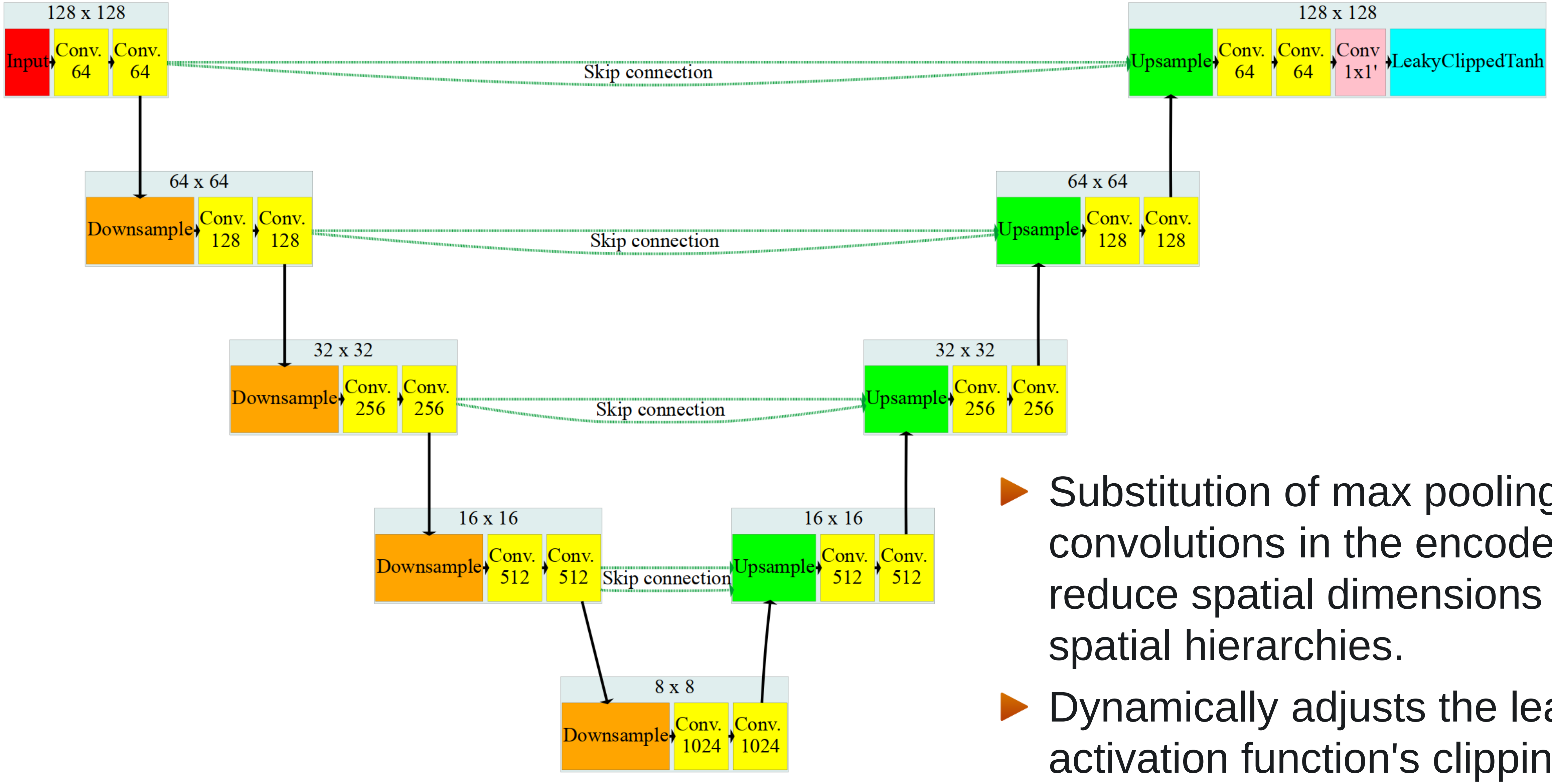
Our approach: incorporating analytical solutions as predictors in U-Net models

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

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.

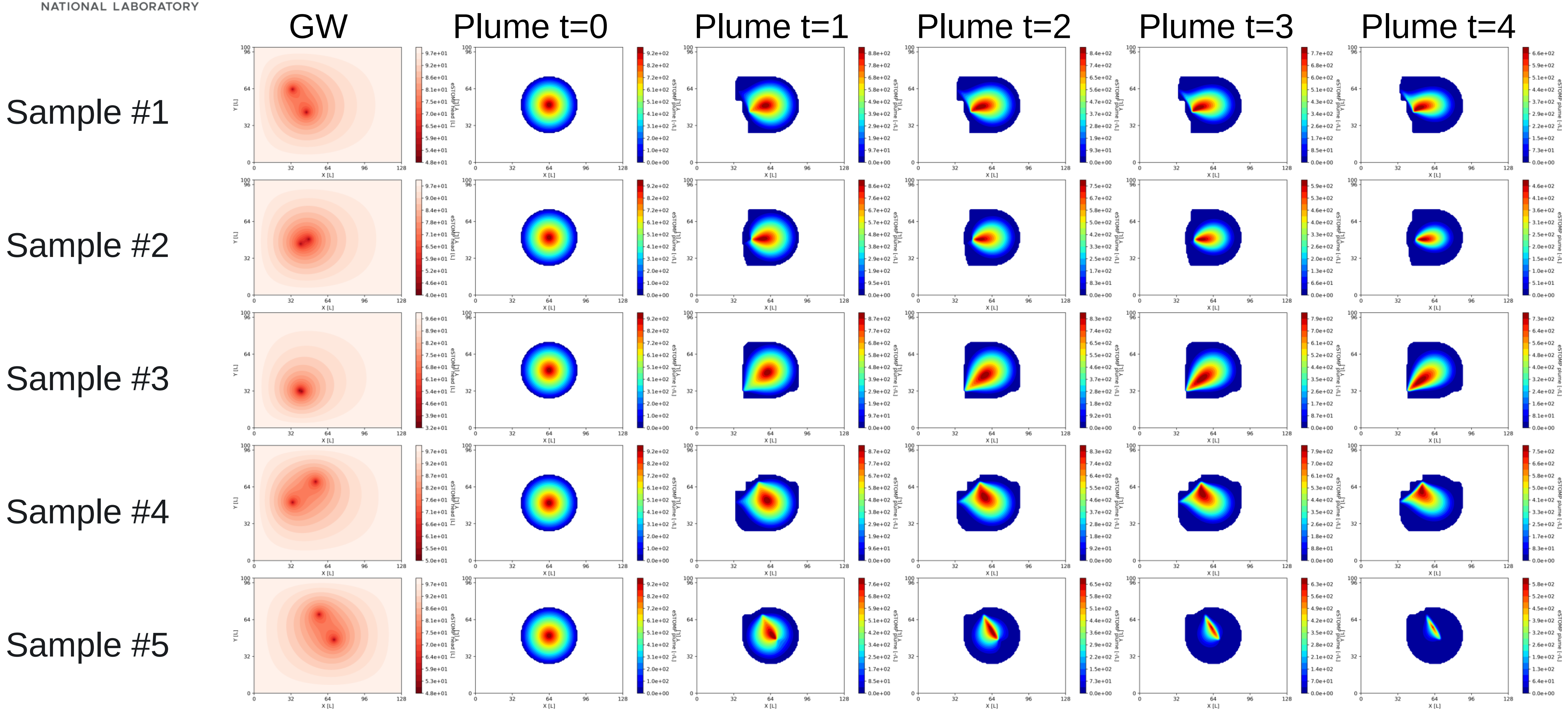
U-Net Architecture for 2-D Plume Prediction



