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Integration and Demonstration of Monitoring, Modeling, and Prediction of DV-1 Amendment Performance at the Bench Scale

DV-1 Amendment Demonstration

September 2025

Tim Johnson
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U.S. DEPARTMENT of ENERGY

Prepared for the U.S. Department of Energy
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Summary

During fiscal years 2024 and 2025, the U.S. Department of Energy's Hanford Field Office commissioned Pacific Northwest National Laboratory to conduct applied research aimed at reducing the cost, time, and uncertainty associated with in situ treatment of vadose zone contaminants at the Hanford Site. This report outlines the integration of three key research efforts into a meso-scale demonstration designed to advance field-scale solutions that aim to (1) optimize the delivery of chemical amendments to contaminated soils, (2) reduce uncertainty in amendment delivery performance assessment using advanced monitoring techniques, and (3) provide real-time insights into when and where amendment-induced precipitation reactions occur in the subsurface.

To achieve these objectives, the tank-scale (~ 1 cubic meter) Geophysical Imaging of Flow and Transport (GIFT) system was developed. GIFT enables experimental testing of amendment delivery while incorporating automated multi-modal monitoring approaches, including pressure measurements, direct fluid sampling, and remote time-lapse geophysical imaging. The data generated from these monitoring techniques will serve as inputs for a generative artificial-intelligence-driven digital twin – a numerical simulation model designed to honor observed data while quantifying uncertainty in simulation accuracy.

Using this simulator, researchers will refine an amendment injection strategy to maximize delivery efficiency within a low-permeability soil zone. Monitoring data will be interpreted through simulated outputs to enhance understanding of the injection process. The efficacy of this integrated approach will be evaluated through direct sampling at the conclusion of the experiment.

Acknowledgments

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Quality Assurance

The work described 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. This work emphasized acquiring new theoretical or experimental knowledge. The information associated with this publication should not be used as design input or operating parameters without additional qualification.

Acronyms and Abbreviations

AI	artificial intelligence
CDM	conditional diffusion model
ERT	electrical resistivity tomography
FY	fiscal year
GIFT	Geophysical Imaging of Flow and Transport
HFO	Hanford Field Office
IP	induced polarization
ML	machine learning
PNNL	Pacific Northwest National Laboratory
TDIP	time-domain induced polarization

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1.0 Introduction

Over the last 3 to 5 years, the U.S. Department of Energy Hanford Field Office (HFO) and Pacific Northwest National Laboratory (PNNL) have invested heavily in new technologies focused on enhancing capabilities to monitor subsurface behavior, including geochemical interactions, and to use monitoring data to calibrate numerical models that enable long-term predictability. In parallel, HFO has commissioned PNNL to evaluate remedial amendment technologies and quantify their performance.

In fiscal year (FY) 2024, HFO supported the development of the Geophysical Imaging of Flow and Transport (GIFT) system, an approximately 1-m^3, highly instrumented testbed that enables controlled testing of heterogeneous subsurface systems at the laboratory scale. In FY25, HFO supported the integration of these new capabilities to develop and demonstrate the efficacy of a DV-1 performance monitoring strategy that is transferable to the field scale. This report documents the progress of integration elements completed in FY25 and experimental demonstrations planned for the future.

GIFT system integration progressed along two parallel tracks in FY25: (1) system assembly and testing and (2) numerical model development. Physical system assembly involved a continuation of efforts initiated in FY24 to construct the testbed and implement monitoring systems. Those efforts were completed in FY25, including testing of the flow control system, the borehole pressure monitoring system, the borehole fluid conductivity monitoring system, and the electrical resistivity tomography (ERT) monitoring system, and packing of the testbed with sediments meant to represent basic field conditions at the Hanford Site. All control and monitoring systems were designed to operate autonomously and represent capabilities available for field-scale deployment.

A numerical PFLOTRAN simulator of the GIFT system was also completed in FY25. PFLOTRAN is a high-performance subsurface modeling software originally designed to simulate reactive flow and transport processes like those anticipated for DV-1 remediation. PFLOTRAN was recently augmented with the capability to simulate ERT monitoring data arising from those processes. Future GIFT system demonstrations will focus on using generative artificial intelligence (AI)-based inversion capabilities to generate PFLOTRAN models that honor borehole pressure, fluid conductivity, and 3-D ERT monitoring data. By so doing, we aim to generate an ensemble of models that represent the true subsurface in terms of the hydrogeologic properties that govern amendment migration, including uncertainty. Once calibrated, these models will be used predictively to optimize liquid amendment delivery to a low-permeability region. The approach will be established first with a conservative saline tracer. The demonstration will culminate by treating a low-permeability zone with calcium polysulfide and/or polyphosphate amendment and monitoring the delivery and regions of precipitation over time. Subsequent numerical predictions of amendment delivery and performance will be validated through periodic direct sampling of GIFT system sediments at the conclusion of the demonstration.

This report is organized as follows:

- Section 2.0 describes the physical characteristics and capabilities of the GIFT system, including flow control and monitoring systems. The GIFT system is packed with a three-layer sediment structure meant to provide a relatively simple base case for developing, testing, and validating the approach without the burden of extensive heterogeneity. We anticipate future sediment packing schemes will be directed at specific Hanford Site areas that are being considered for amendment-based remediation, such as the perched water or the BY Cribs area in the B Complex.

