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Decision Support for Aquifer Impact Remedial Response to CO₂ and Brine Leakage (A Web-App Tool Overview)

November 13-17, 2023

Presenter: Eusebius J Kutsienyo
Earth Scientist



**2023 Global Summit
on Environmental Remediation
@REMPLEX**



PNNL is operated by Battelle for the U.S. Department of Energy

Team Members: Pejman Rasouli, Eusebius J Kutsienyo, Ashton Kirol, Kyle Wilson, Nicolas J Huerta, Delphine Appriou





Outline

- National Risk Assessment Partnership (NRAP)
- Objectives of the environmental remediation response tool
- Approaches and remediation response strategies
- User interactive features of tool



About the National Risk Assessment Partnership

- **Goal:** develop computational tools and workflows to quantitatively assess risks and potential liabilities associated with geologic carbon storage and address critical stakeholder questions in **support of commercial CCUS deployment.**
- Research collaboration between five U.S. DOE national laboratories supporting geologic carbon storage deployment goals (2010 – present)

Approach:



Build the engine to identify and quantify risks associated with CO₂ injection, and design risk-based monitoring



Mature workflows to support stakeholder decision making on risk management and liability

Outcome:



Reduce uncertainty in risk and liability



Decrease cost for operators



Expedite risk evaluation





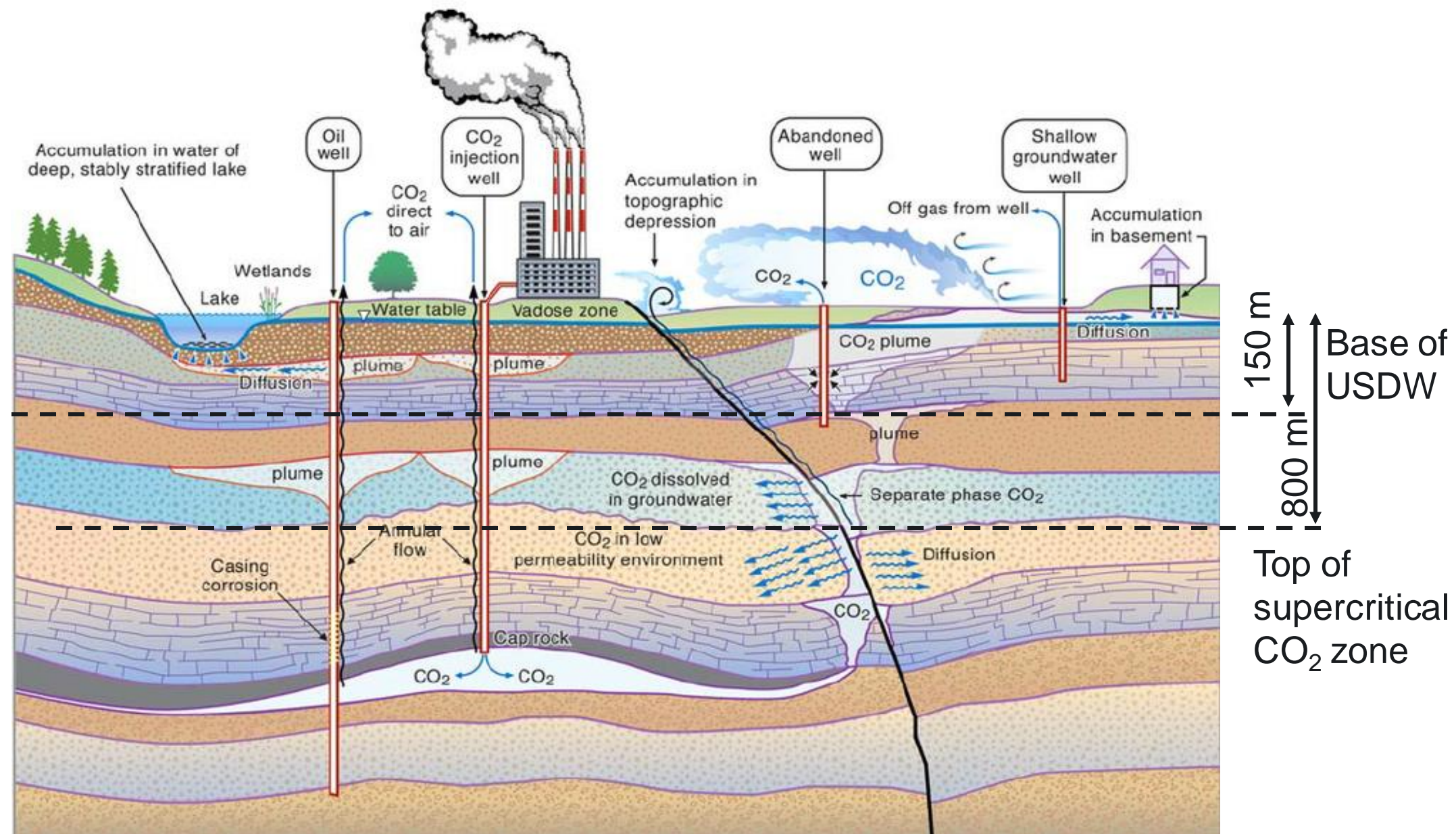
CO₂ Storage and Leakage Risk

Potential Pathways

- Wellbores
- Natural fractures and faults
- Caprock integrity
- Reservoirs boundaries

Potential Risks

- Aquifer impact
- Greenhouse gas emission
- Human health
- Economic risks
- Induced seismicity
- Infrastructure risks
- Ecological risks
- Reputational and public perception



Objectives

What are we developing?

- Decision support system for Environmental Remedial Responses (ERR) design and costs estimate for CO₂ and brine leakage risks in Geologic Carbon Storage (GCS) sites.
- Focus on CO₂ and brine leakage impacts on Underground Sources of Drinking Water (USDW) per EPA definition.
- Evaluates CO₂ or brine plume distribution over time in the impacted aquifer.
- Estimates potential leaked mass treatable, remediation time, and remediation costs.



Approach

How are we doing it?

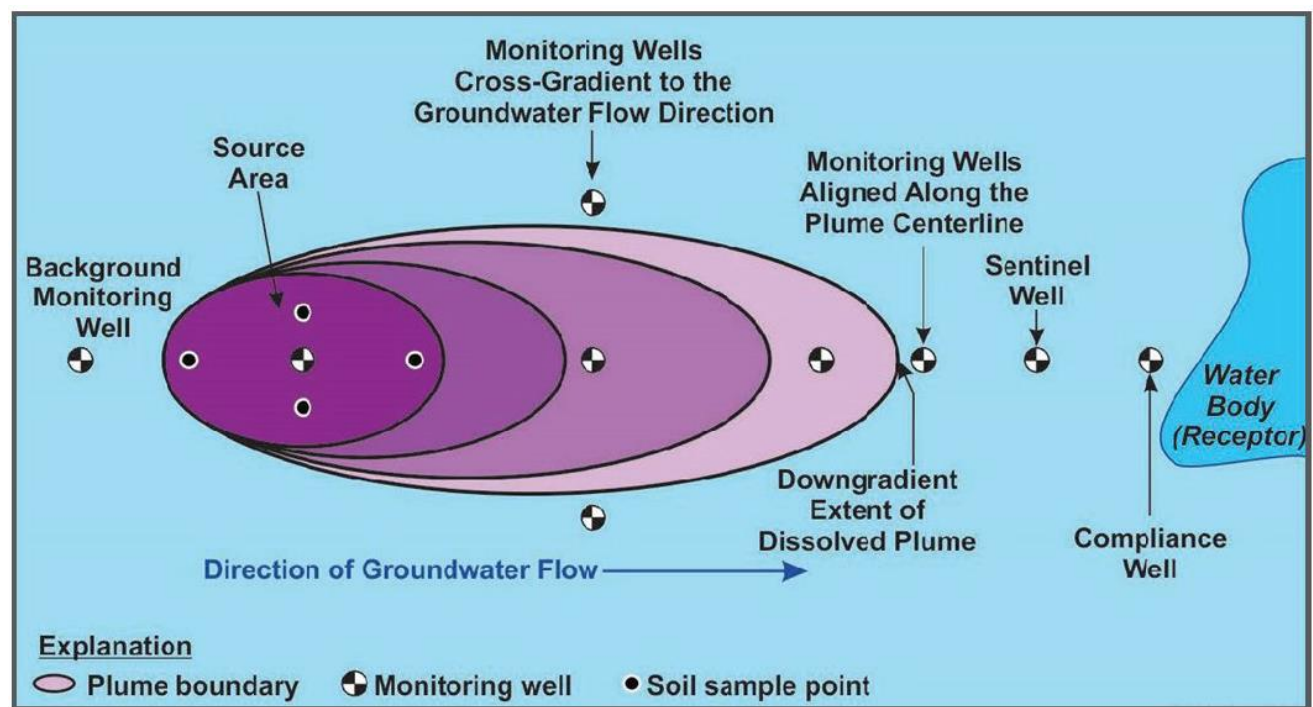
- Using analytical solutions to model fate and transport and extraction well capture zone.
- Utilizing interactive user interface and web-hosting capability to define the ERRs and compare their costs.
- Run Technoeconomic analysis (TEA) on the results to model the project cost.