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 tanh activation function's clipping threshold based on the maximum concentration.

U-Net Architecture for 2-D Plume Prediction

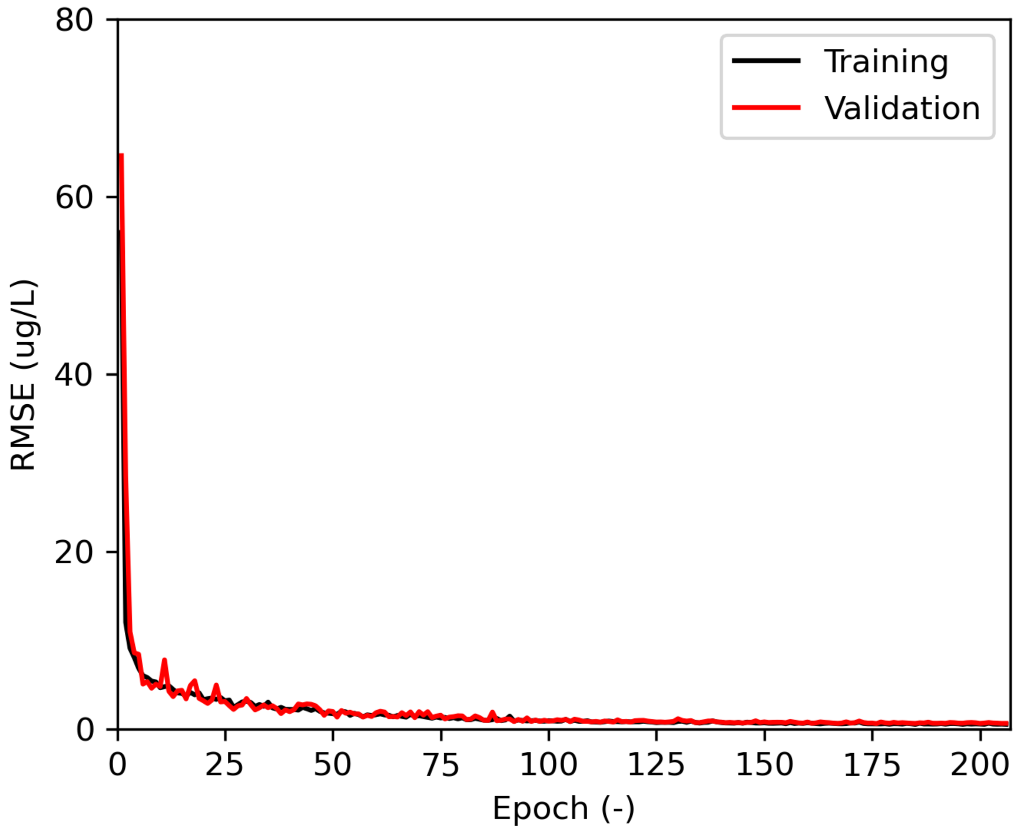


Samples of training data images

- 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.