- Section 3.0 describes the GIFT system PFLOTRAN simulator, which will be used to train the AI-based inversion and design an optimal treatment strategy. Predictions from the calibrated simulator will be compared to GIFT system monitoring data to assess the performance of the inversion.
- Section 4.0 provides an overview of the conditional diffusion-based AI-model that will be trained to invert monitoring data collected during the saline tracer test and calibrate the flow model.
- Section 5.0 presents the demonstration and performance assessment for planned experiments, including the saline tracer test, flow model calibration, treatment design and execution, long-term monitoring, and destruction analysis for performance evaluation.

2.0 Geophysical Imaging of Flow and Transport (GIFT) System

The GIFT system is a laboratory-scale tank testbed with inner dimensions of 193 cm long, 74 cm wide, and 97 cm deep (Figure 1). For the current campaign, GIFT is instrumented with eight monitoring boreholes and one injection borehole. Each monitoring borehole (MI-1 through MI-8) contains 10 ERT imaging electrodes and three fluid ports, positioned as shown in Figure 1. The fluid ports are used by the hydraulic system to autonomously monitor pressure and fluid conductivity. They can also be used for fluid injection and extraction. The injection borehole (I-1) contains three fluid ports with the same functionality as the monitoring wells but does not include ERT imaging electrodes.

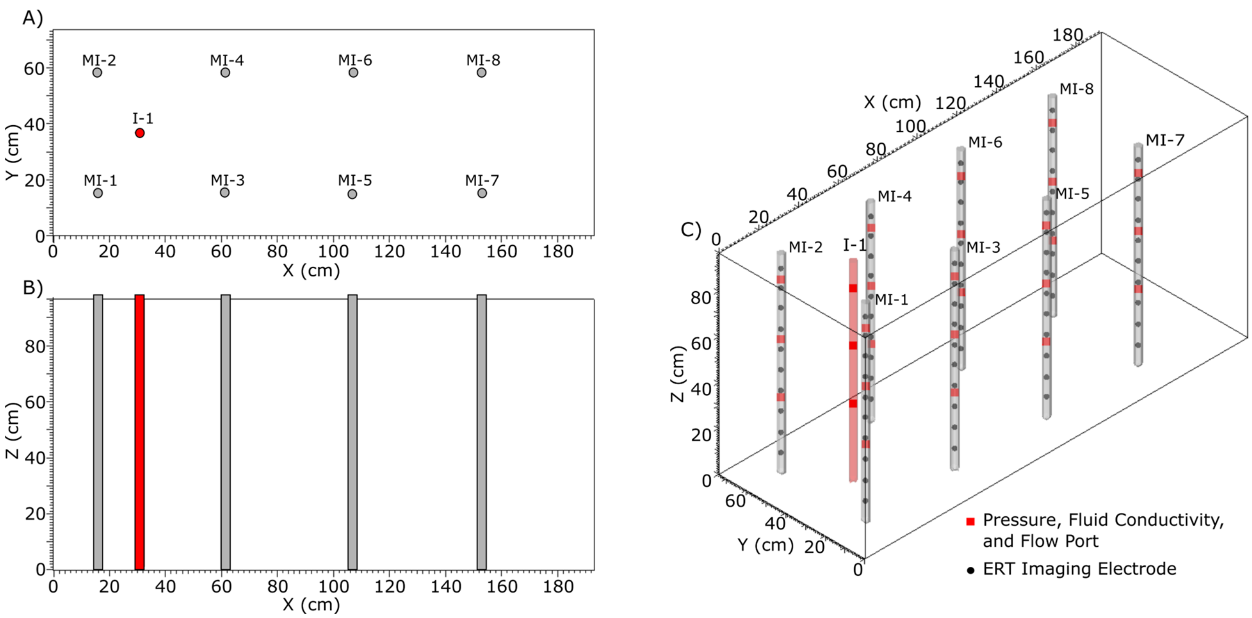

Figure 1. A) plan, B) section, and C) oblique diagrammatic views of the GIFT system. Eight monitoring boreholes (MI-1 through MI-8) are instrumented with fluid ports and ERT electrodes. The injection well (I-1) is instrumented only with fluid ports.

2.1 Flow Control

Fluid reservoirs at X = 0 cm and X = 193 cm (i.e., the bounding x-normal faces) are implemented to enable precise, automated control of the y-normal pressure gradient to mimic the effects of a local groundwater flow field. The fluid inflow rate is precisely controlled (nL/min precision) using a pair of syringe pumps (Teledyne-ISCO 500HP) configured to operate in tandem for continuous flow (Figure 2). In addition to pump flow-through control, a second pair of syringe pumps are used to deliver tracer or amendments to the injection well, or to any flow port.