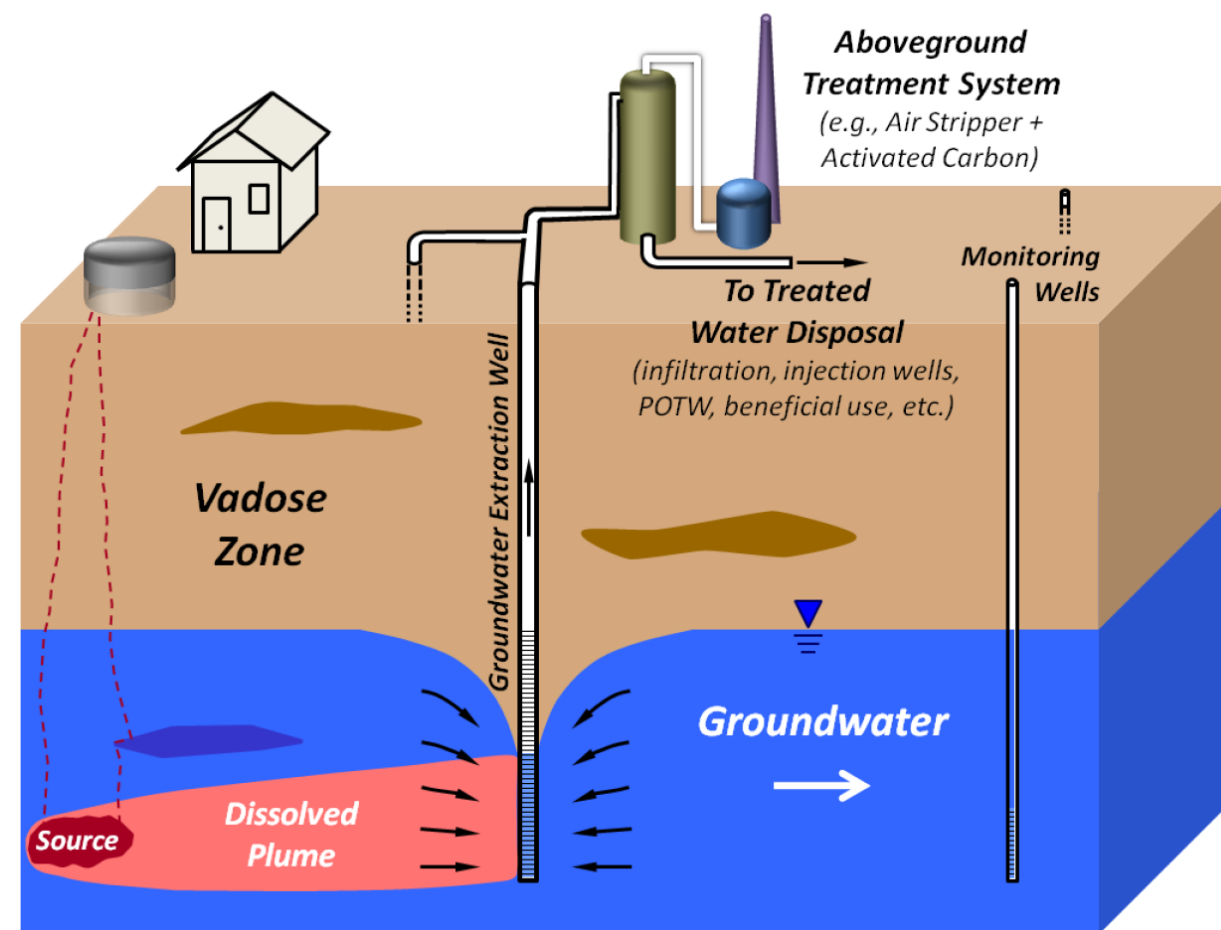
ERR Strategies & Designs

Supports two major environmental remediation response strategies:

1. Monitored Natural Attenuation (MNA)
2. Pump and Treat (P&T)



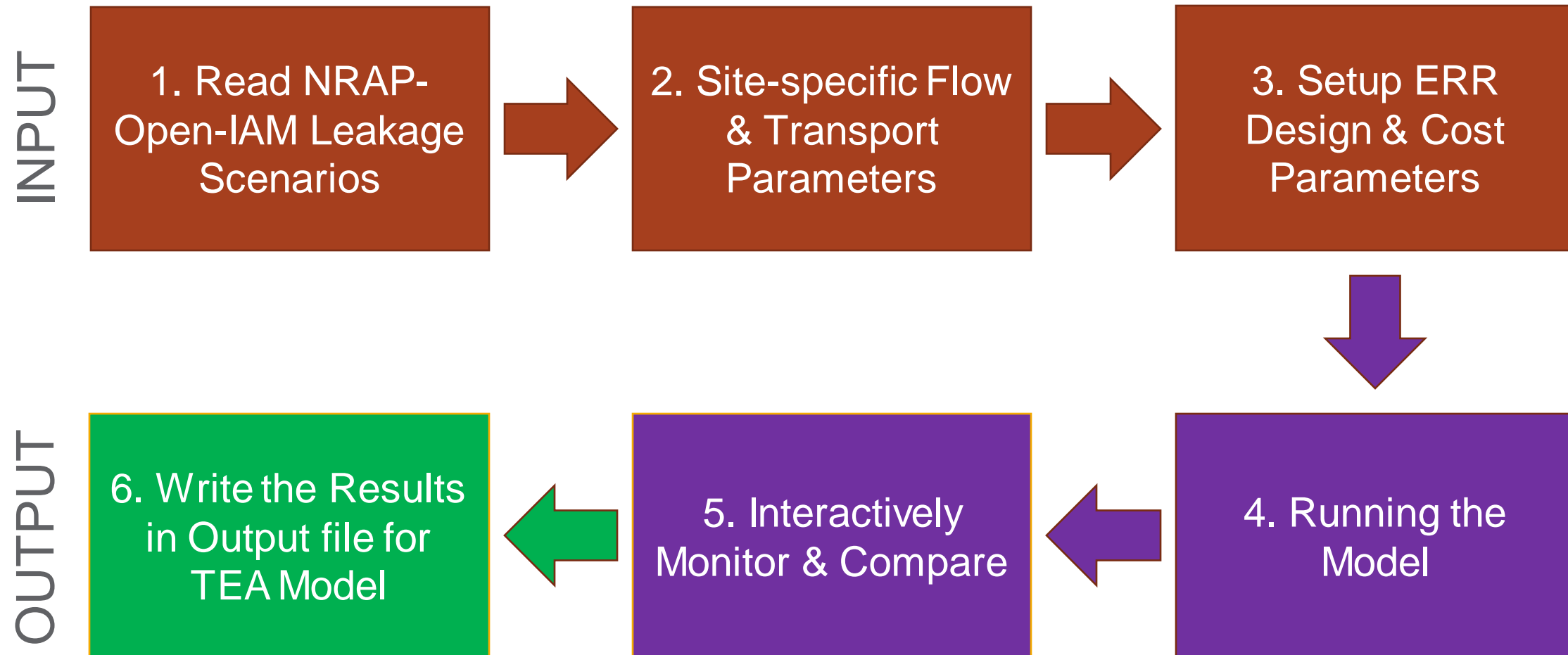
MNA schematic (Source: Federal Remediation Technologies Roundtable)



P&T profile (Source: PNNL-24696RPT-DVZ-AFRI-029)



User Interaction Workflow





Graphical User Interface



Select Response Method:

Pump and Treat

Input Parameters for Pump & Treat

Release Model:

- Impulse Release
- Continuous Release

Max. Concentration Level (MCL) [kg/m³]: Plot MCL

Pumping Rate [m³/day]:



Aquifer Thickness [m]:

Porosity:

Specific Storage [1/m]:

Hydraulic Conductivity [m/day]:

Hydraulic Gradient:

Mass [kg]:

Longitudinal Dispersivity [m]:

Transverse Dispersivity [m]:

Decay Coefficient [1/day]:

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Well Configuration

Well Name	X [m]	Y [m]	
Pumping Well	<input type="text" value="500"/>	<input type="text" value="0"/>	<input type="checkbox"/>
Monitoring Well 1	<input type="text" value="260"/>	<input type="text" value="-60"/>	<input type="checkbox"/>
Monitoring Well 2	<input type="text" value="320"/>	<input type="text" value="60"/>	<input type="checkbox"/>
Monitoring Well 3	<input type="text" value="94"/>	<input type="text" value="50"/>	<input checked="" type="checkbox"/>
Monitoring Well 4	<input type="text" value="94"/>	<input type="text" value="50"/>	<input type="checkbox"/>
Monitoring Well 5	<input type="text" value="605"/>	<input type="text" value="17"/>	<input type="checkbox"/>
Number of Additional Monitoring Wells:		<input type="text" value="5"/>	<input type="checkbox"/>
Well Sampling Option:	<input type="text" value="Set Universally"/>		
Sampling Frequency:	<input type="text" value="Quarterly"/>		
Number of Analytes:	<input type="text" value="10"/>		