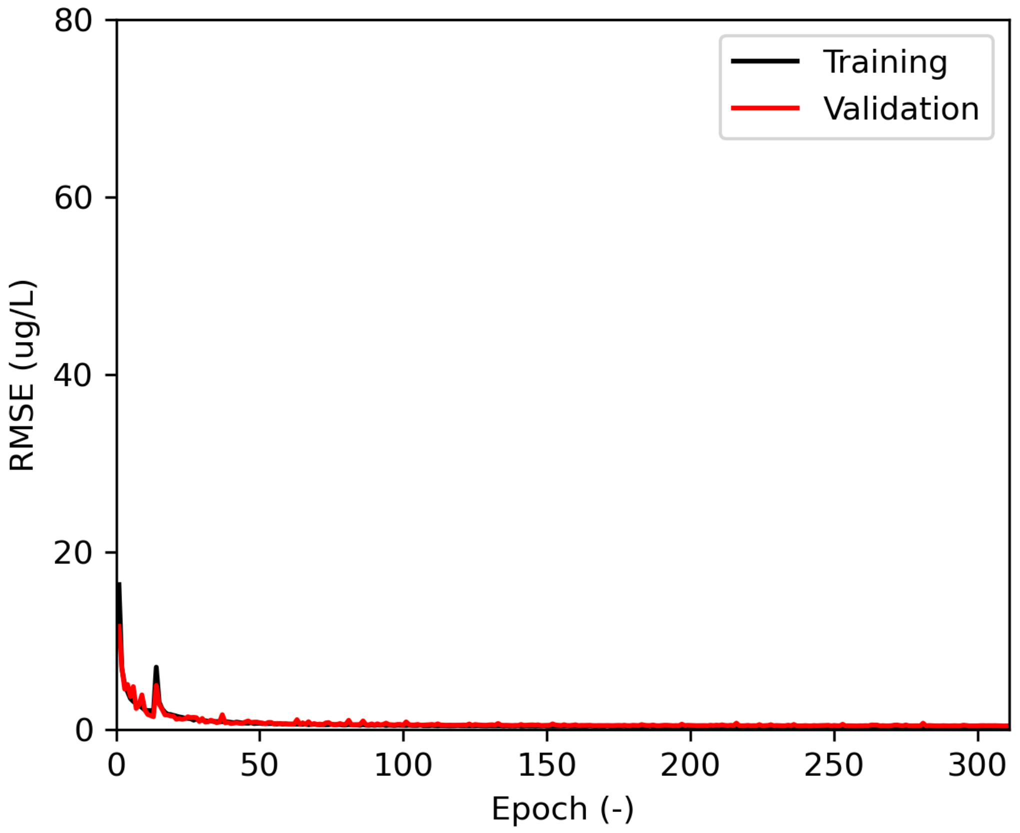
2-D Mode Training Results

- Case #1 validation RMSE: 0.62



Model training results of case #1

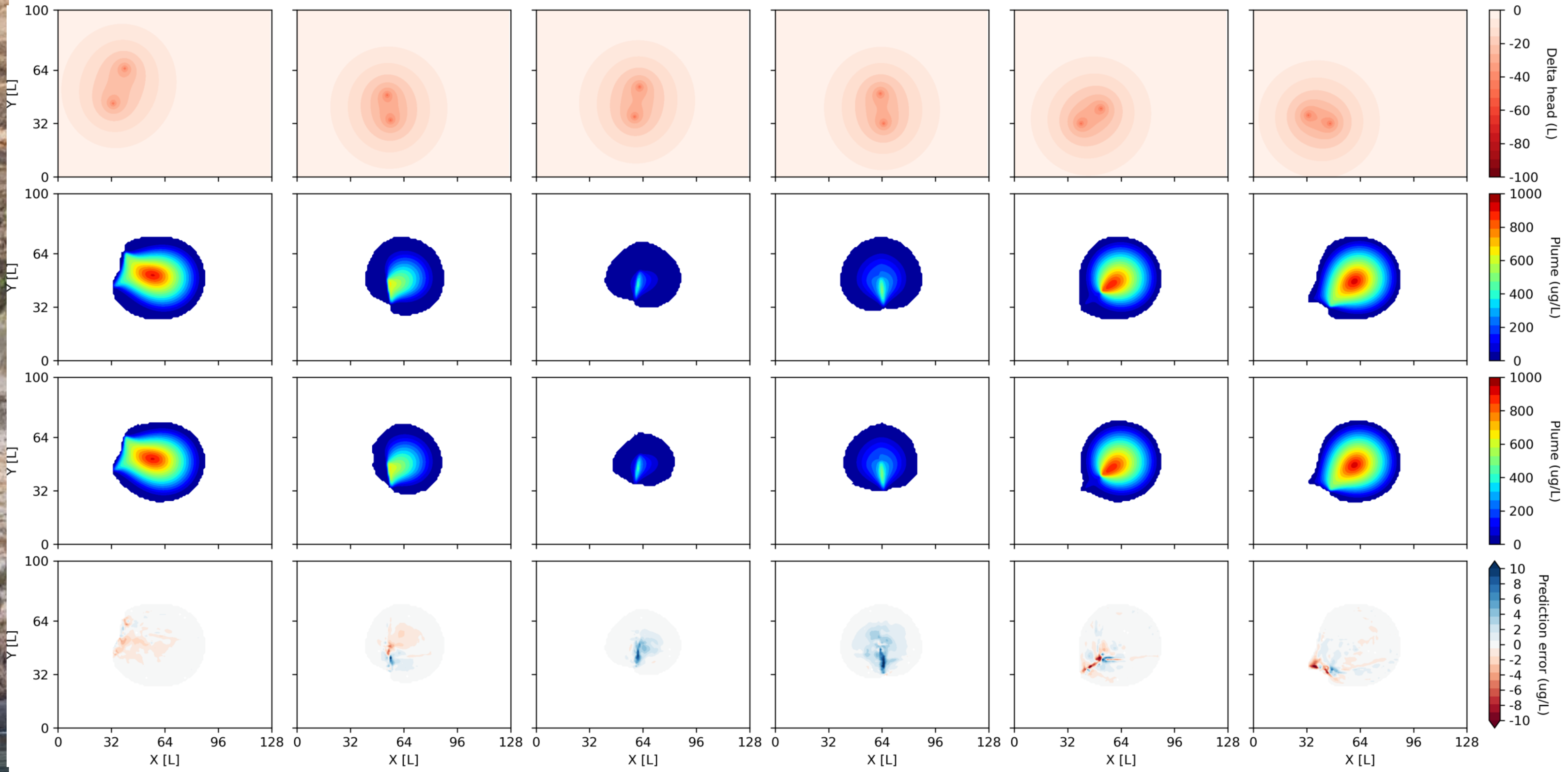
- Case #2 validation RMSE: 0.41



Model training results of case #2

- 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.

