

DOE-FIU Cooperative Agreement Annual Research Review – FIU Year 2

Tuesday, September 27, 2022

9:30 - 9:35 am EDT	Kick-Off /Welcoming Remarks (DOE-EM)	Kurt Gerdes (Director, Technology Development) – DOE EM-3.2
9:35 - 9:40 am EDT	Welcoming Remarks (DOE-LM)	Leonel Lagos on behalf of DOE Office of Legacy Management
9:40 - 10:00 am EDT	Projects 4 & 5: STEM Workforce Development and Training	FIU, DOE HQ (EM & LM), SRNL, PNNL, WIPP, SRS, ORP, LBNL, WRPS, INL, Grand Junction
BREAK		
11:00 - 12:00 pm EDT	Projects 4 & 5 (cont'd): STEM Workforce Development and Training	FIU, DOE HQ (EM & LM), SRNL, PNNL, WIPP, SRS, ORP, LBNL, WRPS, INL, Grand Junction
BREAK		
1:00 - 2:30 pm EDT	Project 1: Chemical Process Alternatives for Radioactive Waste	FIU, DOE HQ, PNNL, WRPS, SRNL, SRS
2:30 - 4:00 pm EDT	Project 3: Waste and D&D Engineering & Technology Development	FIU, DOE HQ, SRNL, PNNL, LBNL, INL, ANL

Wednesday, September 28, 2022

10:00 - 11:30 am EDT	Project 2: Environmental Remediation Science & Technology	FIU, DOE HQ, SRNL, PNNL, ORNL, LANL, CBFO
11:30 - 1:00 pm EDT	Wrap Up (FIU Projects 1, 2, 3, 4 & 5)	FIU, DOE HQ (EM & LM)



DOE-FIU Cooperative Agreement Annual Research Review – FIU Year 2

PROJECT 2

Environmental Remediation Science & Technology





FIU Personnel and Collaborators

Principal Investigator: Leonel Lagos

Project Manager: Yelena Katsenovich

Faculty/Staff: Ravi Gudavalli, John Dickson, Vadym Drozd, Angelique Lawrence, Pieter Hazenberg

Postdoctoral Fellows: *Hamid Bazgirkhoob

DOE Fellows/Students: *Juan Morales, *Gisselle Gutierrez, Mariah Doughman, Phuong Pham, Stevens Charles, Angel Almaguer, Caridad Estrada, Aubrey Litzinzger.

DOE-EM: Genia McKinley, Kurt Gerdes, *Paul Beam, Skip Chamberlain, Nick Machara, John Mocknick, Karen Skubal

DOE-SRS: Jeff Crenshaw, Nixon Peralta

SRNL: Brian Looney, Hansell Gonzalez-Raymat, Carol Eddy-Dilek, Mark Amidon, Bruce Wiersma, Connie Herman, Brady Lee

SREL: *John Seaman, Daniel Kaplan

LBNL: Haruko Wainwright, Zexuan Xu

PNNL: *Vicky Freedman, Rob Mackley, Nik Qafoku, Jim Szecsody, Hilary Emerson, Matthew Asmussen

LANL: Paul Dixon, Don Reed, Juliet Swanson, David Moulton

DOE-CBFO: Anderson Ward

ORNL: Eric Pierce, Alexander Johs

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*Former staff/student contributors



Project Tasks and Scope

TASK 1: REMEDIATION RESEARCH AND TECHNICAL SUPPORT FOR THE HANFORD SITE

- | | |
|--------------------|---|
| Subtask 1.2 | Re-oxidation of Redox Sensitive Contaminants Immobilized by Strong Reductants |
| Subtask 1.3 | Eval. of Competing Attenuation Processes for Mobile Contaminants in Hanford Sediments |
| Subtask 1.4 | Experimental Support of Lysimeter Testing |

TASK 2: REMEDIATION RESEARCH AND TECHNICAL SUPPORT FOR THE SAVANNAH RIVER SITE

- | | |
|--------------------|---|
| Subtask 2.1 | Environmental Factors Controlling the Attenuation and Release of Contaminants in the Wetland Sediments at Savannah River Site |
| Subtask 2.2 | Investigating the Effect of KW-30 (Humate Material) on the Removal of Uranium |