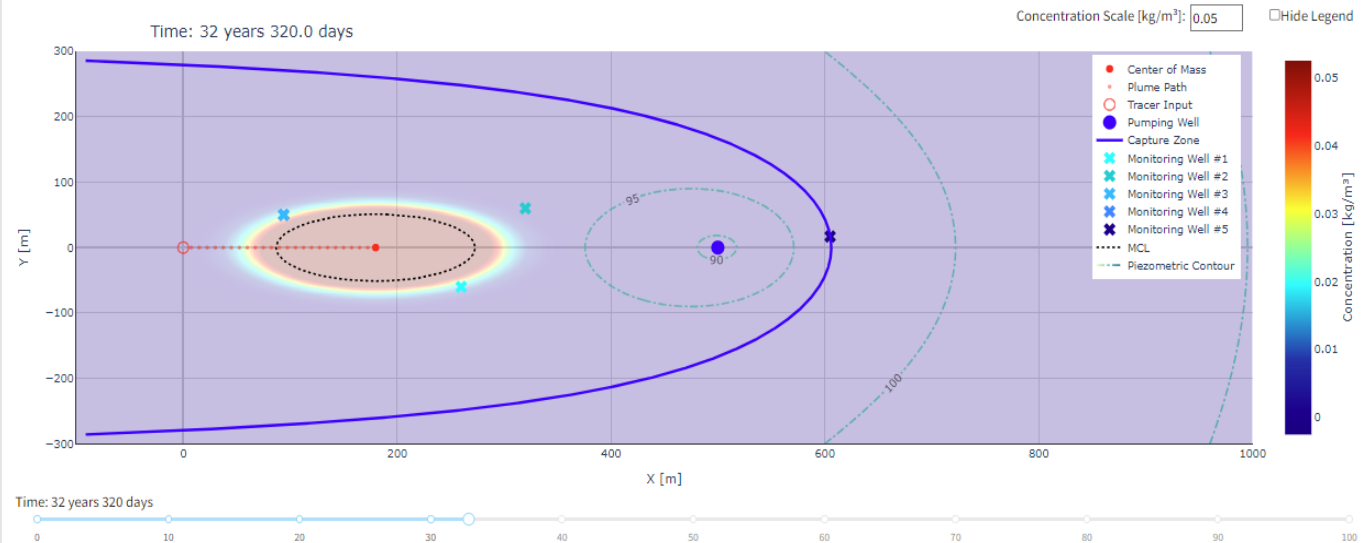
Information

Pejman Rasouli

Ashton Kirol

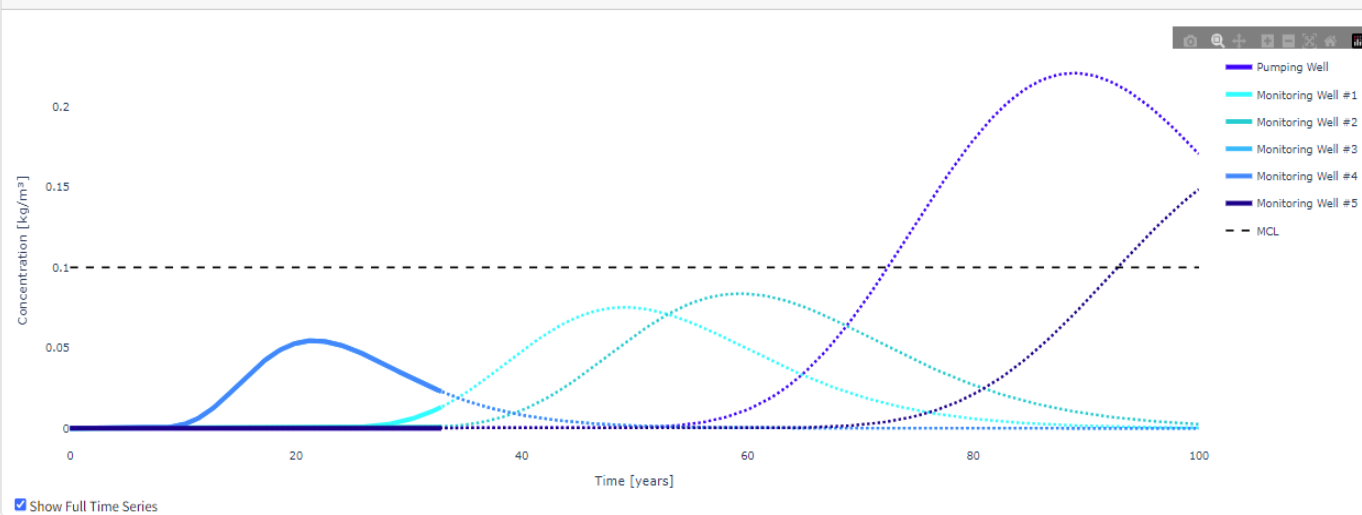
Eusebius Kutsienyo

Plume Migration and Capture Zone



Play/Stop Final Simulation Time (years): Time Step (days):

Monitoring Wells



System Performance Summary

Max. Concentration Level Area: 14,873.11 m²

Estimated Contaminant Mass: 834.10 kg

Estimated Cleanup Time: 91.78 Years

Estimated GW Removal Volume: 3,000,000 m³

Cost Analysis - Estimation

Cost Parameter	Unit Cost	
Subtotal		
Upfront Costs		\$1,220,000.00
Investigation and design cost:	<input type="text" value="150000"/>	\$150,000.00
Bench and Pilot Scale Tests:	<input type="text" value="500000"/>	\$500,000.00
Regulatory Program/ Oversight and Document Preparation:	<input type="text" value="20000"/>	\$20,000.00
Construction and Startup Costs:	<input type="text" value="550000"/>	\$550,000.00
Operational Costs		\$2,900,002.00
Process Activities:	<input type="text" value="1"/>	\$1.00
Performance Monitoring:	<input type="text" value="100"/>	\$2,400,000.00
Utilities, Raw Materials, and Waste Products:	<input type="text" value="150000"/>	\$150,000.00
Maintenance cost, routine and non-routine maintenance:	<input type="text" value="350000"/>	\$350,000.00
Demobilization and Site Restoration:	<input type="text" value="1"/>	\$1.00
Overall Total Cost:		\$4,120,002.00



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User Interface Workflow

1

Site Parameters for Monitored Natural Attenuation Pump & Treat

Input Parameters for Monitored Natural Attenuation

Release Model:
 Impulse Release
 Continuous Release

Max. Concentration Level (MCL) (kg/m³): Plot MCL

Aquifer Thickness (m):

Porosity:

Specific Storage (1/m):

Hydraulic Conductivity (m/day):

Hydraulic Gradient:

Mass (kg):

Longitudinal Dispersivity (m):

Transverse Dispersivity (m):

Decay Coefficient (1/day):

Input Parameters for Pump & Treat

Release Model:
 Impulse Release
 Continuous Release

Max. Concentration Level (MCL) (kg/m³): Plot MCL

Pumping Rate (m³/day):

Aquifer Thickness (m):

Porosity:

Specific Storage (1/m):

Hydraulic Conductivity (m/day):

Hydraulic Gradient:

Mass (kg):

Longitudinal Dispersivity (m):

Transverse Dispersivity (m):

Decay Coefficient (1/day):

Additional Monitoring Well

Well Configuration

Well Name	X [m]	Y [m]
Pumping Well	500	0
Number of Additional Monitoring Wells:	<input type="text" value="3"/>	
Monitoring Well 1	70	-70
Monitoring Well 2	440	-60
Monitoring Well 3	250	30

ERR Method Selection

Select Response Method:

Pump and Treat

Monitored Natural Attenuation

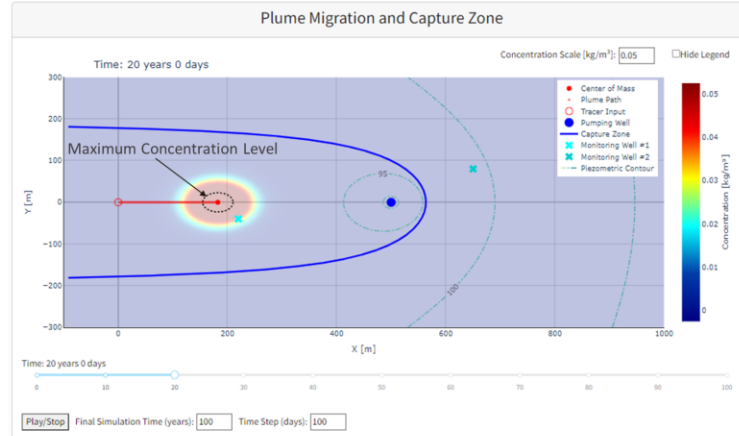
Design Parameters for MNA

Well Configuration

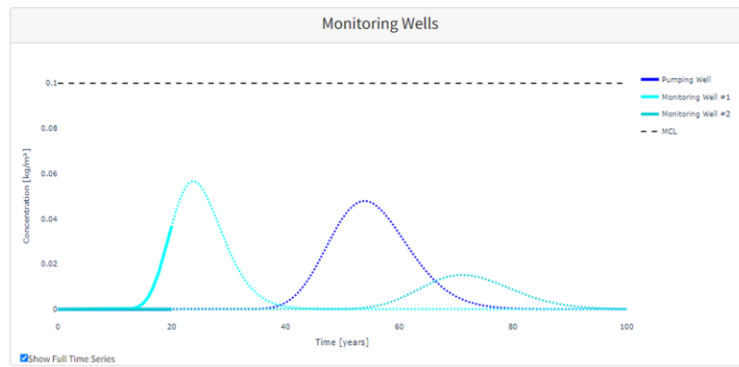
Well Name	X [m]	Y [m]
Background Monitoring Well	50	0
Source Area Well	0	0
Cross Gradient Wells	200	150
		0
		-150
Centerline Well #1	400	0
Centerline Well #2	500	0
Sentinel Well	600	0
Compliance Well	700	0
Number of Additional Monitoring Wells:	<input type="text" value="3"/>	
Monitoring Well 1	70	-70
Monitoring Well 2	440	-60
Monitoring Well 3	250	30