2-D Mode Predictions



Input :thiem solution

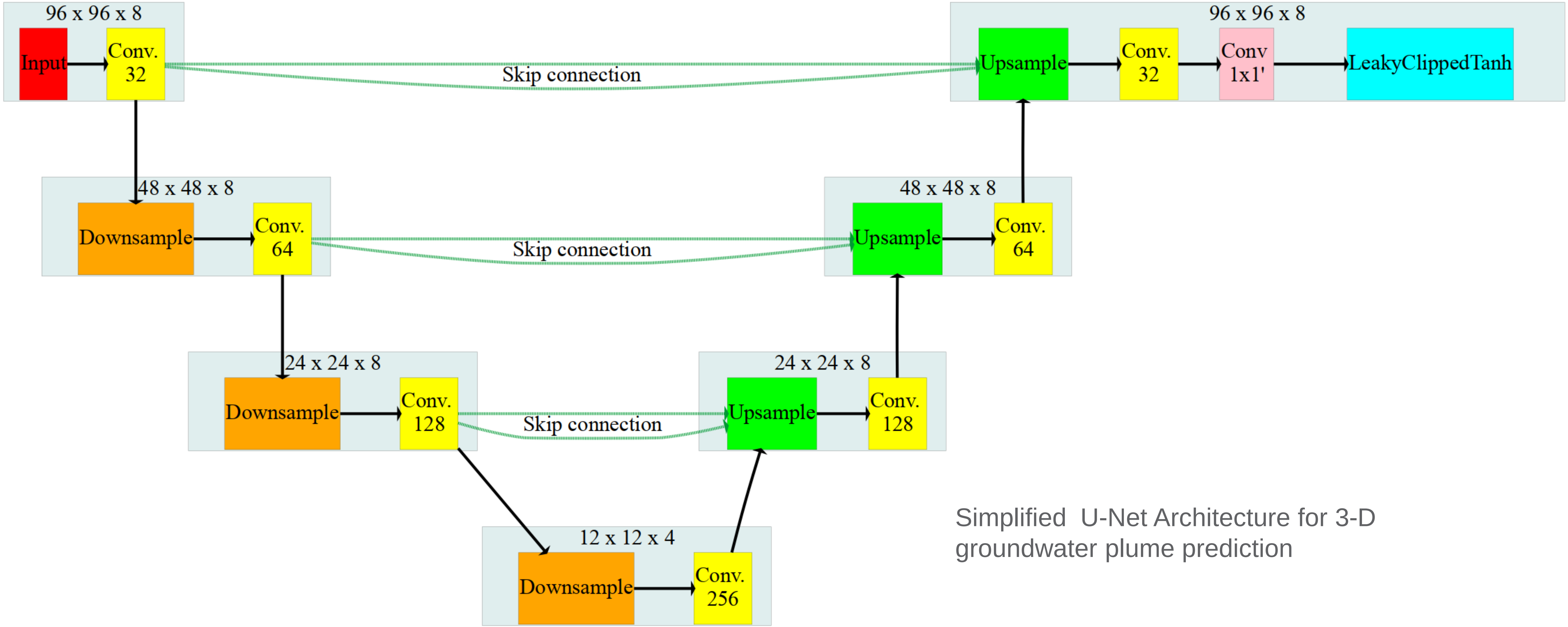
Target: final plume

Prediction

Error

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

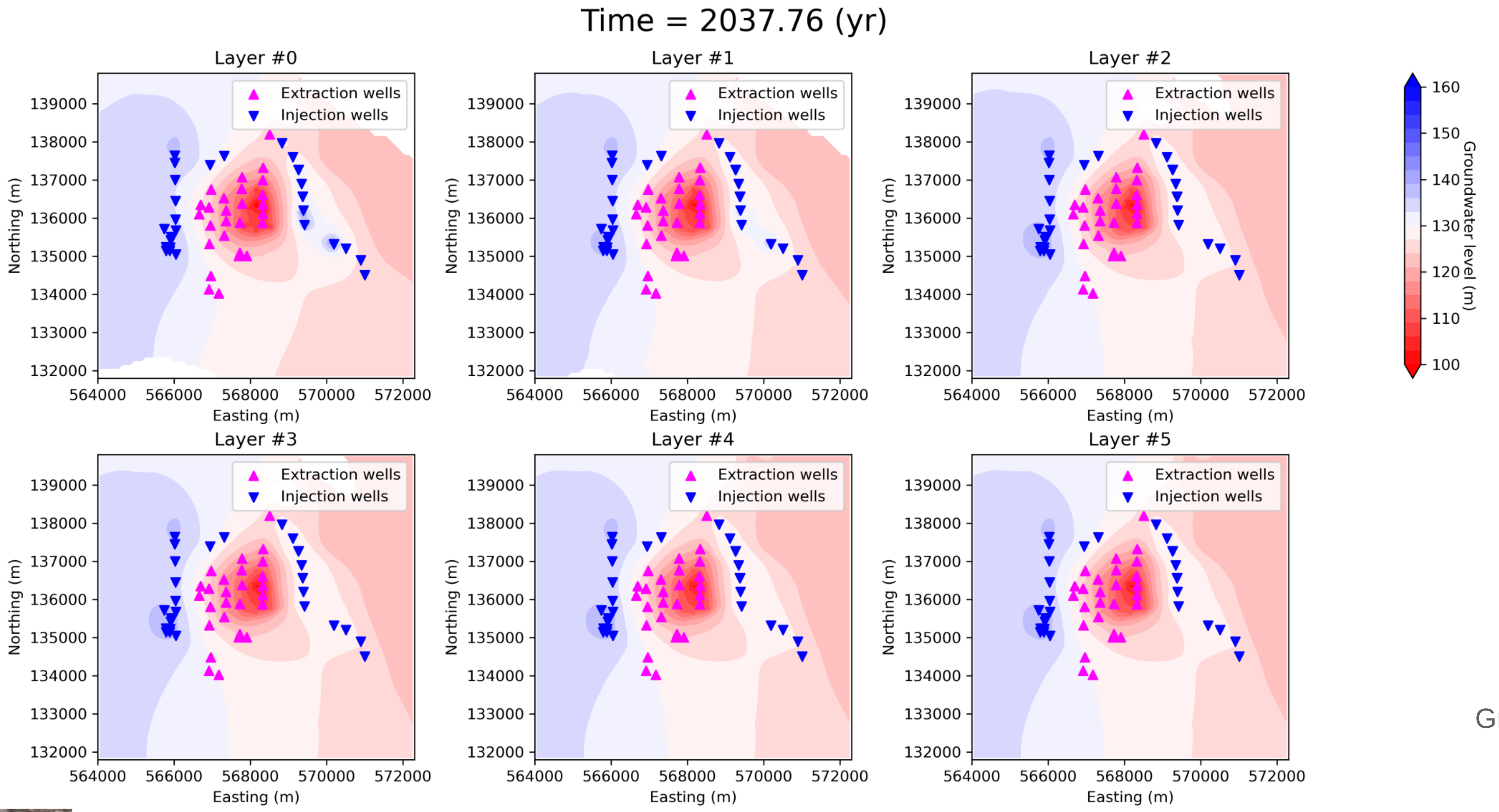
U-Net Architecture for 3-D Plume Prediction