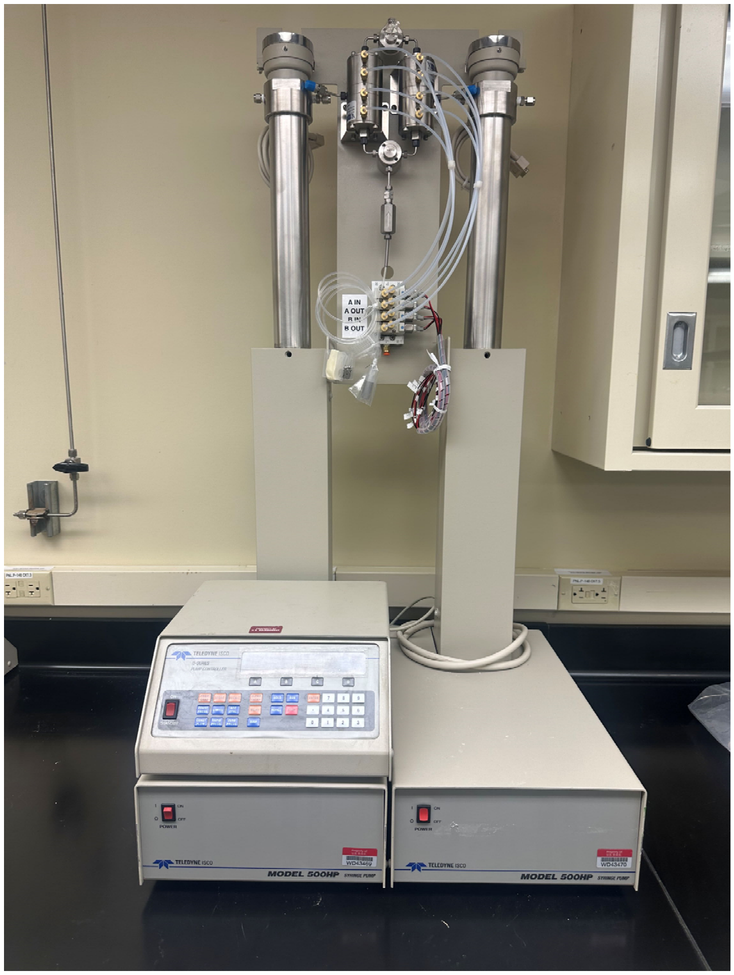

Figure 2. Dual ISCO syringe pumps used for flow control.

2.2 Pressure and Fluid Conductivity

Each fluid port is connected through tubing extending from the inside of each borehole to a circulation pump (Boxer 10KDL Diaphragm Pumps) with integrated pressure (Omega PX-429 +/- 5 psi) and fluid electrical conductivity sensors (Cole-Parmer Conductivity Cell, K=0.01, 10 Kohm ATC). Each port uses three tubes: two that form a recirculation loop for fluid electrical conductivity measurements and one non-flowing pressure-sensing line. The pumps have integrated flow control, and the flow rate was determined through laboratory testing to minimize disturbance to the flow streams surrounding each port.

Fluid sensing and flow control are accomplished using two enclosures: one containing all the liquid sensing and control components and another with a data acquisition system (National Instruments cRIO-9045). Figure 3 illustrates the connections between various GIFT experimental systems, and Figure 4 shows internal components of the liquid control and sensing system.

Figure 5 shows annotated photographs of the GIFT system during testing of the flow control and fluid sensing systems with the tank filled with water. Closeup views of boreholes show electrodes and screened portions of the PVC boreholes that serve as fluid access ports.

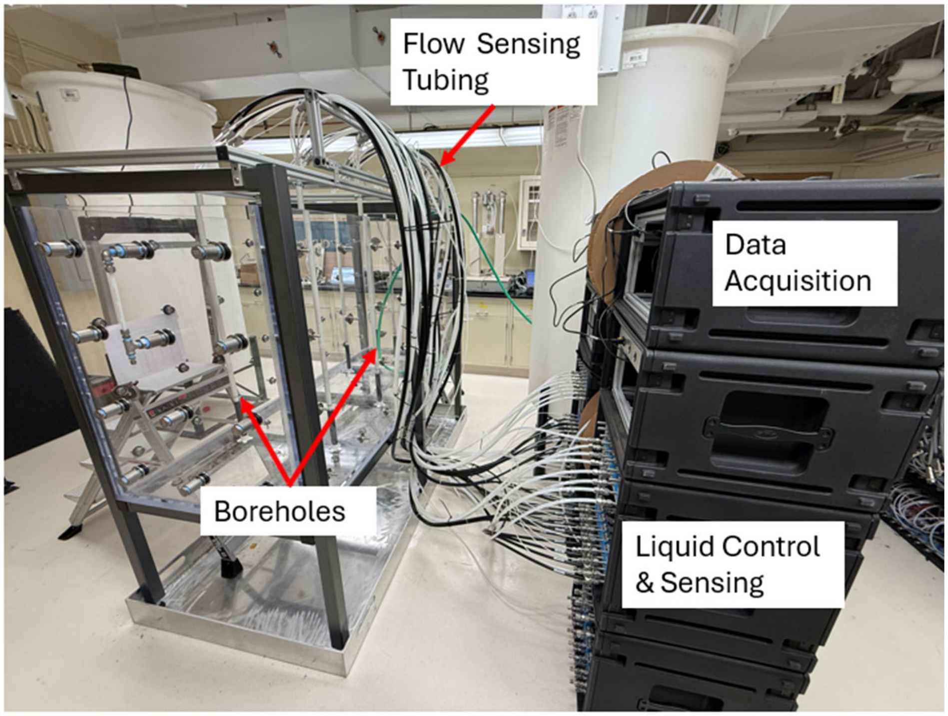

Figure 3. GIFT experimental setup.

