An Online Prototype Toolset for Predicting and Optimizing P&T Performance FY23 Status Report

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Summary

A new web-based toolset is being developed to support ongoing remediation optimization efforts and implementation of an adaptive site management strategy for the 200 West Area Pump-and-Treat (P&T) system at the Hanford Site. This toolset, comprising the well performance index tool and the well optimization pre-screening tool, will offer a user-friendly interface to predict and optimize the P&T well network's performance at a preliminary level.

Efforts in fiscal year (FY) 2023 focused on three main components: updating the existing deep learning model for predicting P&T performance, designing and developing a prototype of a web-based performance index tool, and initiating the conceptual design of the well optimization pre-screening tool. The well performance index tool is based on a pre-trained deep learning model that allows users to select a target contaminant and well screen length, then visualize the predicted performance of potential new wells across the site. The well optimization pre-screening tool includes two separate modules: the pre-computed scenario viewer, which organizes and visualizes offline optimization simulation results, and the quick analysis module, which provides real-time model prediction using user-specified well locations.

In FY24, the plan is to add web-based applications to SOCRATES for both the well performance prediction tool and the optimization prescreening tool, with accompanying user and theory guides. These tools are intended to enable an accessible, easily applied, and transparent approach to remedy planning and decision-making.

Introduction

The 200 West P&T system at the Hanford Site is one of the key components of the final remedy selected for the 200-ZP-1 operable unit (OU) and the interim remedial decisions selected for the 200 UP-1 (DOE/RL 2009), 200-BP-5, and 200-PO-1 OUs (EPA, Ecology, and DOE 2021), all of which are groundwater OUs located in the Central Plateau area. The P&T system consists of a network of extraction and injection wells that are designed to capture contaminated groundwater for aboveground treatment and to prevent further migration of contaminants. A comprehensive effort for the 200 West P&T remedy optimization for the 200-ZP-1 OU was initiated at the end of FY19 under a formal optimization study plan (DOE/RL 2019). Continuous tracking of P&T well network performance and developing dynamic, performance-based optimization approaches are important to maintaining effectiveness and efficiency of the remedy over time.

Recent tasks performed under the Deep Vadose Zone (DVZ) project have focused on developing a data-driven deep learning model for predicting extraction well performance and a performance-based remedy optimization pre-screening tool. The deep learning model can predict the extraction well performance for

a given location using historical P&T records and site characterization data. The deep learning model is trained using image-based machine learning techniques that can capture the spatial patterns and relationships of the data (Song et al. 2023). The optimization pre-screening tool is designed to provide preliminary cost and benefit analysis evaluation. These evaluations, which include factors such as time and cost needed to achieve remedial action objectives, are intended to serve as a starting point for further detailed analysis. Both the deep learning model and the optimization pre-screening tool are hosted on local workstations, and thus lack accessibility for users and connection to ongoing data updates. Migrating the optimization tool and deep learning models to the SOCRATES web-based software platform will increase the feasibility and transparency of remedy planning and will thus facilitate timely and informed decision-making. This tool is intended for use by The U.S. Department of Energy Richland Operations Office (RL) staff and contractors involved in decision-making or analyses related to the 200 West P&T system. Featuring a user-friendly interface and up-to-date data, the tool will enable users to efficiently pre-screen a variety of remediation strategies based on predicted well performance and projected optimization outcomes. The chosen strategies can undergo more thorough and computationally demanding modeling evaluations, thereby facilitating informed decision-making.

The FY23 scope included:

- Deep learning model update: revise and update the previously published machine learning model to integrate new data and to reduce its dependency on numerical simulations.
- Web-based well performance index tool development: design web-based user interface and develop prototype web application.
- Design the web-based well optimization pre-screening tool webpage.

This status report describes the progress achieved for these three aspects in FY23. The deep learning model was updated, the user interface design for the well performance index tool was completed, a static prototype web application was developed, and the conceptual design for the well optimization pre-screening tool was initiated.