2

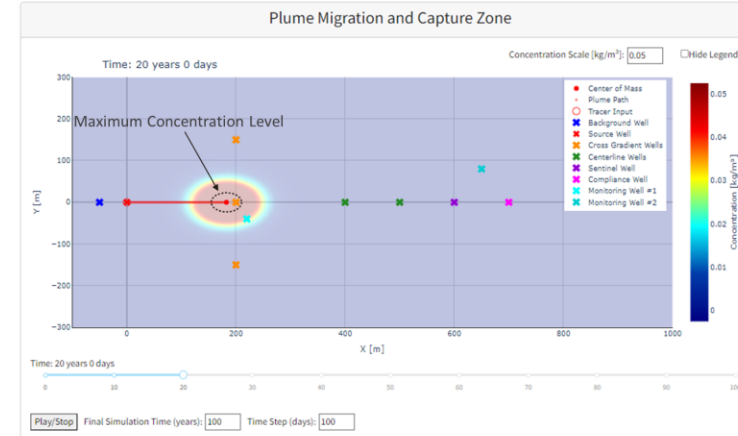
Plume Migration Output for Pump and Treat



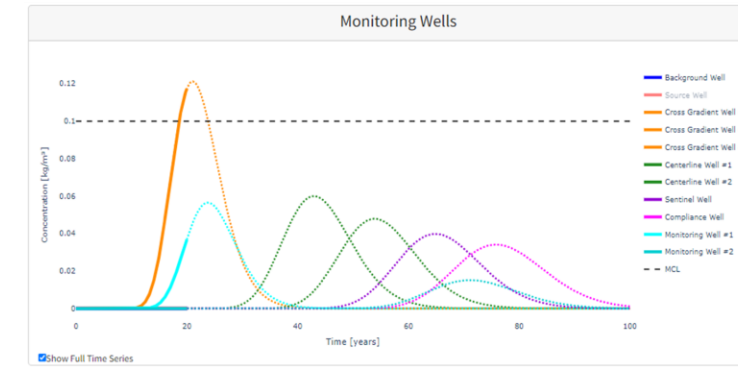
Concentration Breakthrough Output for Pump and Treat



Plume Migration Output for Monitored Natural Attenuation



Concentration Breakthrough Output Monitored Natural Attenuation



3

System Performance Summary

Max. Concentration Level Area: 1,952.58 m²

Estimated Contaminant Mass: 222.60 kg

Estimated Cleanup Time: 1,000.00 Years

Estimated GW Removal Volume: 1,000.00 m³

Response Method Information

Pump and Treat

Upfront Costs

- Investigation and design cost:
- Bench-and Pilot Scale Tests:
- Regulatory Program/ Oversight and Document Preparation:
- Construction and Startup Costs:

Operational Costs

- Process Monitoring:
- Performance Monitoring:
- Utilities, Raw Materials, and Waste Products:
- Maintenance cost, routine and non-routine maintenance:
- Demobilization and Site Restoration:

Panels Guide

- 1 Input Parameters Cards
- 2 Output Graphic Results
- 3 System Performance & Cost Parameters Output



NRAP-Open-IAM Interface

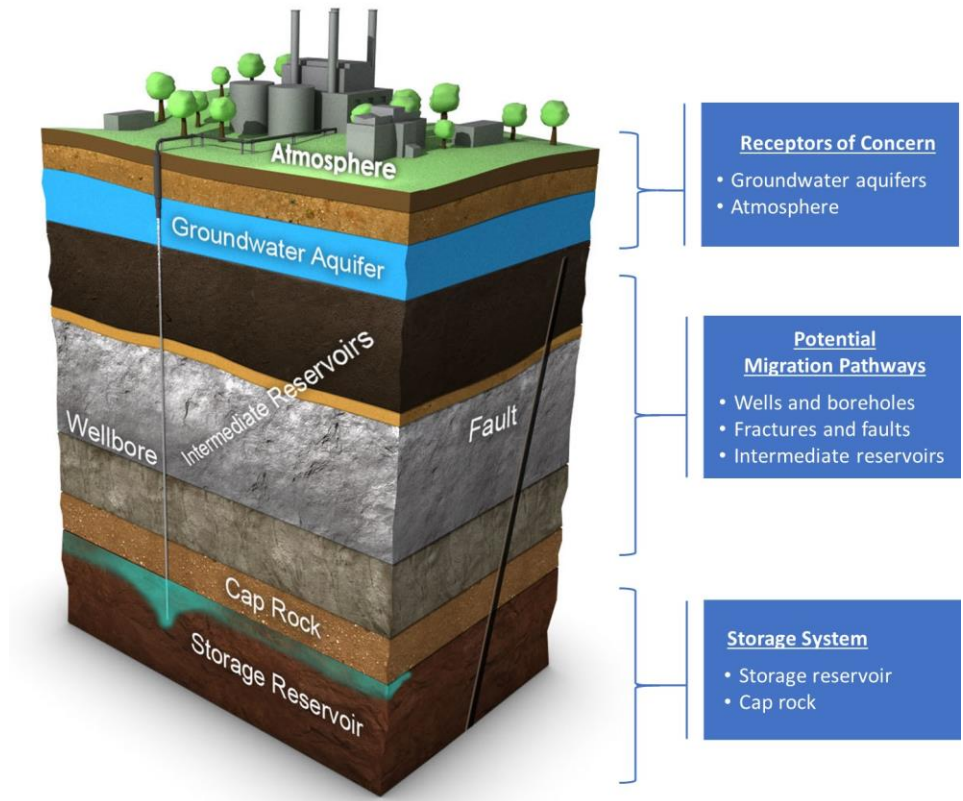
NRAP-Open-IAM answers questions about potential GCS site's ability to:

- Contain injected CO₂
- Protect groundwater and other environmentally sensitive areas
- Reduce atmospheric greenhouse gas emissions

By:

- Characterizing system features (reservoir, confining zones, leakage pathways, potential receptors)
- Defining potential unintended migration pathways
- Simulating response to planned injection
- Quantifying unintended migration risks and potential impacts

Vasyukivska, V., R. Dilmore, G. Lackey, Y. Zhang, S. King, D. Bacon, B. Chen, K. Mansoor and D. Harp (2021). "NRAP-open-IAM: A flexible open-source integrated-assessment-model for geologic carbon storage risk assessment and management." Environmental Modelling & Software 143. <https://gitlab.com/NRAP/OpenIAM>





User Interaction Features

Interactive web-based functionality let the user to:

- Input site-specific parameters:
 - hydraulic conductivity
 - aquifer thickness
 - porosity
 - gradient
 - dispersivity
 - decay rate
 - and more ...
- Select between scenarios:
 - continuous release
 - impulse release

➤ **Change parameters/scenarios on the fly and see the effect on the fly**

Select Response Method:

Monitored Natural Attenuation ▾

Pump and Treat

Monitored Natural Attenuation

Monitored Natural

1 Site Parameters for Monitored Natural Attenuation Pump & Treat

Input Parameters for Monitored Natural Attenuation

Release Model:
 Impulse Release
 Continuous Release

Max. Concentration Level (MCL) [kg/m³]: 0.1 Plot MCL

Aquifer Thickness [m]: 25

Porosity: 0.2

Specific Storage [1/m]: 0.0025

Hydraulic Conductivity [m/day]: 0.5

Hydraulic Gradient: 0.006

Mass [kg]: 1000

Longitudinal Dispersivity [m]: 0.1

Transverse Dispersivity [m]: 0.07

Decay Coefficient [1/day]: 0

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Input Parameters for Pump & Treat

Release Model:
 Impulse Release
 Continuous Release

Max. Concentration Level (MCL) [kg/m³]: 0.1 Plot MCL

Pumping Rate [m³/day]: 250

Aquifer Thickness [m]: 25

Porosity: 0.2

Specific Storage [1/m]: 0.0025

Hydraulic Conductivity [m/day]: 0.5

Hydraulic Gradient: 0.006

Mass [kg]: 1000

Longitudinal Dispersivity [m]: 0.1

Transverse Dispersivity [m]: 0.07

Decay Coefficient [1/day]: 0

Upload File

Additional Monitoring Well

Well Configuration

Well Name	X [m]	Y [m]
Pumping Well	500	0
Number of Additional Monitoring Wells:	3	
Monitoring Well 1	70	-70
Monitoring Well 2	440	-60
Monitoring Well 3	250	30

ERR Method Selection

Select Response Method:

Pump and Treat

Pump and Treat

Monitored Natural Attenuation

Design Parameters for MNA

Well Configuration

Well Name	X [m]	Y [m]
Background Monitoring Well	-50	0
Source Area Well	0	0
Cross Gradient Wells	200	150
		0
		-150
Centerline Well #1	400	0
Centerline Well #2	500	0
Sentinel Well	600	0
Compliance Well	700	0
Number of Additional Monitoring Wells:	3	
Monitoring Well 1	70	-70
Monitoring Well 2	440	-60
Monitoring Well 3	250	30