TASK 3: CONTAMINANT FATE AND TRANSPORT MODELING FOR THE SAVANNAH RIVER SITE

- | | |
|--------------------|---|
| Subtask 3.1 | Modeling of Surface Water Flow and Contaminant Transport in the Tims Branch Ecosystem |
| Subtask 3.2 | Model Development for Fourmile Branch with Specific Focus on the F-Area Wetlands |

TASK 5: RESEARCH AND TECHNICAL SUPPORT FOR WIPP

- | | |
|--------------------|---|
| Subtask 5.2 | Fate of Actinides in the Presence of Ligands in High Ionic Strength Systems |
|--------------------|---|

TASK 6: HYDROLOGY MODELING OF BASIN 6 OF THE NASH DRAW NEAR THE WIPP

- | | |
|--------------------|--|
| Subtask 6.1 | Basin 6 DEM Development and Delineation of Surface Hydrological Features |
| Subtask 6.2 | Model Development |

TASK 7: ENGINEERED MULTI-LAYER AMENDMENT TECHNOLOGY FOR HG REMEDIATION ON OAK RIDGE RESERVATION

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Task 1

Remediation Research and Technical Support for the Hanford Site

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Subtask 1.2: Re-oxidation of Redox Sensitive Contaminants Immobilized by Strong Reductants

Site Needs:

- Subtask supports evaluation of potential *in situ* treatment technologies for the vadose zone, groundwater and perched water zone located within the 200 Area at Hanford. This research evaluates re-oxidation kinetics of ^{99}Tc in the presence of other co-contaminants (e.g., ^{238}U and nitrate) after initial immobilization via reduction. The results from these batch experiments will be used to determine the rate and extent of Tc remobilization in the presence of co-contaminants and provide insights for remedial actions.

Objectives:

- To study re-oxidation kinetics of perched (PW) and groundwater (GW) contaminants, such as $^{99}\text{Tc}^{(\text{VII})}$, in the presence of ^{238}U , and NO_3^- , that have been initially reduced by strong reductants such as ZVI, SMI and CPS in batch-scale experiments under anaerobic initial conditions followed by aerobic conditions. Sediment samples that evaluated in these experiments include ^{99}Tc comingled with uranium and nitrate.



Subtask 1.2: Re-oxidation of Redox Sensitive Contaminants Immobilized by Strong Reductants

FIU Year 2 Research Highlights & Accomplishments:

- Studied re-oxidation behavior of ^{99}Tc , U(VI), and NO_3^- after treatment with strong reductants:
 - 1% zero valent iron (ZVI) and
 - 1% sulfur modified iron (SMI) (per mass of GW or PW)
- Ringold Formation sediment <2 mm in triplicate samples
- Two phases of experiments for reduction of ^{99}Tc , U(VI), and NO_3^- :
 - In presence of strong reductants and anaerobic conditions for up to **28 days**
 - In aerobic conditions for up to **40 days with aeration 2x/week for 30 s.**Total testing = 68 days.
- Measured pH, ORP, DO, Tc, U, Fe, NO_3^- concentrations at each sample point.
- Test matrix:
 - Prepared synthetic solutions of GW and PW
 - Purged with N_2 , pH adjusted, and spiked with ^{99}Tc , U(VI), and NO_3^-
 - PW: pH 8.2, 10 $\mu\text{g/L}$ Tc, 150 mg/L U.
 - GW: pH 7.8, 420 $\mu\text{g/L}$ Tc, 124 mg/L NO_3^-
- Phase 1:
 - DO: ~0.03-0.05 mg/L
 - ORP: -300 mV -400 mV indicative of reducing conditions.
- Phase 2: DO and ORP increased:
 - DO: 5-6 mg/L
 - ORP: +250 to +500 mV consistent with oxidative conditions.