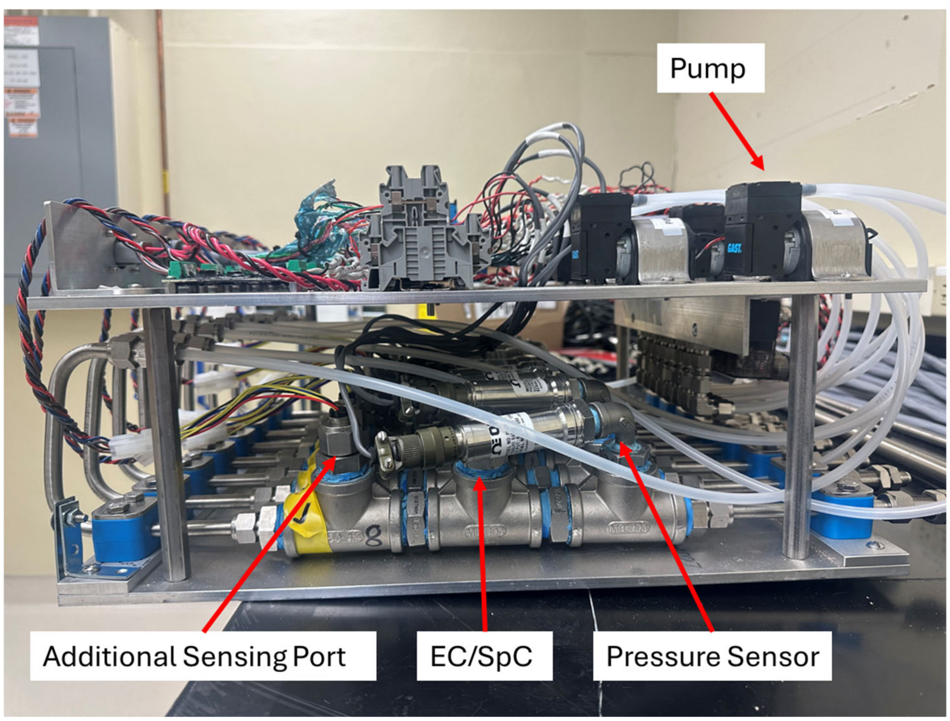

Figure 4. Internal components of GIFT liquid control and sensing system.

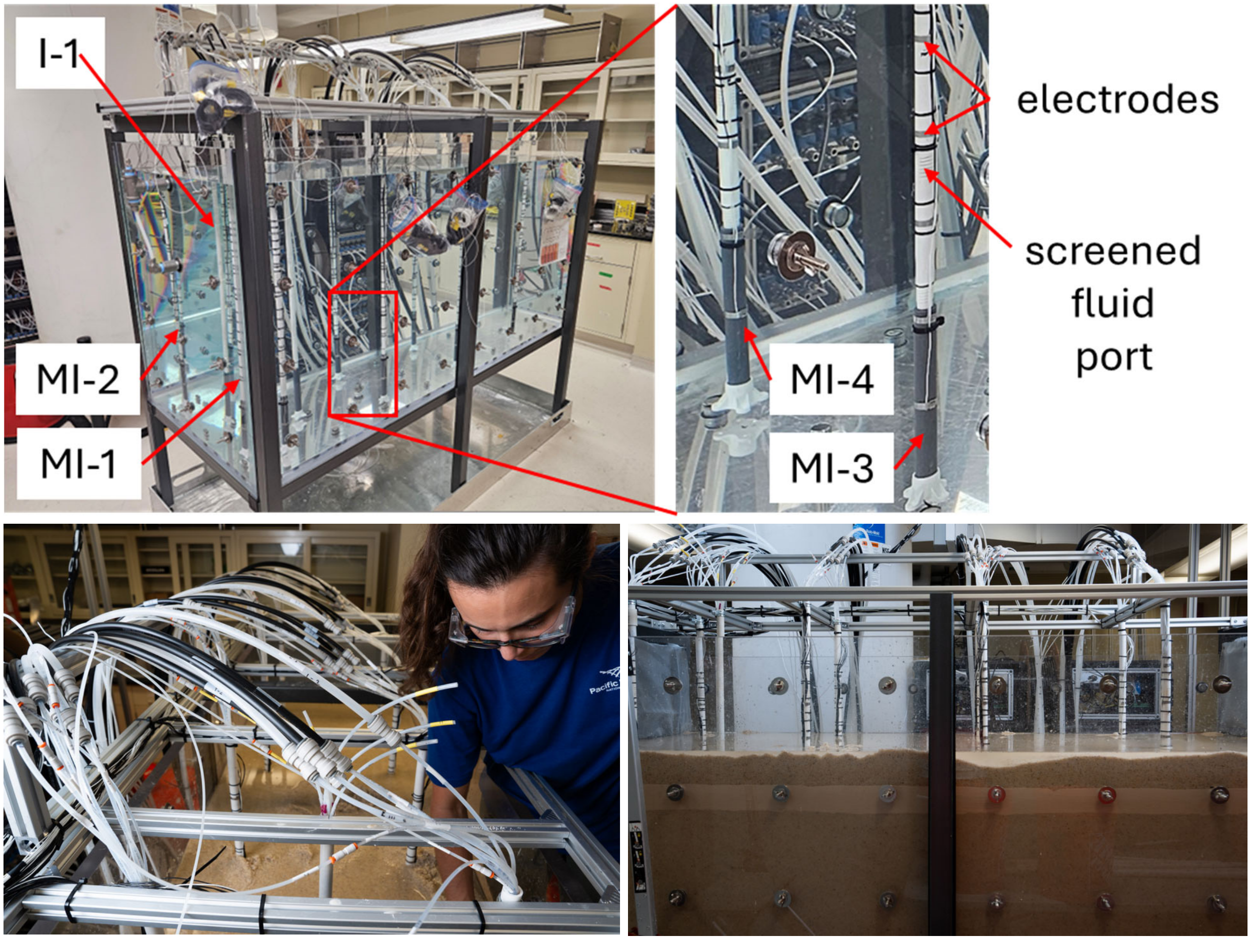

Figure 5. (top) Photograph of GIFT tank and instrumentation during testing of the fluid sensing and control system. Several boreholes are annotated (see Figure 1), with a closeup view of boreholes MI-3 and MI-4 highlighting electrodes and fluid ports. (bottom) Photographs of GIFT tank during sediment packing.