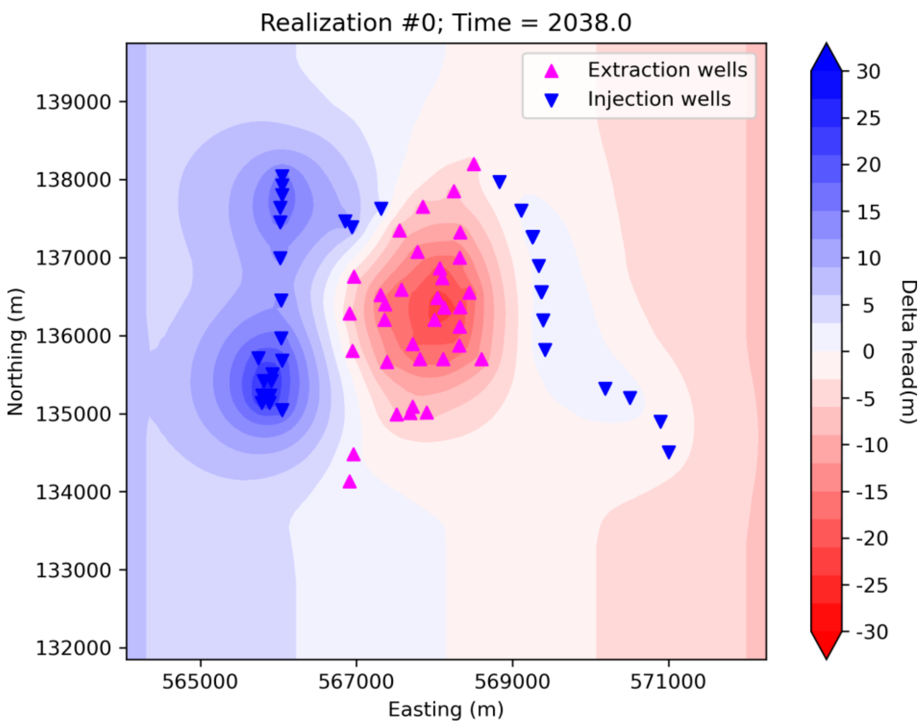
Simplified U-Net Architecture for 3-D groundwater plume prediction

- Justification for simplification:
  - Enhanced memory efficiency by cutting parameters from ~32M down to ~1.7M
  - Simpler field model dynamics compared to the highly transient 2-D model

Thiem Estimation VS. Numerical Model Simulation



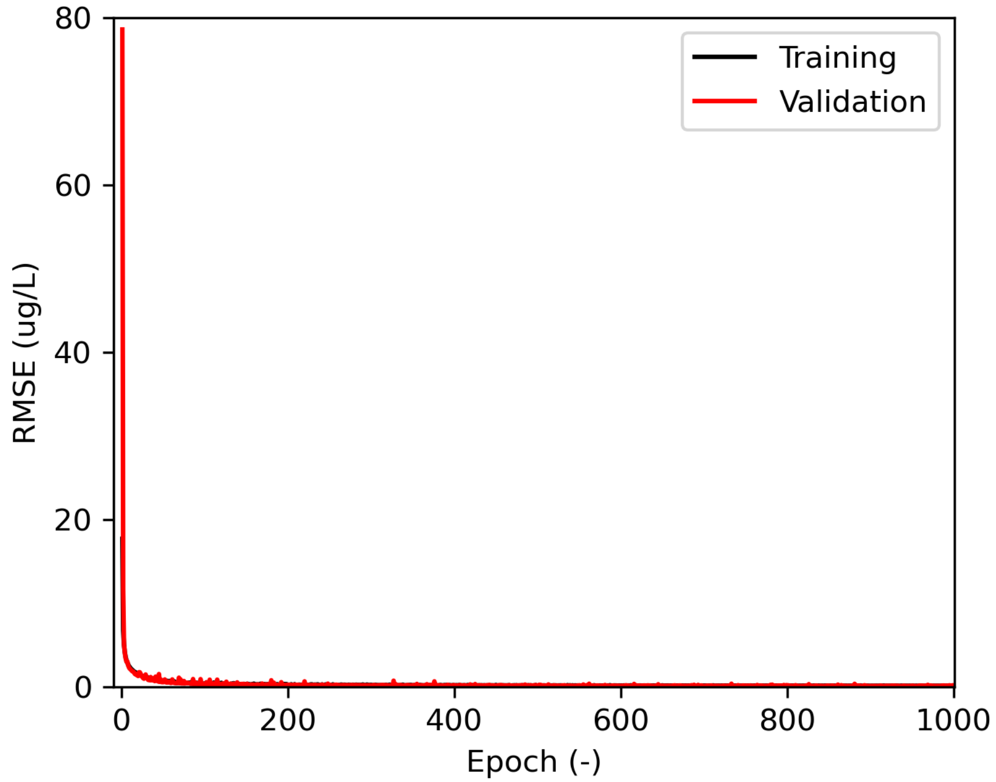
Groundwater level simulation results from P2R MODFLOW model