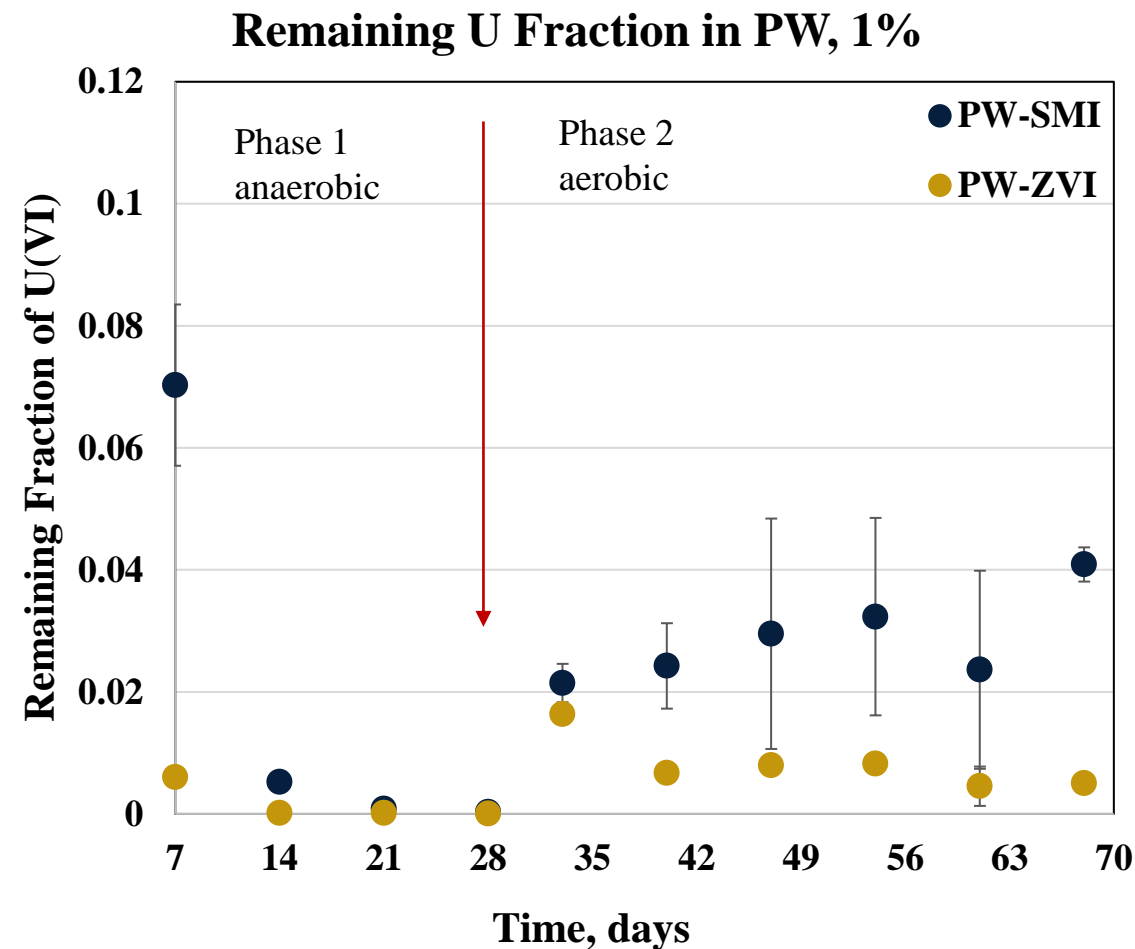
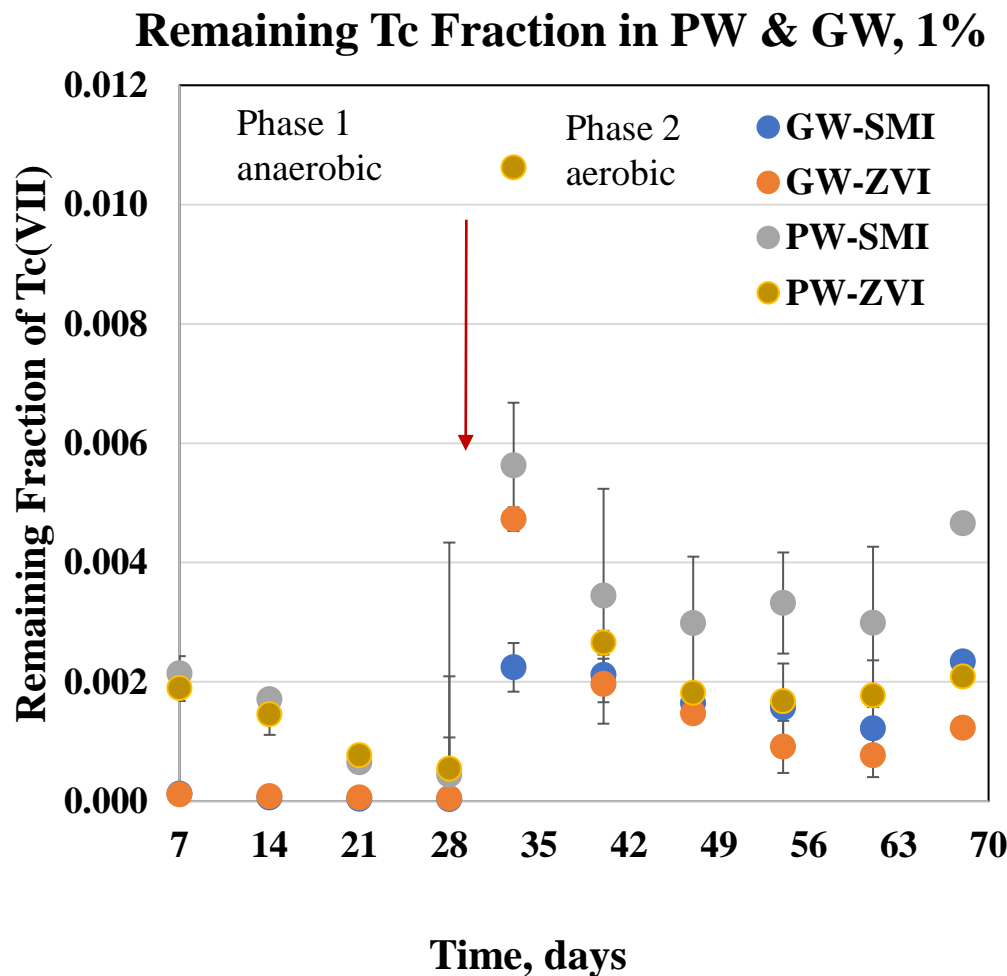
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Subtask 1.2: Re-oxidation of Redox Sensitive Contaminants Immobilized by Strong Reductants