Deep Learning Model Update

The deep learning method used in the well performance index tool was developed in a previous DVZ task (Song et al. 2023). The deep learning method, known as the multi-channel three-dimensional convolutional neural network (MC3D-CNN), integrates transient 3D contaminant plumes and multiple aquifer properties (such as hydraulic conductivity and hydrostratigraphic maps) to identify characteristic patterns that control and represent extraction well mass recovery. The model provides future mass recovery estimates for existing wells and candidate wells at any proposed location within defined Central Plateau bounds. Figure 1 illustrates the general workflow of the MC3D-CNN method, with a more detailed method description available in Song et al. (2023). This year's updates to the deep learning model include:

1. Replacing the hydrostratigraphic data in the original application with the updated Hanford geological framework data (Hanford South GFM, version 6).
    a. Removing the hydraulic conductivity data from the deep learning model to reduce the model's dependence on the P2R (Plateau-to-River) model. Model testing confirmed that removing the hydraulic conductivity data has negligible impacts on the deep learning model training results.
2. Rewriting and modularizing the deep learning code.

3. Updating the output data structure for visualization in a web-based user interface.

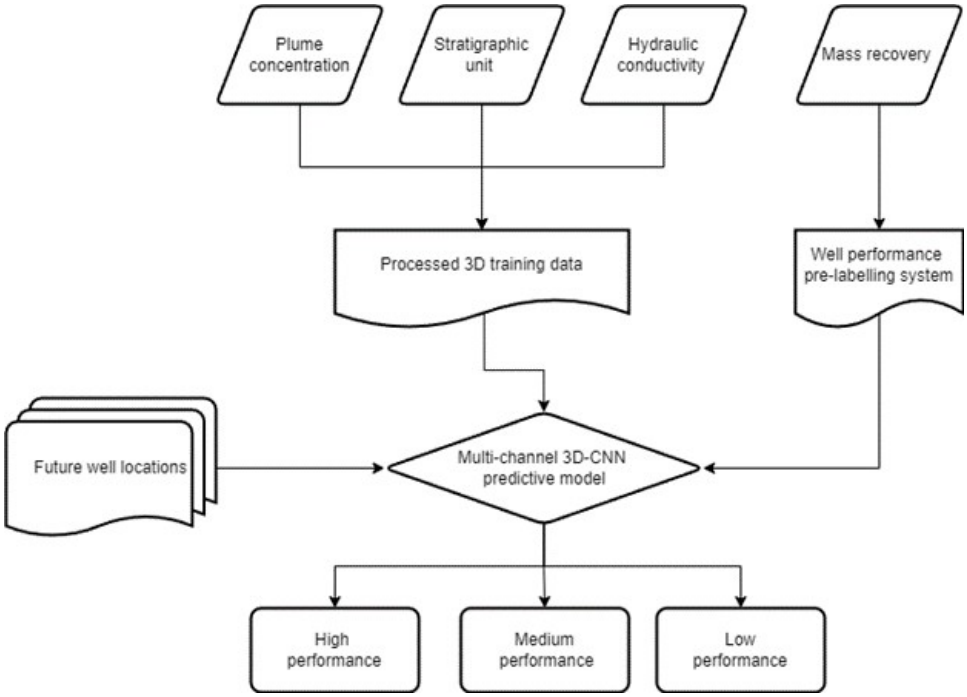

Figure 1. Deep learning-based workflow for ranking well performance (Song et al. 2023).

Development of Web-based Well Performance Index Prototype Tool

The web-based well performance index tool is designed to provide an efficient and user-friendly way to examine the deep learning model results for well performance prediction. More importantly, it offers an easy-to-use interface for planning and selecting well locations on a GIS map, and gives instantaneous well performance prediction for these location selections, making it a useful tool for an initial well field plan. In FY23, the user interface design work for this tool was completed and a static web application prototype was developed to illustrate functionality.