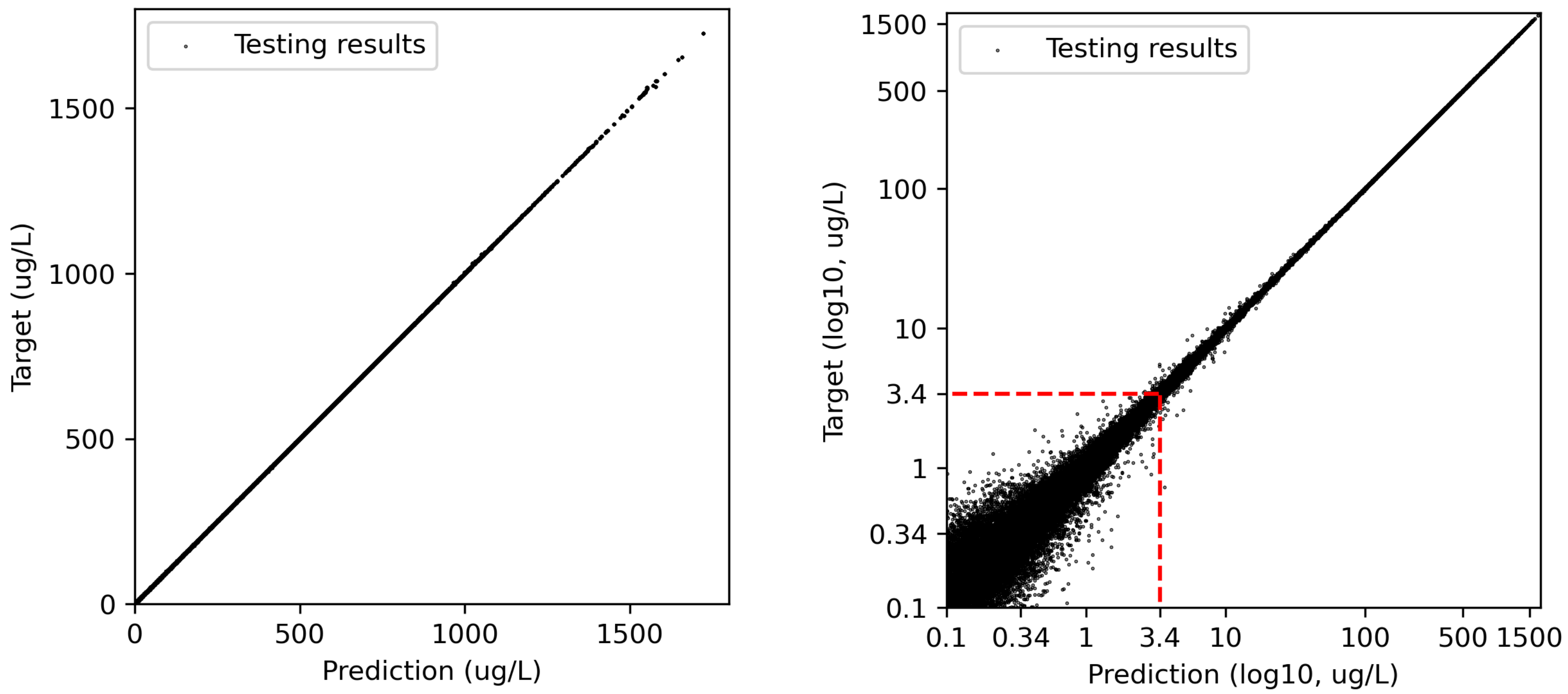
Groundwater level simulation results from Thiem estimation

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

3-D Model Training and Testing Results



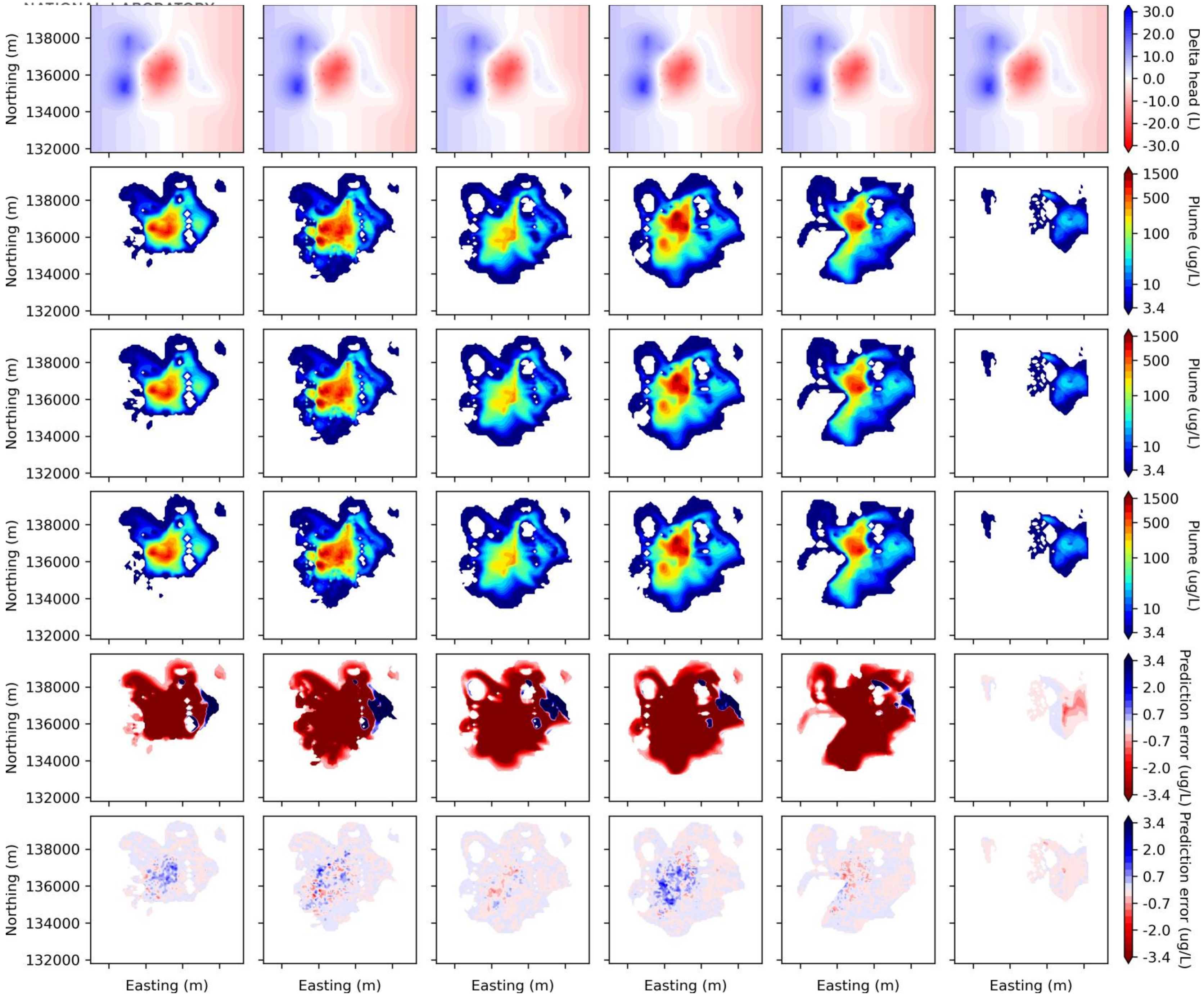
Model training results



Model predictions assessed against actual target values (linear and log scale)