2.3 Electrical Resistivity Tomography

Boreholes MI-1 through MI-8 are each instrumented with 10 equally spaced stainless-steel ERT image electrodes. Each electrode is attached to the outside of the borehole wall and to one insulated copper wire extending up the borehole annulus to the surface (Figure 5), where it is connected to the ERT measurement instrumentation. ERT measurements will be used in two ways. First, they will be used to image migration of injected amendments and amendment reactivity in real time using time-lapse ERT and time-domain induced polarization (IP) imaging. Second, they will serve (along with pressure and fluid conductivity time-series) as conditioning data for the generative AI-based PFLOTRAN model calibration.

2.4 Sediment Profile

The GIFT system is packed with a simplified three-layer sediment profile meant to generally approximate conditions common to the Hanford Site, including a moderate permeability basal unit, which is overlain by a relatively thin low-permeability unit, which is overlain by a high-permeability unit that extends to the surface. The basal unit extends vertically from the bottom of the column to approximately 56 cm. The low-permeability central unit extends vertically from 56 to 61 cm. The upper unit extends from 61 to

96 cm, with hydrogeologic properties as shown in Figure 6 (Zhong et al. 2024). The lower permeability central unit is meant to represent a fine-grained unit that makes it more challenging to treat with injected amendments due to its low permeability.

As described in Section 3.0, the future experiments aim to achieve a comprehensive objective: (1) estimate the hydrogeologic property distribution shown in Figure 6 using monitoring data, (2) construct the corresponding PFLOTRAN model (effectively constituting a digital twin of the GIFT system), (3) use the PFLOTRAN model predictively to design an amendment injection and fluid extraction strategy to optimally treat the low-permeability zone, and finally (4) test and verify that strategy in terms of amendment delivery to the target zone.

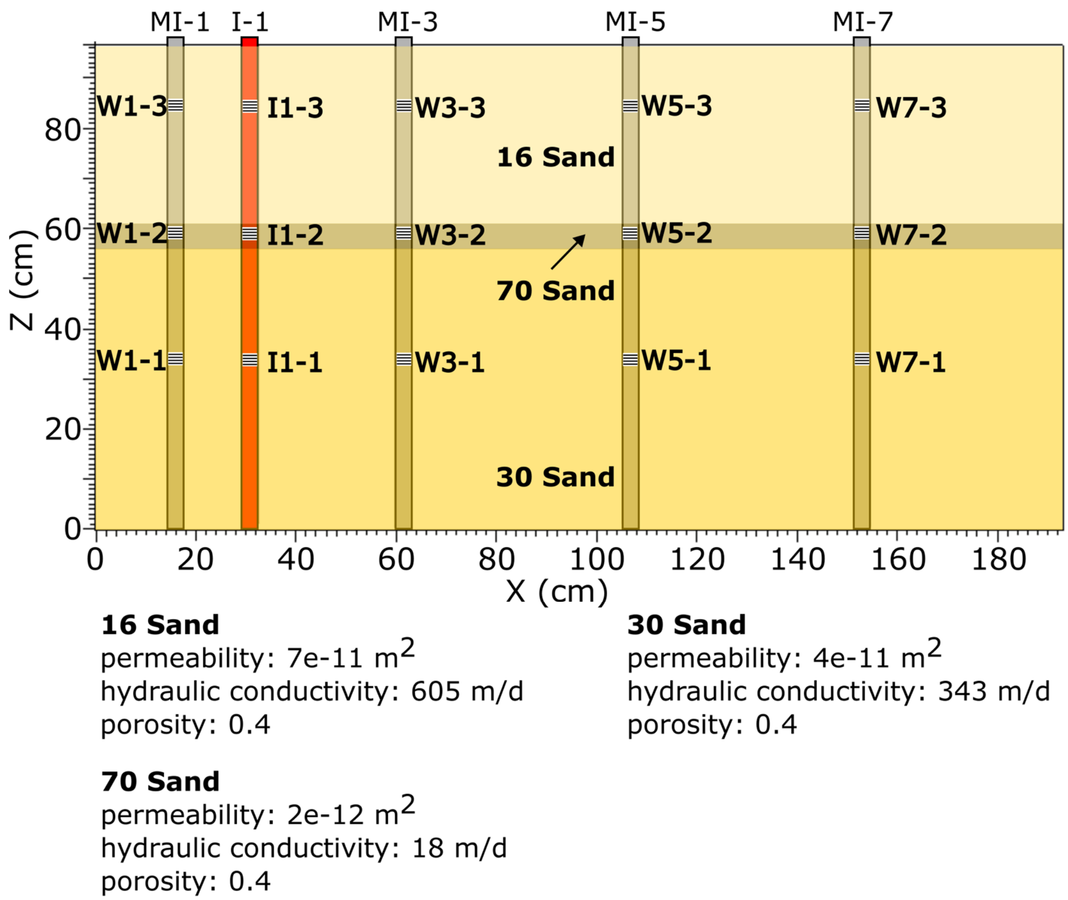

Figure 6. GIFT system sediment hydraulic property profile and port locations. Ports are used to inject, extract, and sample fluid, and to monitor pressure.