Figure 2 shows the main page of the well performance index tool user interface. On the top left, users can select the desired target contaminant (e.g., carbon tetrachloride) and choose the desired well screen length and length units, which are constrained inputs based on the pre-trained deep learning model. At the bottom of the left pane, users can choose to overlay additional contextual layers, such as contaminant plumes and existing wells, as reference information for selection of new wells. In the middle pane, users can visualize the 2D horizontal overview of the well performance prediction. By using the panning and zooming functions, users can also investigate more details on the 2D performance index map. Warm colors in the 2D performance index map represent potential high well performance locations, and cold colors represent low well performance locations. The key feature in this middle pane is the cross-section function, which can be used to select straight lines in the 2D map from which the web application will create 2D vertical cross-sections in the right pane. Users can then open these 2D cross-sections to refine

the well location selection in the vertical direction. In the end, users can save these selected cross-sections by using the export function to finish the workflow (bottom of the right pane).

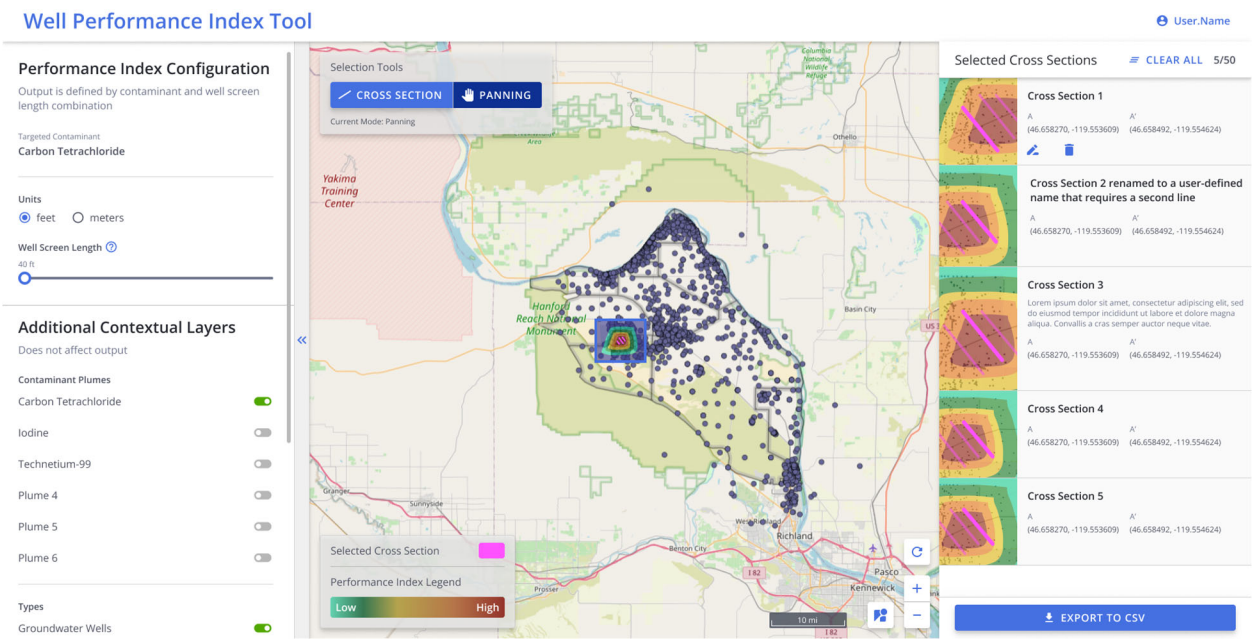

Figure 2. Web-based user interface of the well performance index tool.

Web-Based Well Optimization Pre-screening Tool Design

The purpose of the web-based well optimization pre-screening tool is to integrate the optimization pre-screening simulations into an interactive and user-friendly interface. In FY23, the work primarily focused on the conceptual design of the user interface.