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Monitored Natural Attenuation (MNA)

- ✓ Design Monitoring Network (use template for MNA or modify it)
- ✓ Design Sampling Program: annual, semi-annual, quarterly, etc.
- ✓ Define number of analytes to sample
- ✓ Monitor concentration change over time

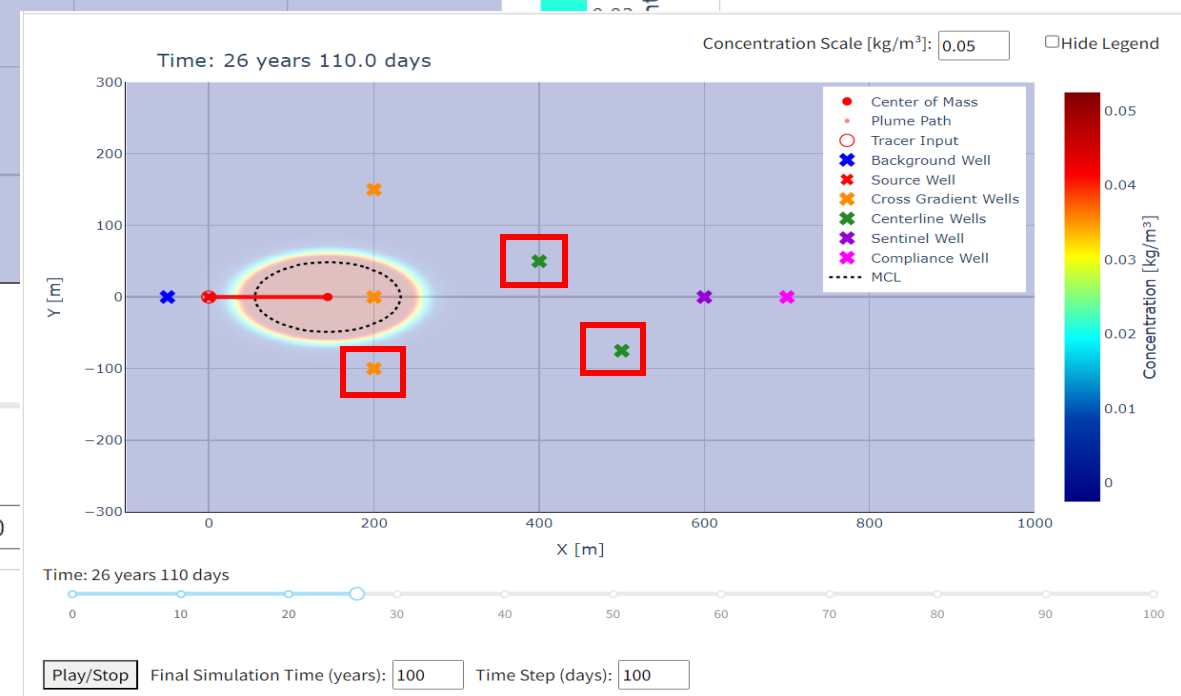
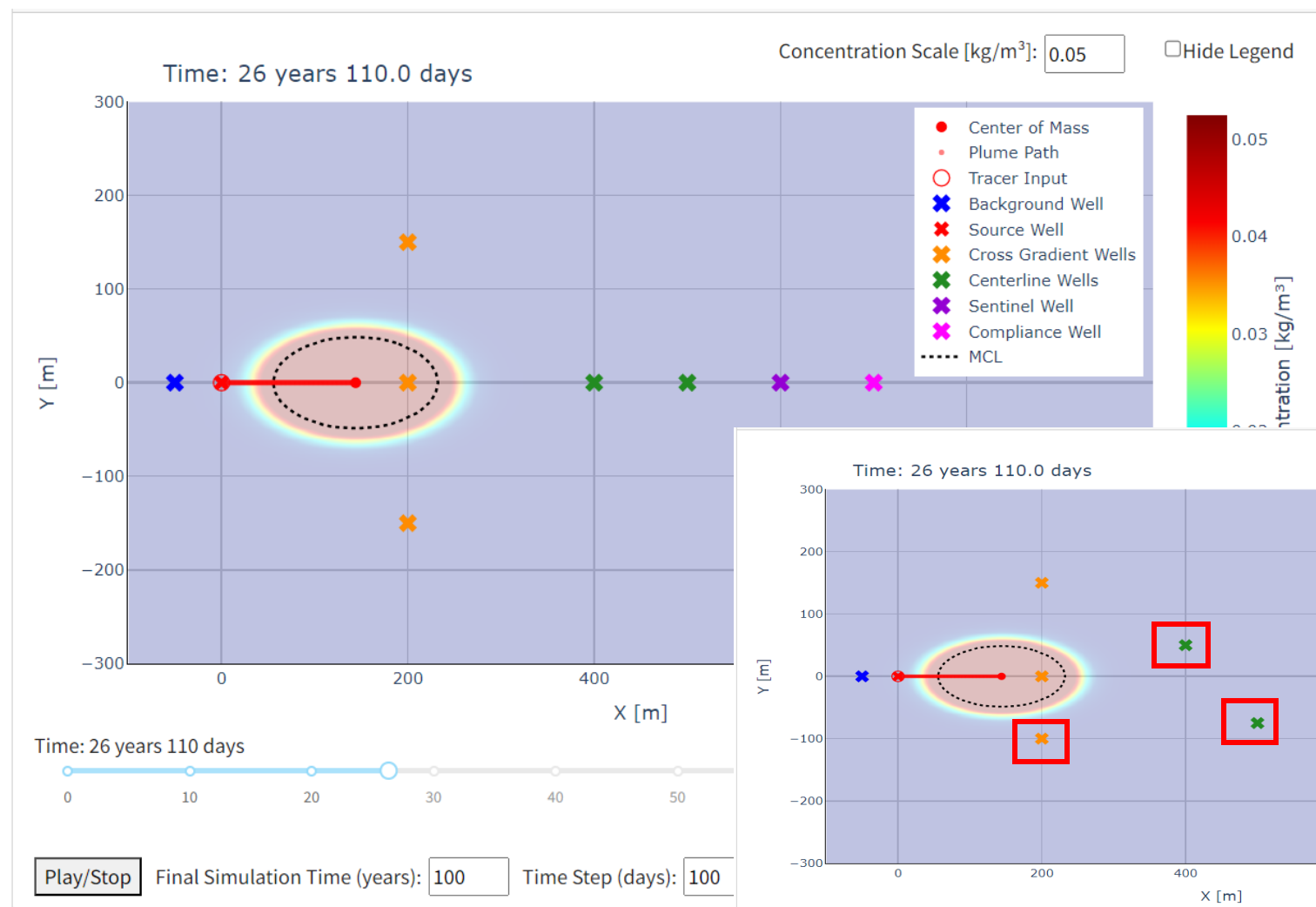
Well Configuration

Well Name	X [m]	Y [m]	
Background Monitoring Well	-50	0	<input type="checkbox"/>
Source Area Well	0	0	<input type="checkbox"/>
Cross Gradient Wells	200	150	<input type="checkbox"/>
		0	<input type="checkbox"/>
		-150	<input type="checkbox"/>
Centerline Well #1	400	0	<input type="checkbox"/>
Centerline Well #2	500	0	<input type="checkbox"/>
Sentinel Well	600	0	<input type="checkbox"/>
Compliance Well	700	0	<input type="checkbox"/>
Number of Additional Monitoring Wells:		0	<input type="checkbox"/>

Well Sampling Option:

Sampling Frequency:

Number of Analytes:





Pump and Treat (P&T)

- ✓ Select extraction well location
- ✓ Adjust extraction rate
- ✓ Assess capture zone
- ✓ Add monitoring wells as needed

Input Parameters for Pump & Treat

Release Model:
 Impulse Release
 Continuous Release

Max. Concentration Level (MCL) [kg/m³]: Plot MCL

Pumping Rate [m³/day]:

Aquifer Thickness [m]:

Porosity:

Specific Storage [1/m]:

Hydraulic Conductivity [m/day]:

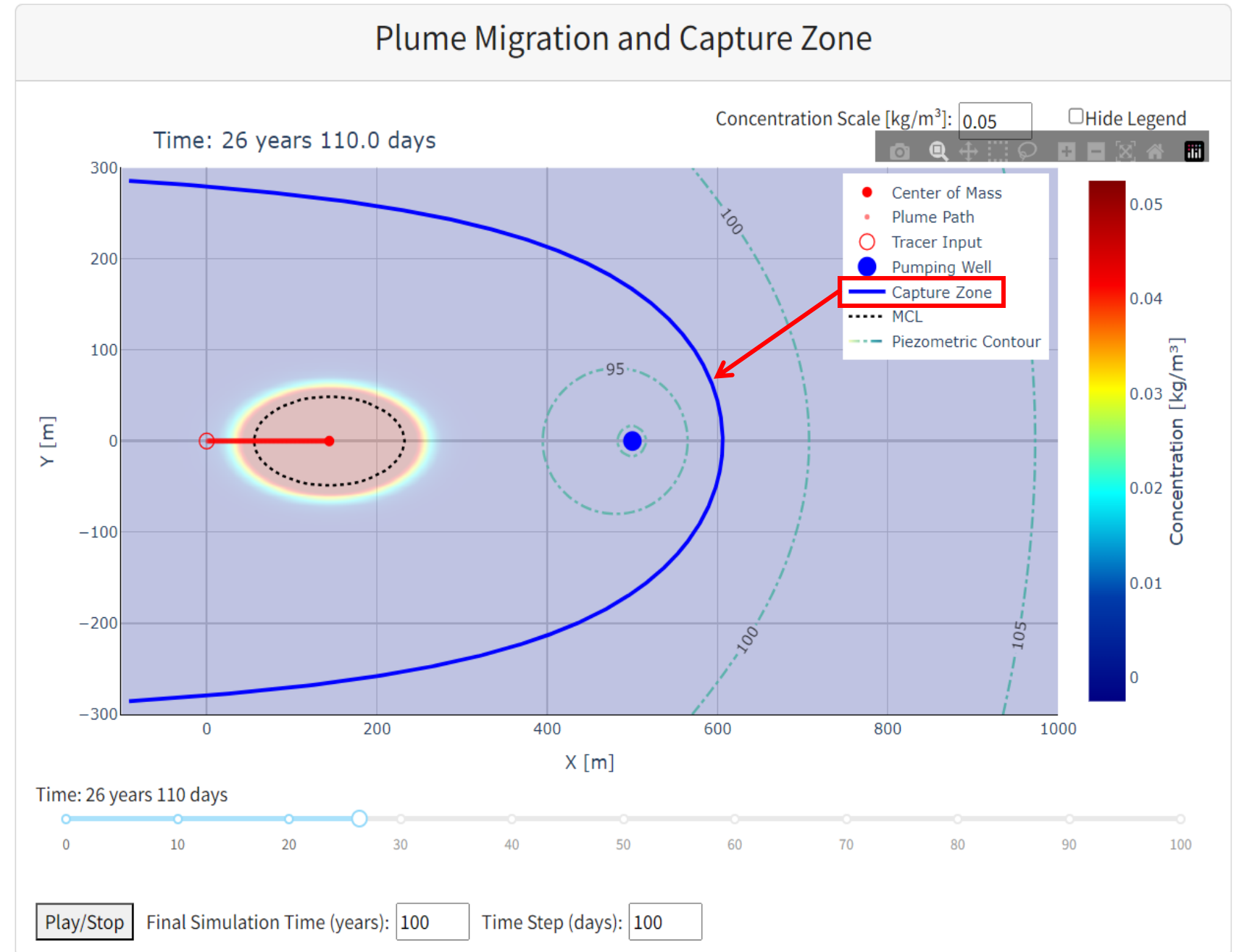
Hydraulic Gradient:

Mass [kg]:

Longitudinal Dispersivity [m]:

Transverse Dispersivity [m]:

Decay Coefficient [1/day]:

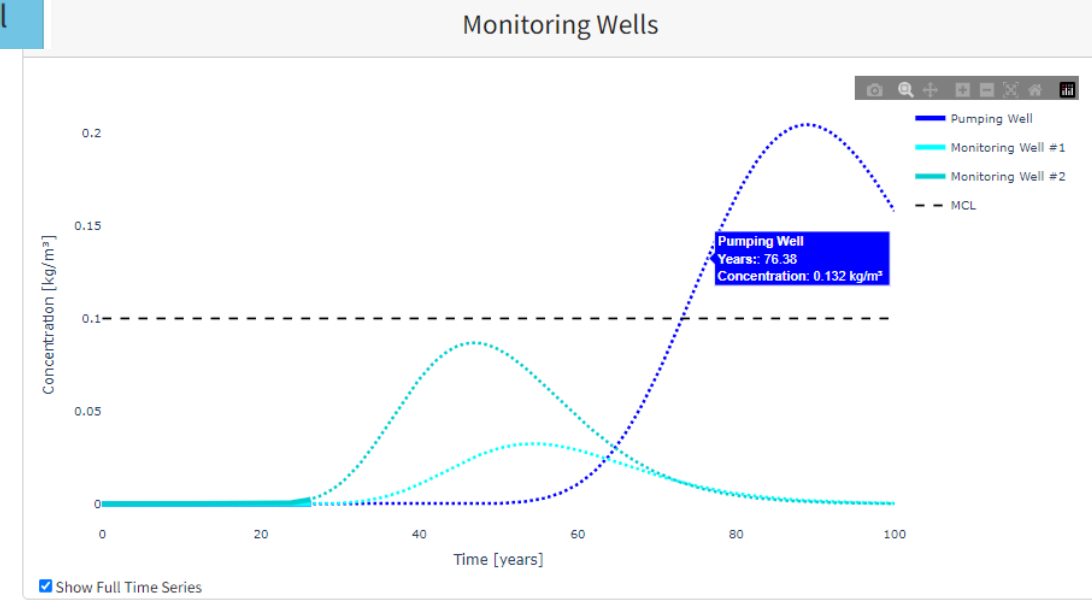
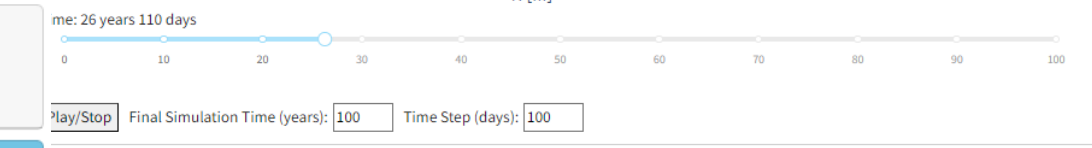
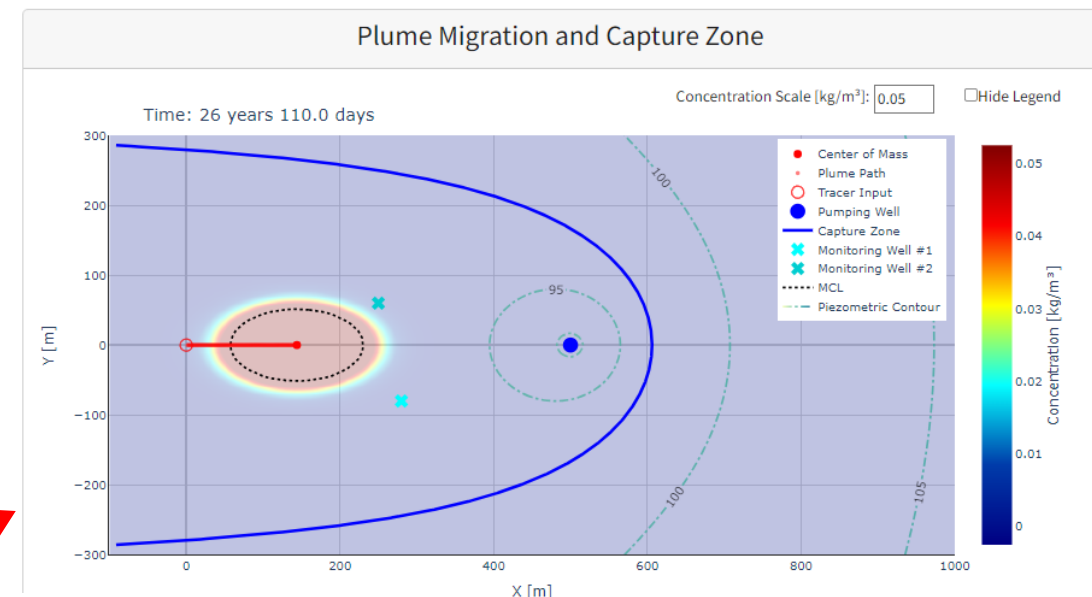
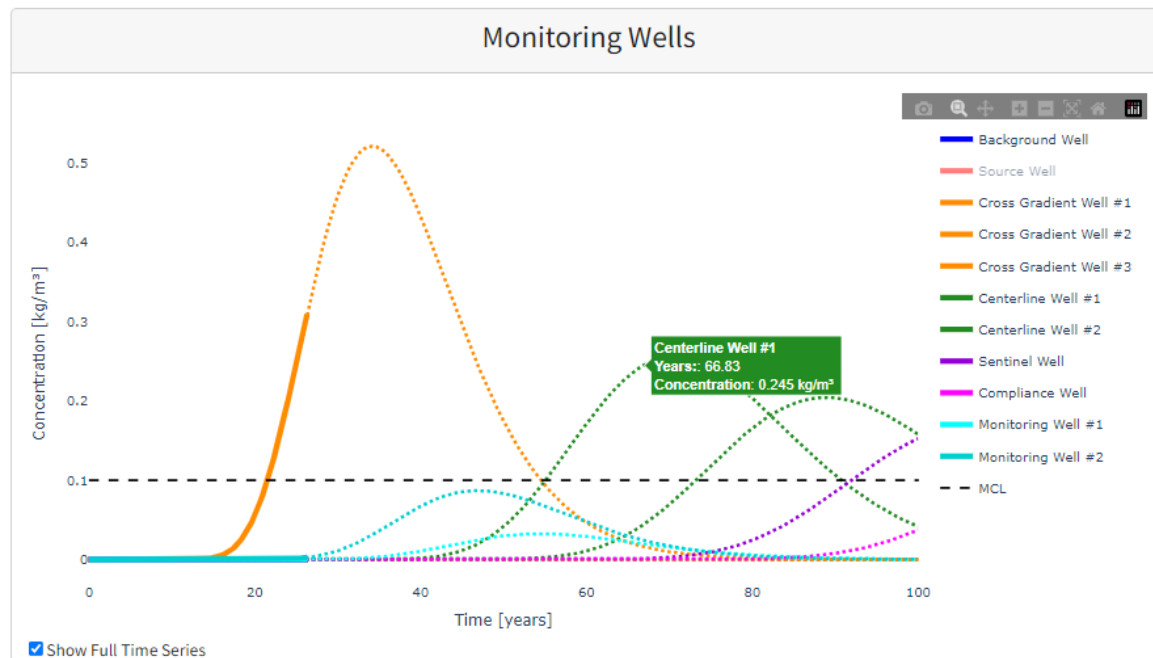
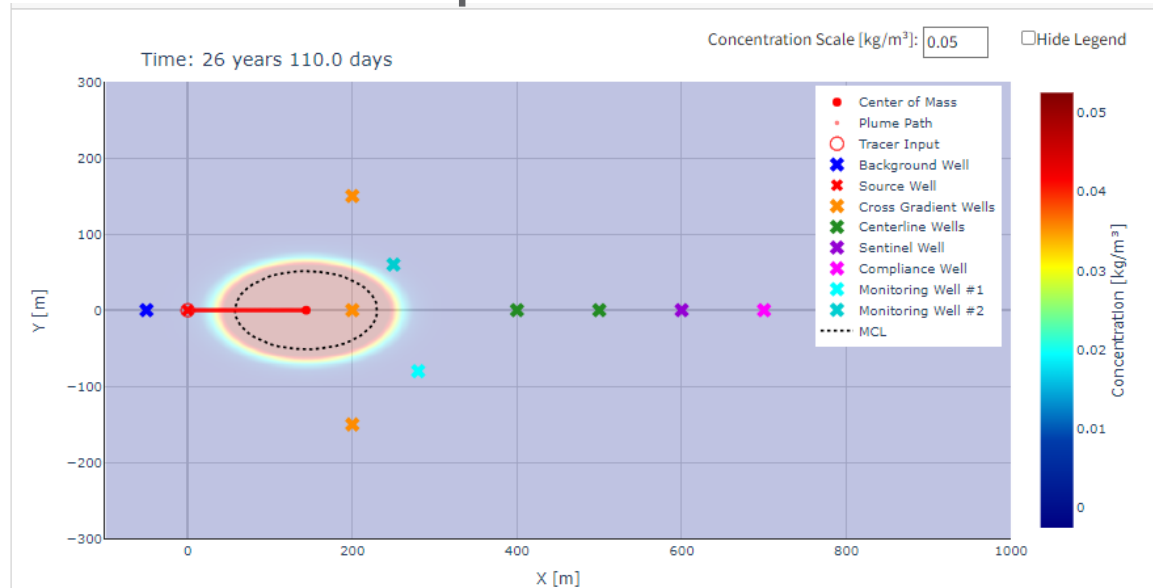