3.0 GIFT System PFLOTRAN Simulator

Numerical simulation plays two central roles in extracting information from monitoring data to produce useful predictions of subsurface behavior. First, it is used to train the AI-based calibration to interpret observation data in terms of the hydrogeologic properties that govern those observations. Second, after being calibrated, it is used predictively to design optimal liquid amendment delivery.

3.1 Forward Modeling

Forward modeling refers to the process of simulating observation data, given a specified set of hydrogeologic parameters, initial conditions, boundary conditions, and induced flow conditions. During the AI training processes, many forward simulations are executed to produce the monitoring observations (i.e., pressure, fluid conductivity, and raw ERT data) corresponding to pseudo-randomly chosen hydrogeologic parameters. The training process then uses the many parameter-observations pairs to teach the AI algorithm to predict tank hydrogeologic parameters (e.g., permeability, porosity) in each of the numerical model cells, given the monitoring observations, or equivalently to invert the monitoring data.

In FY25, a PFLOTRAN model of the GIFT system was constructed that can simulate flow and transport processes in GIFT, as well as the monitoring data resulting from those processes. For example, Figure 7 shows the results of a saline tracer injection simulation, given the hydrogeologic properties shown in Figure 6. Here, a head gradient of -2.0E-6 is established in the x-direction, and a saline fluid is injected at a rate of 50 ml/min into the central port in borehole I-1 for 12 hours, after which the tracer migrates with the pore water flow in the x-direction. The effects of the permeability variations in each of the three sediment layers are evident in this case, particularly the lack of tracer penetration into the low-permeability central zone. One objective of the planned demonstration is to use the AI-calibrated PFLOTRAN model to design an injection and extraction scheme to optimize amendment penetration into the low-permeability zone.

Figure 8 presents the simulated fluid conductivity monitoring data collected at the three monitoring ports in each of the eight monitoring boreholes. Pressure data time-series are also simulated at each port, and time-lapse ERT surveys are simulated every 30 minutes (not shown).

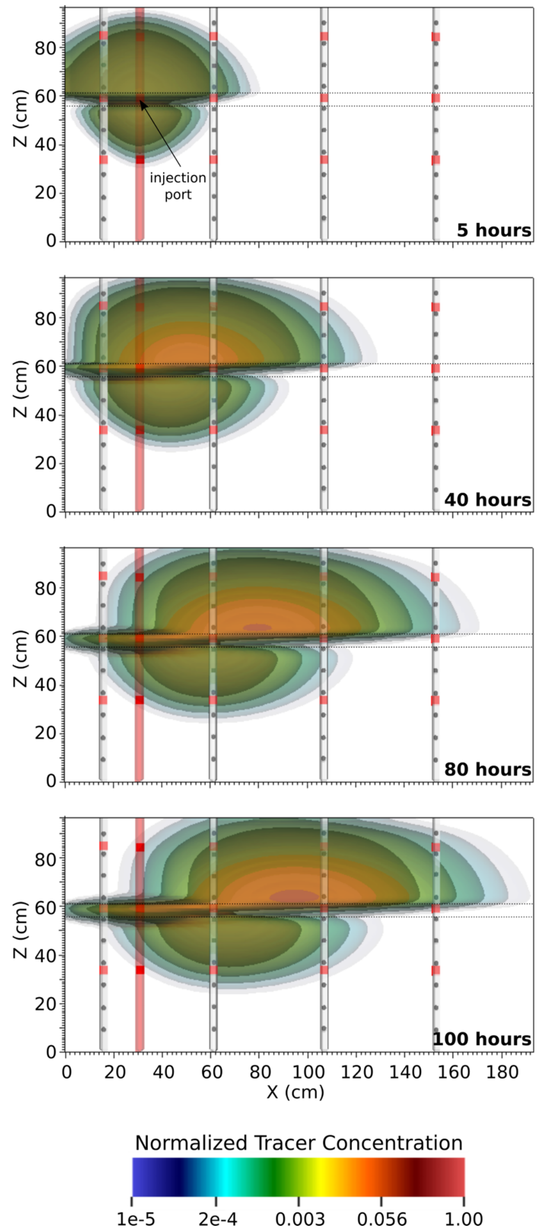

Figure 7. PFLOTRAN simulation of tracer migration given the hydrogeologic properties shown in Figure 6.