Due to the high computational cost of optimization simulations, full-scale optimization runs were not included as part of this web-based application. The optimization simulations might require thousands of simulation runs and long waiting times, which are not conducive to a responsive web application. Instead, the web-based well optimization pre-screening tool was divided into two modules: (1) a pre-computed scenario viewer and (2) a quick analysis tool. The functions of the two modules are as follows.

- The pre-computed scenario viewer will provide a framework that can add new optimization simulations as they are completed and visualize any of the available optimization simulation results (Figure 3). Within the viewer tool, a time slider can be adjusted to view the changes (e.g., new wells, diminished wells) in each scenario over time. This will allow the user to visualize the operational life of each existing and planned well. It can also show the scenario objectives (such as mass recovery and total cost) and input assumptions (such as total treating capacity).

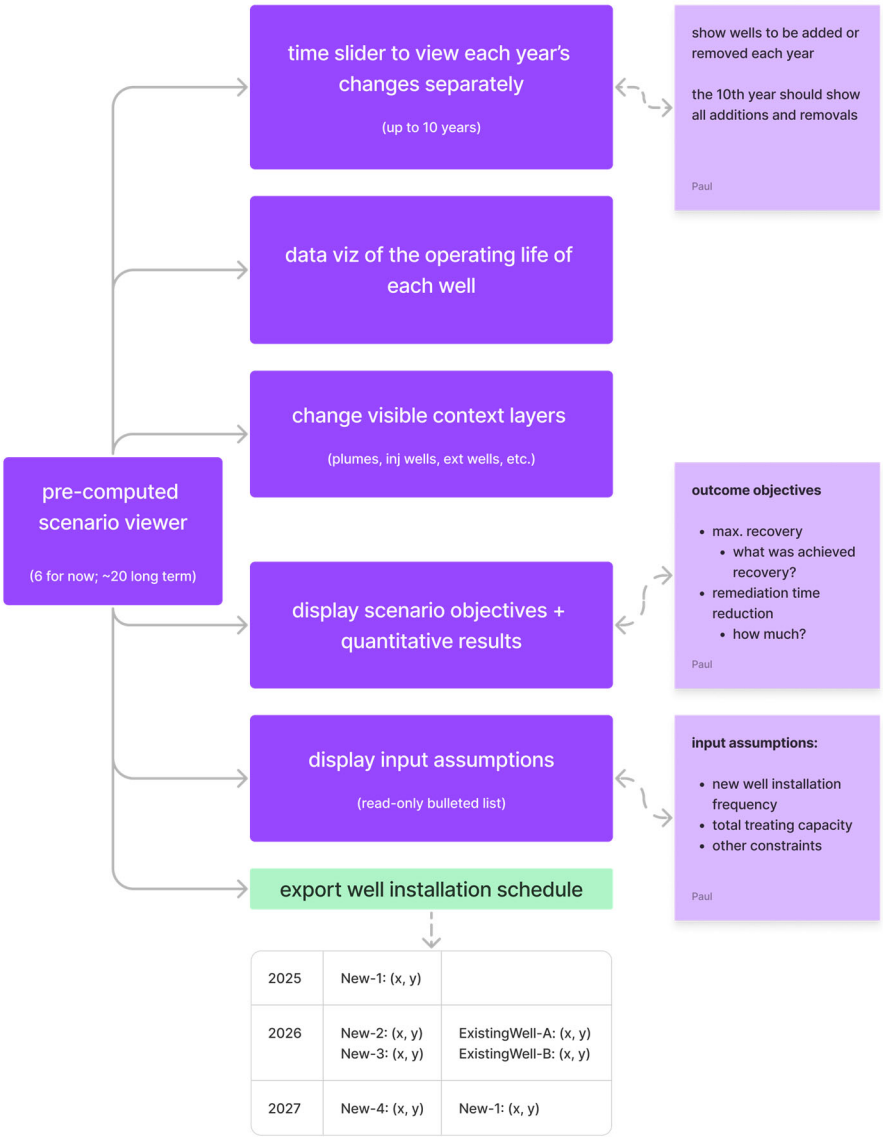

Figure 3. Conceptual design of the pre-computed scenario viewer.