FIU Year 2 Research Highlights & Accomplishments:

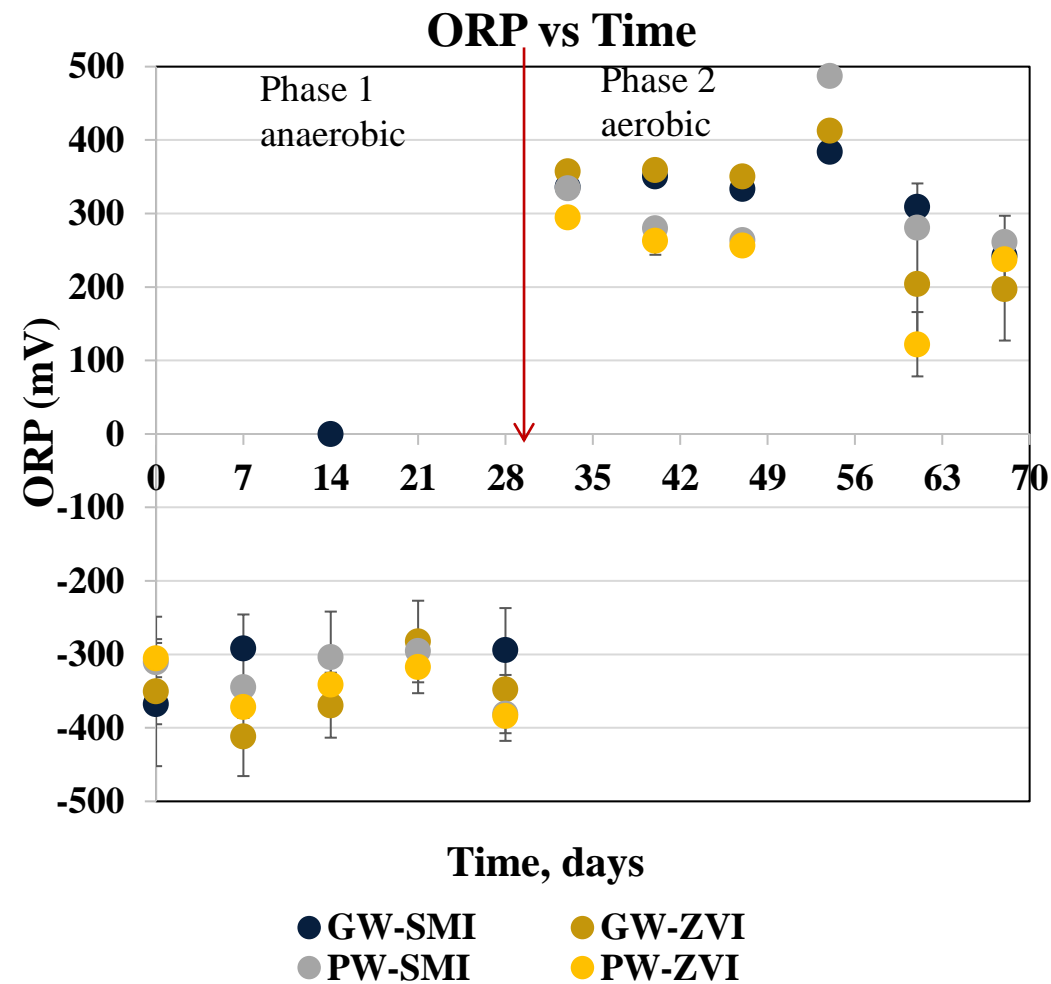
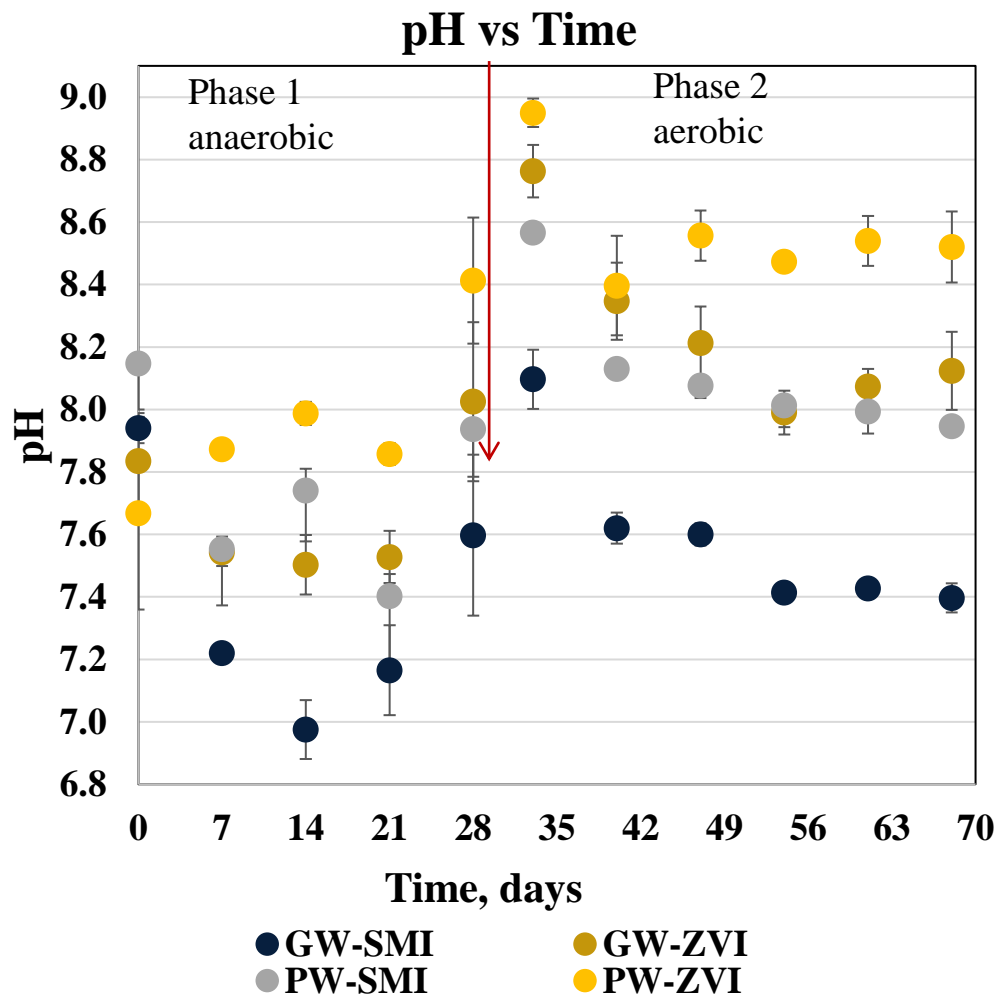