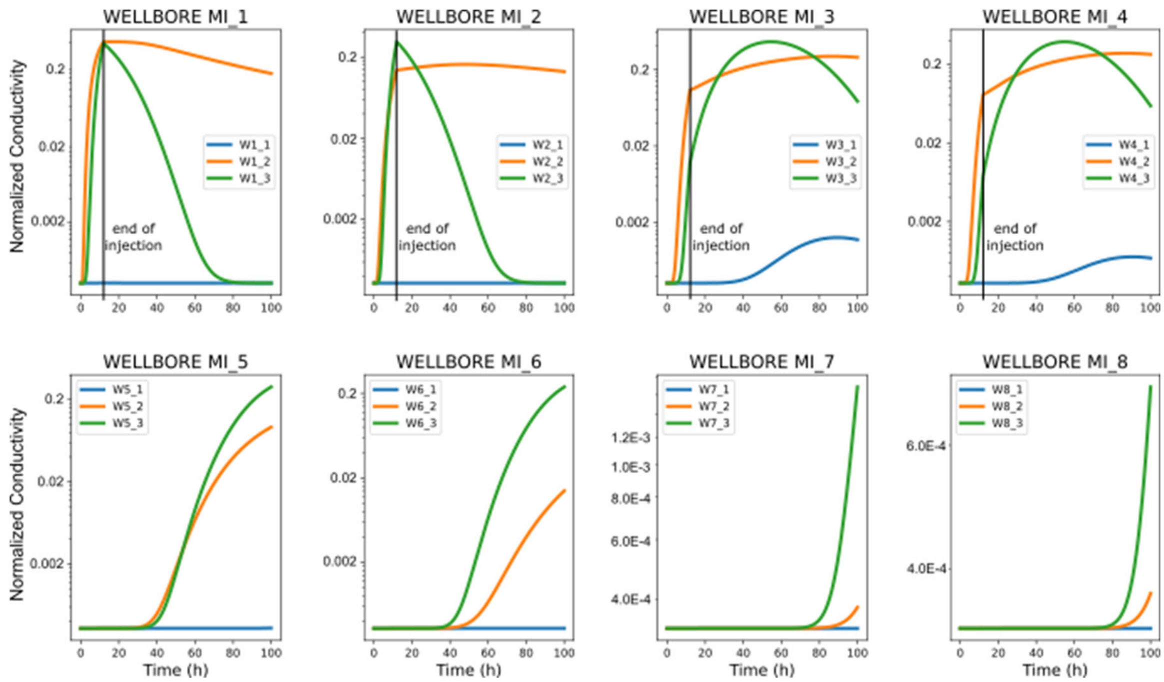

Figure 8. Simulated fluid conductivity (normalized to injectate conductivity) data collected at each fluid port in the eight monitoring borehole wells. Ports WX-1, WX-2, and WX-3 are the top, middle, and bottom ports, respectively, for wellbore MI-X.

4.0 Generative AI Inversion Using Conditional Diffusion Models

Conditional diffusion models (CDMs) have enabled recent breakthroughs in many AI and machine learning (ML) applications. For example, CDMs represent the current state-of-the-art in text-to-image generation, whereby text prompts (i.e., the conditions) are interpreted and a corresponding image matching the text prompt is generated. For the case at hand, the conditions are the observation data collected by the GIFT system, and the image is the corresponding spatial distribution of hydrogeologic properties that, when input into PFLOTRAN, reproduce the observation data.

The CDM will take as input a sequence of random numbers (i.e., noise) and observations, and then sequentially transform the noise into estimates of hydrogeologic properties in each of the numerical model cells. In principle, different random number sequences will produce different hydrogeologic property distributions, but each distribution will accurately reproduce the observations when input into PFLOTRAN. In this manner, an ensemble of equally probable hydrogeologic property distributions can be generated, which can be used to estimate uncertainty in both the hydrogeologic properties and the predictions produced by those properties. If the implicit information in the observations is relatively uninformative, the ensemble will contain a relatively high-variability hydrogeologic property estimate and high variability in the corresponding prediction simulations of tracer or amendment behavior within the tank. Conversely, if the implicit information in the observation data is relatively informative, each hydrogeologic sample in the ensemble will be relatively similar, as will the corresponding simulations of amendment behavior, each approaching true conditions.

The CDM inversion of GIFT observations will leverage a CDM-PFLOTRAN AI/ML framework previously developed on other projects. Applied to a vadose zone fluid problem, the CDM model was able to generate some hydrogeologic property distributions that honored time-lapse ERT observations very well, and others that were marginal. Although the CDM results achieved so far have far outperformed traditional approaches, we anticipate continued advancement in the AI-based inversion using the GIFT data in the future.

Training the CDM model requires many examples of hydrogeologic property distributions and corresponding observations generated by PFLOTRAN. It is anticipated that between 5K and 50K simulations will be required to adequately train the model. Although the computational requirements are easily tractable with a relatively small PFLOTRAN model like the GIFT system model, they may become onerous for larger field-scale applications. One objective of the demonstration will be to implement known approaches for reducing training data requirements. Active learning is one such approach, whereby the AI model will be trained to interpret only the actual observations as opposed to interpreting any possible set of observations.

5.0 Planned Experiments

DV-1 amendment monitoring, modeling, and prediction strategy demonstration will involve two separate injection experiments using the GIFT system: a saline tracer injection and a DV-1 liquid amendment treatment injection scenario.

5.1 Saline Tracer Injection

The primary objective of the saline tracer injection is to generate a monitoring dataset that will be used to calibrate the PFLOTRAN simulator, using the CDM-based joint inversion approach as described in Section 4.0. The injection will be designed based on the hydrogeologic properties shown in Figure 6, with targeted behavior like that shown in Figure 7. Specifically:

1. A y-normal flow gradient will be established within the tank with a targeted pore velocity of 2 cm/hour.
2. A saline tracer with fluid conductivity greater than the native pore fluid conductivity will be injected into the central port of the injection well for 5 to 12 hours, at a rate of 50 ml/min.
3. The saline tracer will be allowed to migrate though the GIFT tank downgradient, where it will exit the system. This is anticipated to require 150 to 200 hours.
4. Fluid pressure at each of the fluid ports will be recorded at 5-second intervals during the injection period, and hourly afterward.
5. Fluid conductivity at each of the fluid ports will be recorded every 30 minutes for the duration of the test.
6. 3D ERT surveys will be collected every 30 minutes for the duration of the test and inverted in real-time to track plume migration through the system.