- Training, validation, and testing dataset sizes are 8400, 1800, and 1800 samples, respectively.
- Validation RMSE for the best-performing model is 0.10 ug/L, with variations among different models ranging from 0.10 to 0.25 ug/L.
- Testing RMSE for the top model is 0.10 ug/L, with a model variation range of 0.10 to 0.27 ug/L.

Model Predictions: Example #1



Input #1:thiem solution

Input #2:plume at year N

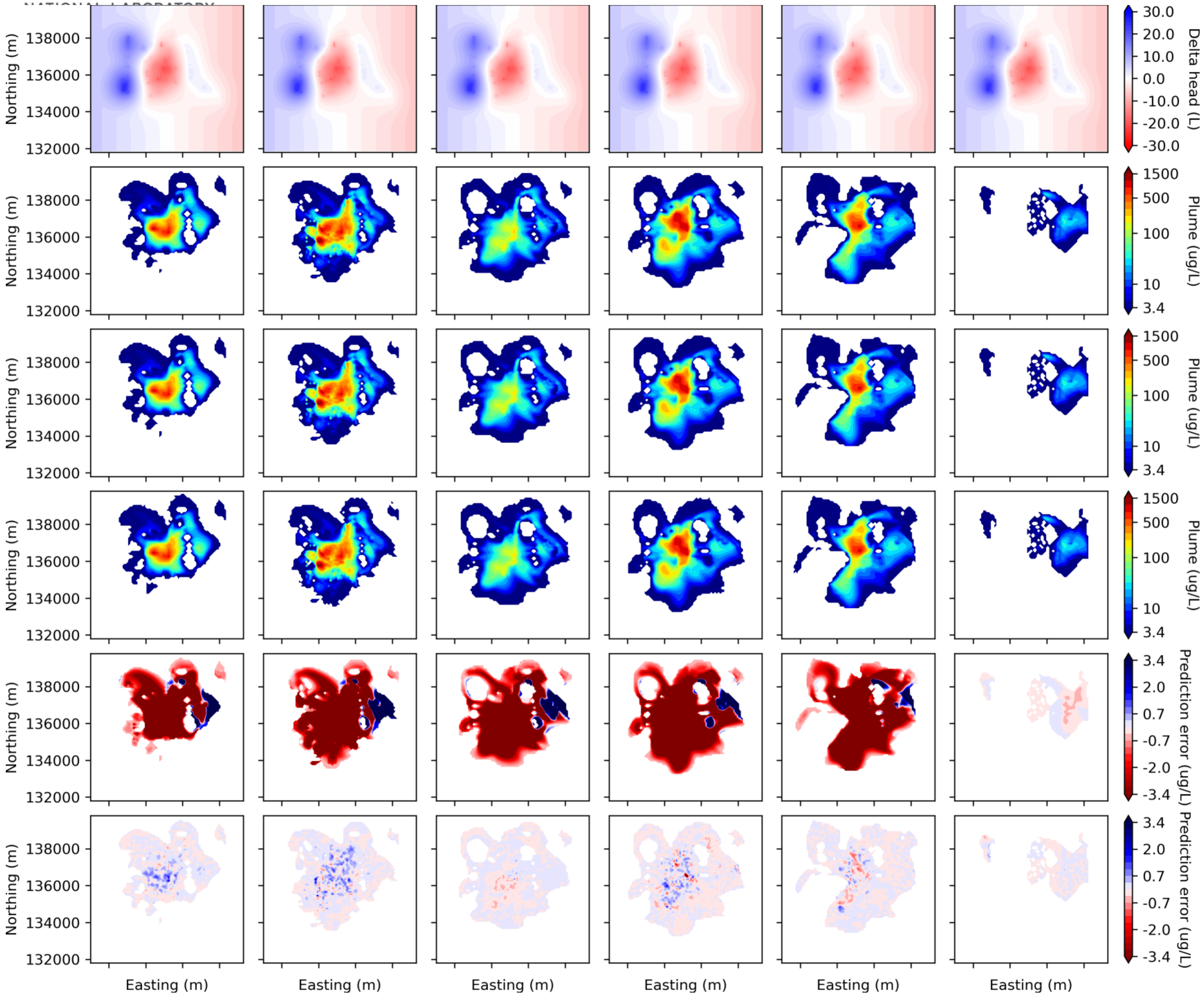
Target: plume at year N+1

Prediction: plume at year N+1

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

Prediction error (row 4-row2)

Model Predictions: Example #2



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)