- Hepure ZVI was a more effective reductant than SMI
- ZVI-treated triplicates contained smaller remaining fraction of U(VI) & Tc(VII) in solution throughout both phases.



Subtask 1.2: Re-oxidation of Redox Sensitive Contaminants Immobilized by Strong Reductants

FIU Year 2 Research Highlights & Accomplishments:



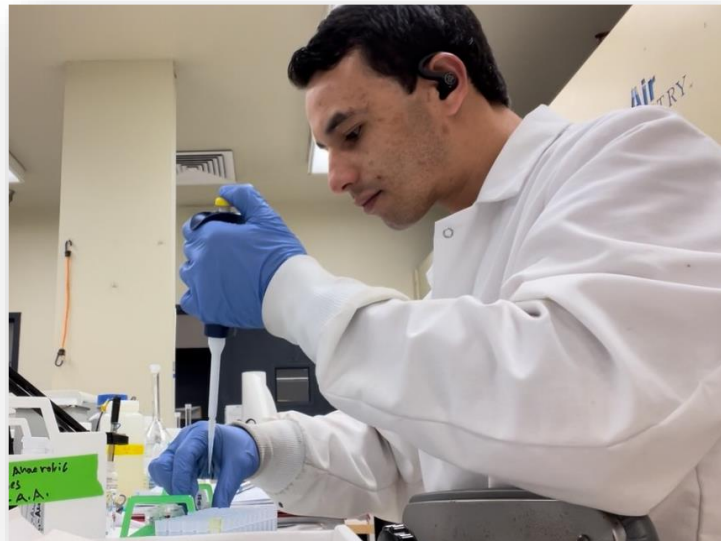
- SMI-amended samples exhibited lower pH compared to ZVI.
- SO_4^{2-} analyses via IC are in progress.



Subtask 1.2: Re-oxidation of Redox Sensitive Contaminants Immobilized by Strong Reductants

FIU Year 2 Research Highlights & Accomplishments:

- Completed analysis of sediment samples amended with 1% ZVI and SMI investigating reoxidation behaviors of U and Tc.
- Completed summer internship at PNNL performing column experiments under mentorship of Drs. Qafoku, Szecsody and Emerson.
- Presented student poster at WM2022 Symposia: "*Re-oxidation of Technetium (^{99}Tc) Comingled with Uranium (^{238}U) and Nitrate (NO_3^-) Immobilized by Strong Reductants*"



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DOE Fellow Angel Almaguer in the laboratories at FIU-ARC and at PNNL during summer internship



Subtask 1.2: Re-oxidation of Redox Sensitive Contaminants Immobilized by Strong Reductants