5.2 Flow Model Calibration

CDM model training will occur in parallel with preparation for and execution of the tracer experiment so that monitoring data can be inverted once the injection is complete. As described in Section 4.0, the CDM model will be used to generate an ensemble of estimated hydrogeologic properties in each cell of the numerical model. These will be used to design a strategy to treat the low-permeability zone with a DV-1 amendment, as described in Section 5.3. Performance assessment of the CDM inversions will be achieved by comparing the CDM-estimated hydrogeologic property distributions with the actual distributions shown in Figure 6.

5.3 Predictive Simulation and Treatment Design

The PFLOTRAN models generated as described in Section 5.2 will be used to design an injection and extraction scheme aimed at optimizing treatment of the low-permeability zone with a DV-1 amendment (calcium polysulfide or polyphosphate). In this case, any of the fluid ports may be used to inject amendment or to extract fluid. Simulations of treatment scenarios will be used to identify those scenarios that are most likely to result in maximum penetration of amendment (in terms of volume contacted by amendment), given the uncertainty represented by the ensemble. Note that the treatment design effort will be human performed. ML-assisted design is not planned for this effort.

5.4 DV-1 Amendment Injection and Monitoring

Once a treatment design has been finalized, it will be executed in the GIFT tank. Like the saline tracer test amendment migration will be monitored using the fluid sampling ports and the ERT monitoring system to enable a comprehensive performance assessment. ERT imaging will be conducted in real-time to monitor amendment migration. At the conclusion of amendment injection, PFLOTRAN simulations will be conducted using the actual treatment metrics (e.g., injection rates and timings) to simulate the actual monitoring data. The actual monitoring data will be compared with the simulated monitoring to assess how well the PFLOTRAN models predicted actual delivery.

5.5 Long-Term ERT and IP Monitoring

Post delivery, the GIFT tank will be continuously monitored by the ERT system for image changes in bulk electrical conductivity and chargeability associated with amendment reactions. The spectral induced polarization (SIP) response of DV-1 amendments has been observed in laboratory experiments as an indicator of precipitation reactions that occur as part of the treatment process. The SIP response is governed by both physical and chemical changes at the pore grain interface and is therefore sensitive to the precipitation reactions anticipated in DV-1 amendment treatments.

One metric that summarizes the SIP response to precipitation reactions is chargeability: the ability of a medium to store electrical energy like a capacitor. Chargeability can also be sensed using a version of SIP called time-domain induced polarization (TDIP). In TDIP, the polarization response (which is measured as frequency dependent phase shift using SIP) is measured as a voltage decay curve when the driving current is turned off. Unlike SIP, TDIP responses can be measured using the ERT system. Although TDIP does not provide the spectral information content that SIP provides, chargeability imaging using TDIP is anticipated to indicate where precipitation (or dissolution) reactions are occurring. Therefore, long-term TDIP monitoring will then be used to determine if reactions are detectable using their chargeability response, and if so, when and where reactions occur.

At the end of the experiment, the GIFT system sediments will be destructively sampled to determine where amendments were delivered, and where reactions occurred. These data will enable an assessment of both the PFLOTRAN delivery predictions and the ERT/IP imaging. Since a 3-D sampling map of the PO_4-precipitated zone is needed, the destructive sampling will involve removing sediment in vertical lifts with samples taken in each vertical zone. Typically, significantly more samples are taken than are analyzed.

Selected samples will then be analyzed to define the precipitated zone. Gaps can be filled with analysis of additional unanalyzed samples in specific locations. For example, if a phosphate amendment was injected, there may be aqueous phosphate and precipitated phosphate. In that case, a water extraction on collected sediment samples is used for aqueous phosphate measurement and a weak acid extraction is used to dissolve the precipitated phosphate. Alternatively, if the calcium polysulfide amendment is used, then aqueous sulfide and sulfate and precipitated sulfides can be obtained from sediment samples post experiment, like what was described for phosphate.

6.0 Conclusions

This report highlights the progress made in FY25 on the development, integration, and application of the GIFT system to support advanced subsurface remediation strategies at the Hanford Site. Through simultaneous advancements in system assembly, sensor integration, and numerical modeling, including incorporation of AI-based inversion tools, the GIFT system has progressed into a platform for evaluating amendment injection and performance monitoring strategies in heterogeneous field-scale subsurface environments.

The planned experiments – including saline tracer validation, hydrogeologic property calibration using PFLOTRAN simulations, and subsequent demonstration of DV-1 amendment injection – are aimed at refining a predictive, field-transferable strategy for treating challenging low-permeability zones. The combination of real-time geophysical monitoring, advanced data inversion techniques, and numerical modeling underscores the potential of this integrated approach to reduce uncertainty, improve efficiency, and help validate the long-term efficacy of subsurface treatment technologies.

As the project transitions into its experimental phase, the insights gained will not only inform future field-scale applications but also contribute to the broader development of innovative tools and methodologies for managing vadose zone contamination. The GIFT system serves as a stepping stone in bridging laboratory-scale testing with the complexity of real-world environments, advancing the mission of the U.S. Department of Energy to develop sustainable and cost-effective remediation solutions.

7.0 References

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