- The quick analysis module will provide real-time prediction based on user-specified well configurations (Figure 4). Users will be able to either select specific locations (points on the 2D map) or a set of possible locations (polygon areas on the 2D map) for these locations. The web application will conduct a real-time simulation using these wells and will produce simulation results. To improve the efficiency of the web-based application, two possible backend engines for the simulation are planned. One approach is to use pre-computed simulations as a lookup table. A second option is to employ analytical solutions or machine learning-based surrogate models.

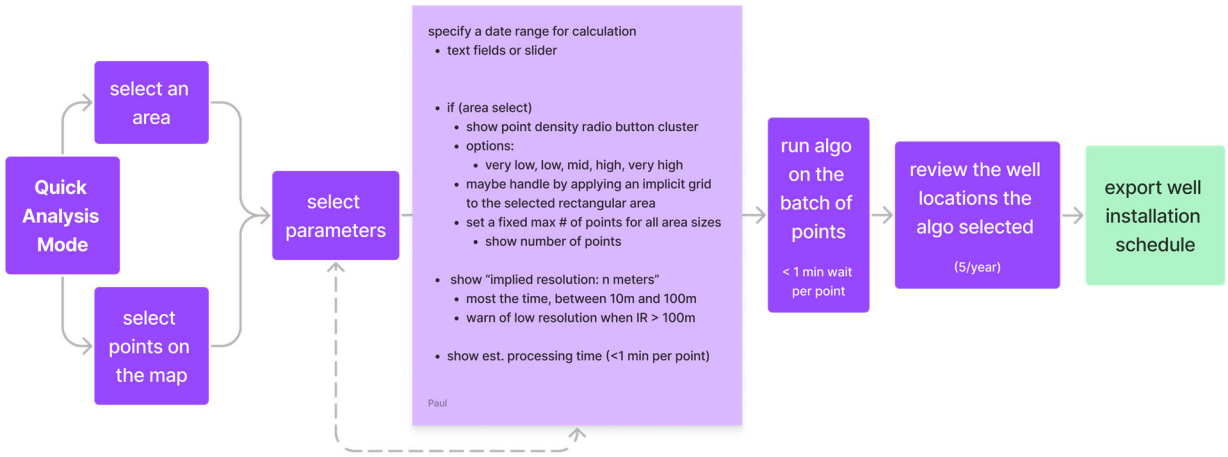

Figure 4. Conceptual design of the quick analysis module.

Conclusion

This status report describes FY23 development of a web-based toolset for predicting and optimizing the performance of P&T systems. This work focused on updating a deep learning model for predicting P&T well performance, developing a prototype web-based tool for visualizing deep learning predictions of well performance, and designing a web-based tool for pre-screening well optimization. Subsequent efforts in FY24 will focus on completing development of the web-based tools. Upon completion, this pre-screening level toolset will be made available to RL and site contractors. It is designed to provide preliminary analyses of remediation strategies based on predicted well performance and projected optimization outcomes. This will aid in narrowing down potential scenarios that warrant further, more detailed evaluation using other models.

Proposed FY24 Activities

In FY24, work to complete the development of two web-based applications is proposed. The key activities would include:

- Moving to a higher quality assurance (QA) technology readiness level (TRL) for the deep learning code and data, which is needed for formal release of the performance index tool. This would involve additional review, testing, and documentation.
- Finalizing development of the web-based application for the well performance index tool, with associated testing, QA, and documentation.
- Completing the design and web-based application development for the optimization pre-screening tool, with associated testing, QA, and documentation.
- Communicating with RL and site contractors about the new tools/capabilities, conducting training sessions as needed, and making revisions to incorporate feedback, as needed.

Quality Assurance

This work was performed in accordance with the Pacific Northwest National Laboratory Nuclear Quality Assurance Program (NQAP). The NQAP complies with 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.

References

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