Conclusions and Implications

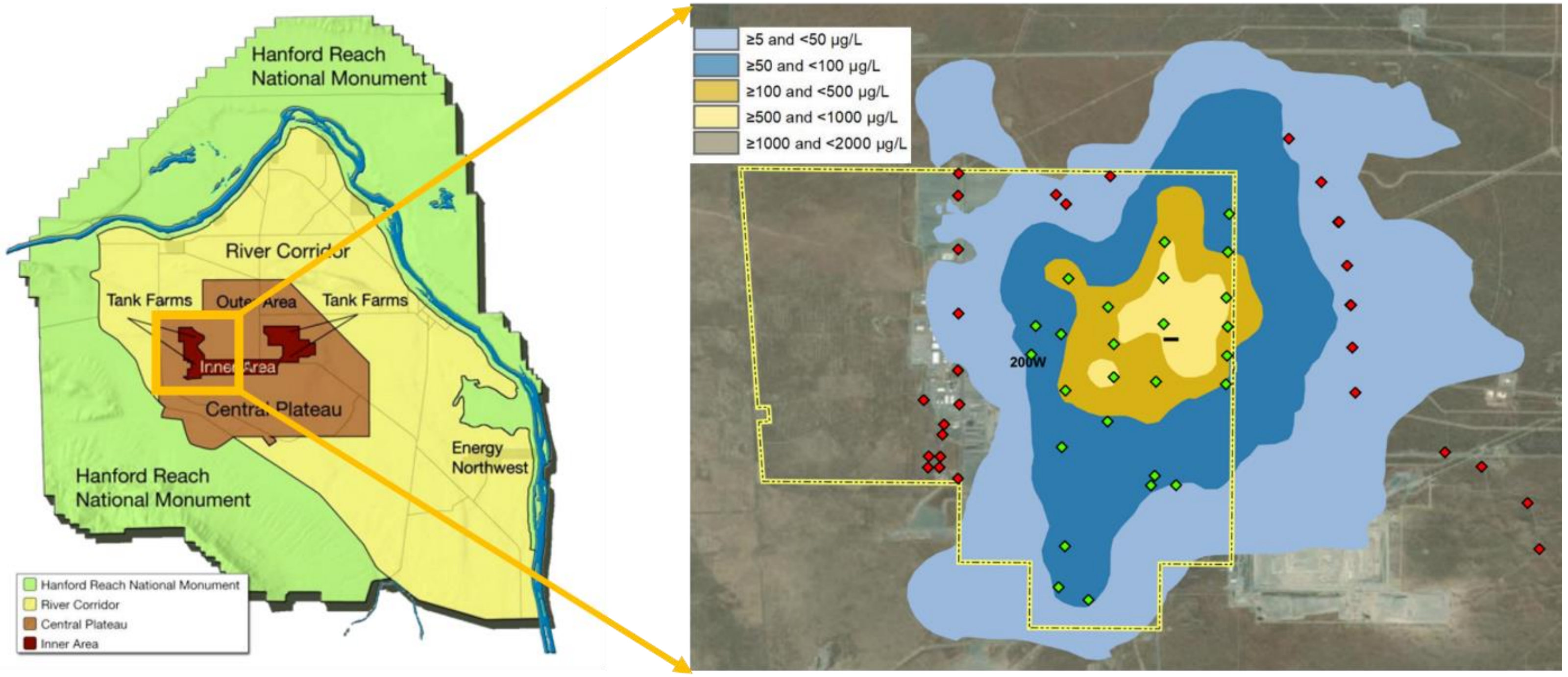
- The U-Net is trained on numerical models then driven by analytical solutions for efficient prediction. The integrated U-Net architecture demonstrates strong performance on both simple yet highly transient 2D model and complex 3D heterogeneous site models.
- With an 8xRTX 2080 Ti GPU setup, the 3D architecture trains each epoch in approximately 20 seconds, totaling under 6 hours for 1000 epochs.
- For a single-step prediction, covering one year and one realization, the model takes 46 milliseconds on a single CPU core, and just 2.2 milliseconds on an 8xRTX 2080 Ti GPU node, a significant improvement over the 3 to 5 minutes required for equivalent numerical simulations on a single CPU core.
- The model's rapid and high-quality predictions pave the way for more complex and time-consuming optimization simulations, such as reinforcement learning applications.
- Additionally, it serves as a swift assessment tool for site evaluation, enhancing responsiveness in environmental management.

Funding for this work was provided by the U.S. Department of Energy Richland Operations 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.

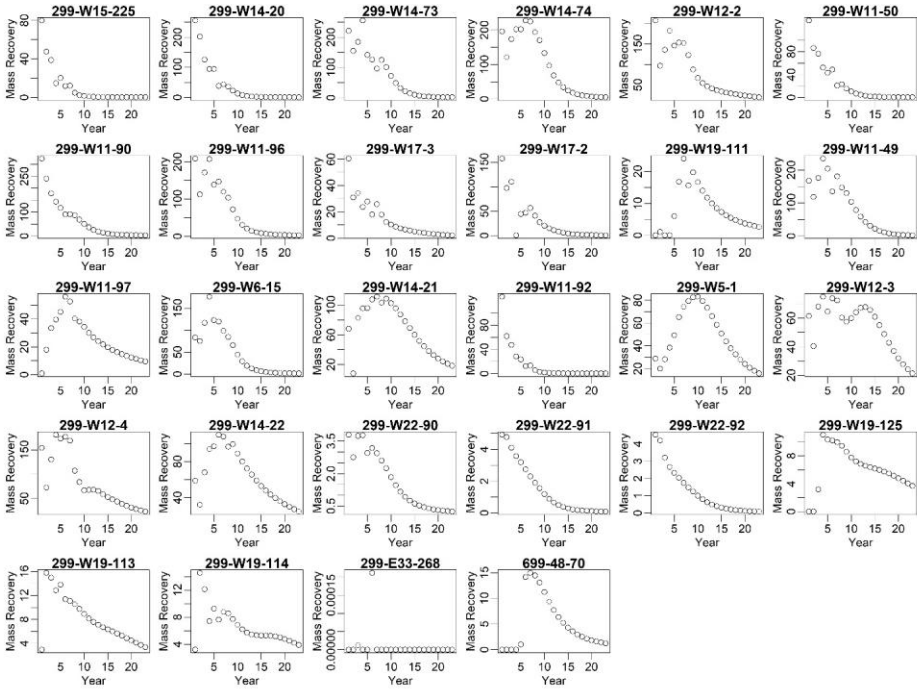
Thank you

200 West Groundwater P&T of the Central Plateau at the Hanford Site

- Contaminant plumes (e.g., CCl4, Tc-99, I-129 and NO_3) resulted from nuclear fuel fabrication from 1943 to 1975.
- 200 West P&T started in 2012, new wells need to be installed based on recent classification data.



CCl4 plume distribution in 200 West Area (Source: https://www.hanford.gov/page.cfm/PHOENIX ; https://www.hanford.gov/files.cfm/Attachment_5_Approach_CP_Cleanup_handout.pdf)



Annual CCT4 recovery from 28 extraction wells