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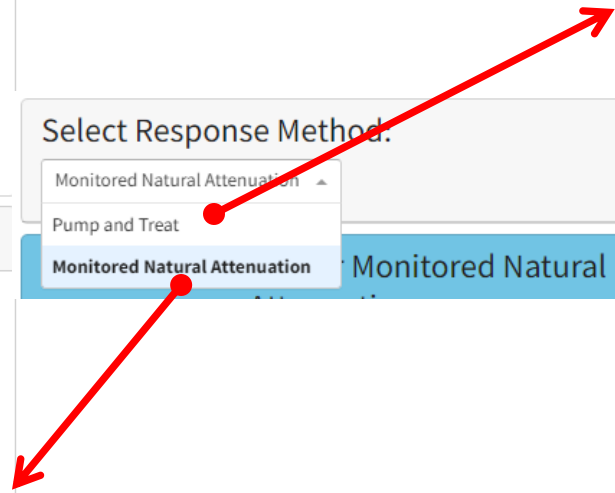
User Interaction Features

Run and compare scenarios simultaneously and switch between ERRs



Select Response Method:

- Monitored Natural Attenuation
- Pump and Treat
- Monitored Natural Attenuation**
- Monitored Natural





User Interaction Features

- Compare different ERR system performances and costs and see the system performance metrics:
 - Impacted area
 - Impacted water volume
 - Estimated mass to remove
 - Estimated remediation time
- Cost outputs are fed into a Technoeconomic Model to calculate Net Present Value (NPV) for the project.

3

System Performance Summary

Max. Concentration Level Area: 14,873.11 m²
Estimated Contaminant Mass: 834.10 kg
Estimated Cleanup Time: 91.51 Years
Estimated GW Removal Volume: 3,000,000 m³

Cost Analysis - Estimation

Cost Parameter		Unit Cost
Subtotal		
Upfront Costs		\$640,000.00
Investigation and design cost:	<input type="text" value="15000"/>	\$15,000.00
Bench and Pilot Scale Tests:	<input type="text" value="50000"/>	\$50,000.00
Regulatory Program/ Oversight and Document Preparation:	<input type="text" value="20000"/>	\$20,000.00
Construction and Startup Costs:	<input type="text" value="555000"/>	\$555,000.00
Operational Costs		\$510,002.00
Process Activities:	<input type="text" value="1"/>	\$1.00
Performance Monitoring:	<input type="text" value="100"/>	\$10,000.00
Utilities, Raw Materials, and Waste Products:	<input type="text" value="150000"/>	\$150,000.00
Maintenance cost, routine and non-routine maintenance:	<input type="text" value="350000"/>	\$350,000.00
Demobilization and Site Restoration:	<input type="text" value="1"/>	\$1.00
Overall Total Cost:		\$1,150,002.00

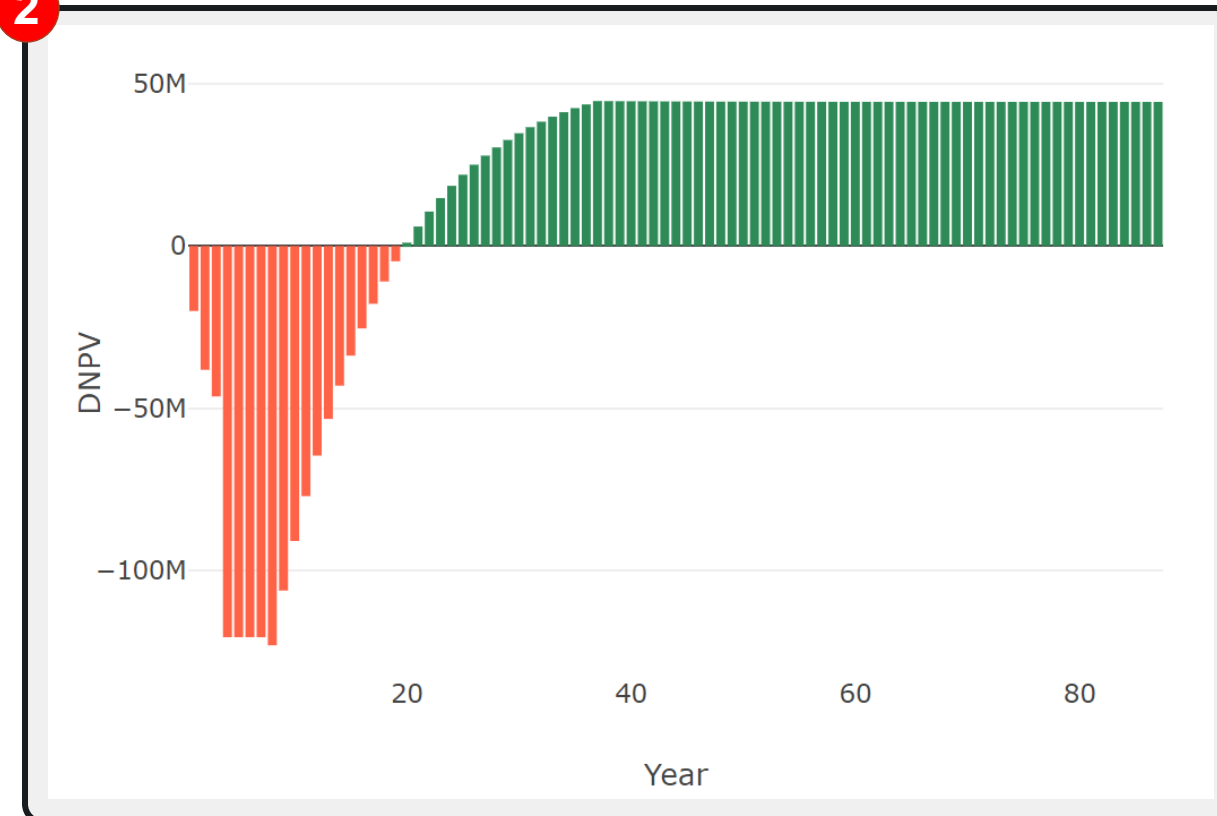


Technoeconomic Model Interface

1

Input Parameters for TEA	Financial Parameters	Event Parameters
Project Size (tons/Year) 30000	Price received (\$/ton) 19	Year that Event Begins (1 = first year of operation) 0
Construction Costs (\$) 1000000	Discount Rate (Equity) 0.15	Duration of Event (Years) 0
Construction Time (Years) 4	Discount Rate (Debt) 0.06	Initial (Fixed) Costs of Event (\$) 0
Operation Costs (\$/Year) 5000000	Percent Funding from Equity 0.5	Ongoing annual costs of event (\$/Year) 0
Operation Time (Years) 30	Federal Tax Rate 0.21	Plant Operation Parameters
Post-Injection Costs (\$/Year) 1000000	State Tax Rate 0.0884	Uptime (Days/Year) 365
Post_Injection Time (Years) 50		Efficiency at Start (%) 100
Siting Cost (\$/Year) 2000000		Efficiency Loss (%/Year) 0
Siting Time (Years) 2		
Site Selection and Screening Cost (\$/Year) 1000000		
Site Selection and Screening Time (\$/Year) 1		

2



3

Economic Metrics
levelized cost: 15.69 \$/tonne
NPV: \$ 44,349,715.48
Benefit-Cost-Ratio: 1.21



Concluding Remarks & Future Developments

- This tool is designed to enhance the decision-making capabilities of stakeholders and operators by providing a rapid and accessible means to assess potential environmental and economic impacts of CO₂ and brine leakage.
- It serves as a supplementary estimator, aiding in the decision-making process, rather than replacing the development of a Conceptual Site Model (CSM) or the in-depth analysis by numerical modeling.
- **Future Developments:**
 - More integration with NRAP-Open-IAM capabilities
 - Add more analytical solutions for other release scenarios and source terms
 - Coupling with numerical simulators
 - Deployment on-scale



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Thank you, Questions & Discussion

Acknowledgement:

Team Members: Pejman Rasouli, Eusebius J Kutsienyo, Ashton Kirol, Kyle Wilson, Nicolas J Huerta, Delphine Appriou.



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Supporting Slides



Future Developments

- Future Developments:
 - More integration with Open-IAM Capabilities
 - Extend to more analytical solutions for other release scenarios and source terms
 - Coupling with numerical simulators
 - Deployment on-scale



Monitored Natural Attenuation (MNA)

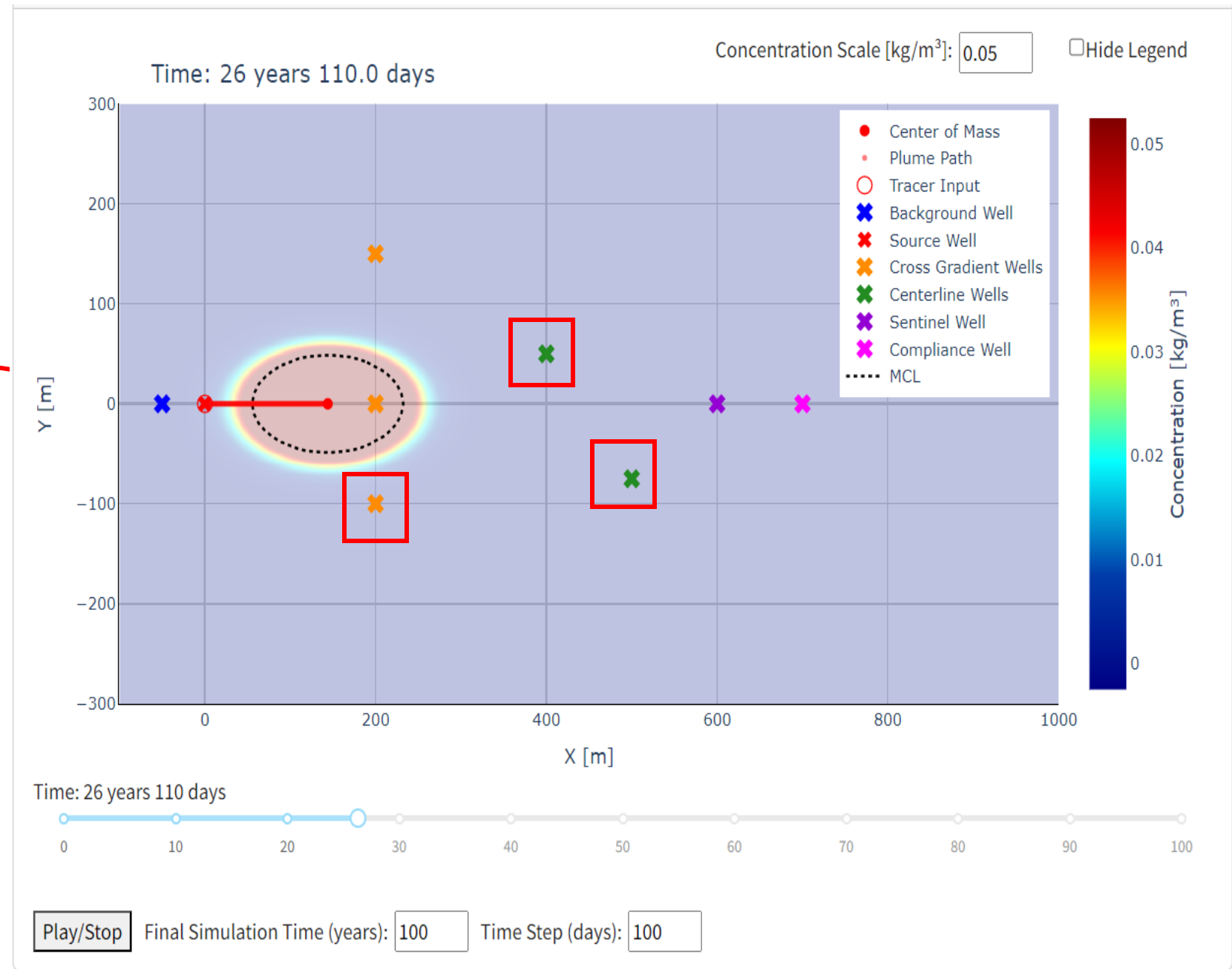
Well Configuration

Well Name	X [m]	Y [m]	
Background Monitoring Well	-50	0	<input type="checkbox"/>
Source Area Well	0	0	<input type="checkbox"/>
Cross Gradient Wells	200	150	<input type="checkbox"/>
		0	
		-100	
Centerline Well #1	400	50	<input checked="" type="checkbox"/>
Centerline Well #2	500	-75	<input type="checkbox"/>
Sentinel Well	600	0	<input type="checkbox"/>
Compliance Well	700	0	<input type="checkbox"/>
Number of Additional Monitoring Wells:		0	<input type="checkbox"/>

Well Sampling Option:

Sampling Frequency:

Number of Analytes:





Technoeconomic Model Interface

- Technoeconomic Model (TEA):
 - Combines technical and economic data.
 - Assesses viability and feasibility of CCS technology.
 - Aids in decision-making by predicting costs, benefits, and risks.

Many parameters go into a TEA such as performance metrics, operational costs, capital expenditures, and projected revenues.

Project Parameters
Project Size (tons/Year)
Construction Costs (\$)
Construction Time (Years)
Operation Costs (\$/Year)
Operation Time (Years)
Post-Injection Costs (\$/Year)
Post Injection Time (Years)
Siting Cost (\$/Year)
Siting Time (Years)
Site Selection and Screening Cost (\$/Year)
Site Selection and Screening Time (\$/Year)
Financial Parameters
Price received (\$/ton)
Discount Rate (Equity)
Discount Rate (Debt)
Percent Funding from Equity
Federal Tax Rate
State Tax Rate
Event Parameters
Year that Event Begins (1 = first year of operation)
Duration of Event (Years)
Initial (Fixed) Costs of Event (\$)
Ongoing annual costs of event (\$/Year)
Plant Operation Parameters
Uptime (Days/Year)365
Efficiency at Start (%)
Efficiency Loss (%/Year)



Introduction: Development Team & Tool

- Developed by Pacific Northwest National Laboratory (**PNNL**), as part of National Risk Assessment Partnership (**NRAP**) program.
- **Team Members:** Eusebius J Kutsienyo, Ashton Kirol, Kyle Wilson, Nicolas J Huerta, Delphine Appriou, Pejman Rasouli.
- Web-based platform for site-specific decision support.



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User Interaction Features

Input and estimate ERR costs:

- Upfront Costs
 - ✓ Investigation and design cost
 - ✓ Bench and pilot scale tests
 - ✓ Regulatory program/ oversight and document preparation
 - ✓ Construction and startup costs:
- Operational Costs
 - ✓ Process activities
 - ✓ Performance monitoring
 - ✓ Utilities, raw materials, and waste products
 - ✓ Routine and non-routine costs
 - ✓ Demobilization and site restoration



User Interaction Features

- Interactive web-based functionality let the user to:
 1. Connect to OPEN-IAM to read Leakage Scenarios by:
 - Using aquifer component of OPEN-IAM to run forward or stochastic leakage scenarios
 - Read OPEN-IAM output files (*.csv) and populates required field
 2. Read site-specific flow and transport parameters (i.e. hydraulic conductivity, aquifer thickness porosity, gradient, dispersivity, decay rate, etc.)



User Interaction Features

Design Environmental Remedial Responses:

- Monitored Natural Attenuation (MNA):
 - ✓ Design Monitoring Network (use template for MNA or modify it)
 - ✓ Design Sampling Program: annual, semi- annual, quarterly, etc.
 - ✓ Define number of analytes to sample
 - ✓ Monitor concentration change over time

- Pump and Treat (P&T):
 - ✓ Select extraction well location
 - ✓ Adjust extraction rate
 - ✓ Assess capture zone
 - ✓ Add monitoring wells as needed