FIU Year 3 Projected Scope

- Finalize analyses for nitrate/nitrite via IC.
- Study the re-oxidation behavior of perched and groundwater contaminants, Tc(VII), U(VI), and NO_3^- , that have been initially reduced by 0.5% and 5% calcium polysulfide (CPS) under anaerobic initial conditions followed by aerobic conditions.
- Conduct solid characterization studies via XRD and SEM-EDS to investigate for changes in sediment mineralogy, surface morphology and elemental composition.
- Initiate preliminary experiments on coupling ZVI approach with ammonium hydroxide and investigate their effect on the re-oxidation behavior of comingled Tc, U and nitrate.
 - Research will follow experimental matrix outlined in DV-1 Operable Unit treatability study ongoing at Hanford Site.

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Subtask 1.3: Evaluation of Competing Attenuation Processes for Mobile Contaminants in Hanford Sediments

Site Needs:

Contaminants [U (VI), ^{129}I , ^{99}Tc , Cr(VI) and NO_3^-] that were released to the environment can potentially impact groundwater. Once active remediation is completed, a transition to monitored natural attenuation (MNA), is needed. Effective MNA requires a thorough understanding of the contaminant immobilization processes that keep the contaminants stable and resistant to remobilization due to changes in environmental conditions or GW chemistry.

Objectives:

Evaluate attenuation processes that affect fate and transport mechanisms of contaminants of concern present in VZ sediment collected from the Hanford Site.

- Conduct competitive adsorption experiments on selected sediment fractions with key contaminants of concern at the max concentrations found at Hanford 200 Area GW and porewater when all contaminants are commingled together to compare adsorption results when each contaminant is present separately.



Subtask 1.3: Evaluation of Competing Attenuation Processes for Mobile Contaminants in Hanford Sediments

FIU Year 2 Research Highlights & Accomplishments:

Dominant U(VI) species:

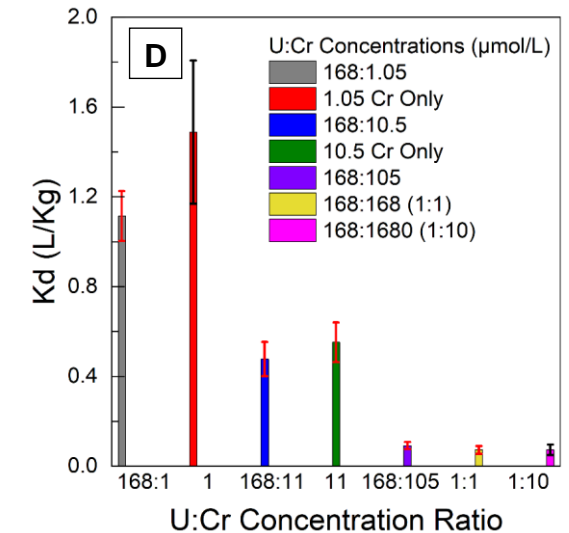
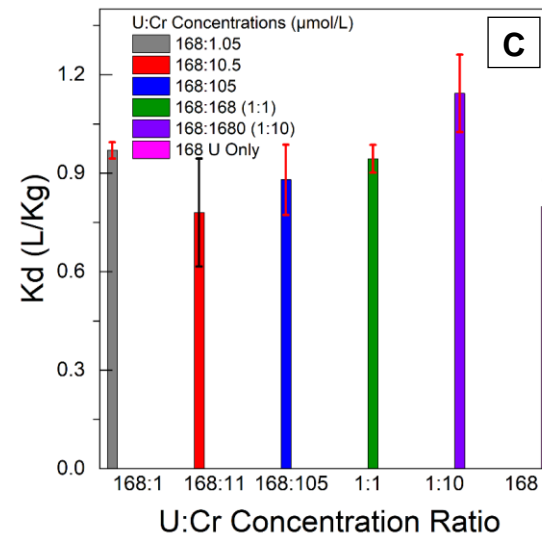
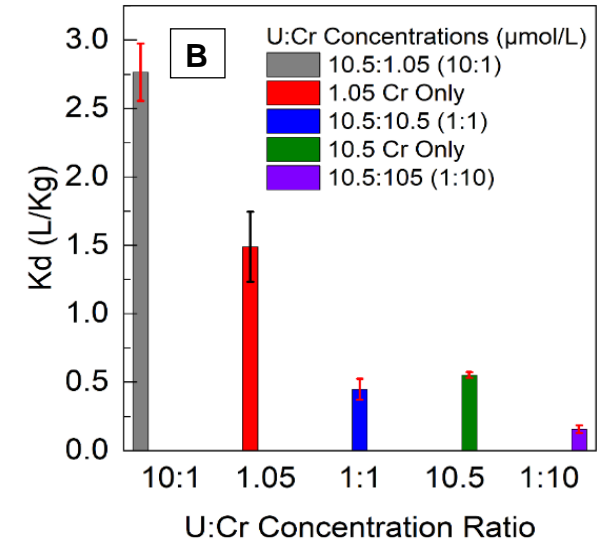
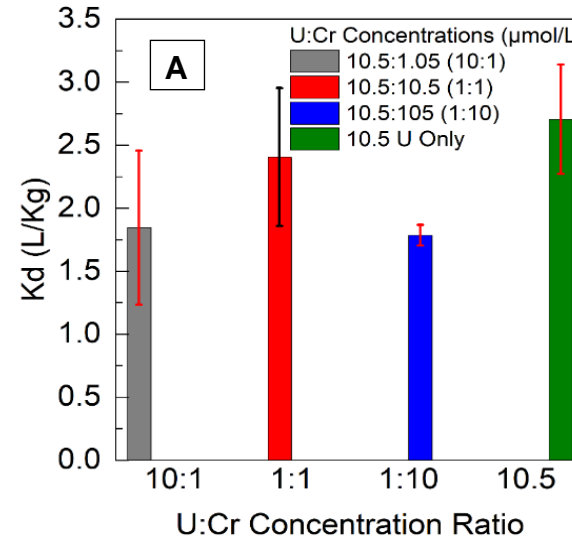
- $\text{Ca}_2\text{UO}_2(\text{CO}_3)_3^0(\text{aq})$ and $\text{CaUO}_2(\text{CO}_3)_3^{2-}$

Dominant Cr(VI) species:

- $\text{CaCrO}_4(\text{aq})$

$$K_d = \frac{[\text{contaminant}]_{\text{sediment}}}{[\text{contaminant}]_{\text{solution}}}$$

A&C: Change in U(VI) K_d B&D: Change in Cr(VI) K_d

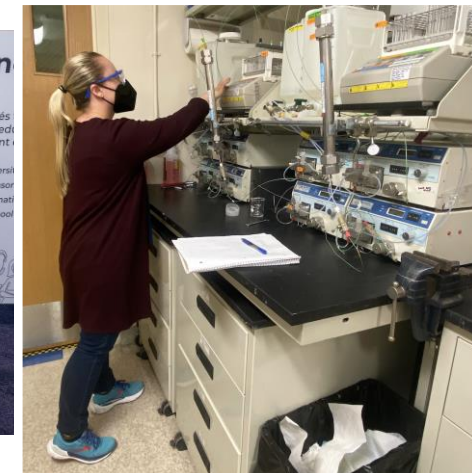




Subtask 1.3: Evaluation of Competing Attenuation Processes for Mobile Contaminants in Hanford Sediments

FIU Year 2 Research Highlights & Accomplishments:

- RemPlex Global Summit PNNL 2021: *“Impact of Major Groundwater Components on the Adsorption of Hexavalent Uranium (VI) to Hanford Formation”* (oral presentation)
- Roy G. Post scholarship recipient
- Waste Management Symposia 2022: *“Impact of Major Groundwater Components on the Adsorption of Hexavalent Uranium (VI) to Hanford Formation”* (poster presentation)
- Summer Internship at PNNL with Drs. Nik Qafoku, Jim Szecsody, and Hilary Emerson



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Subtask 1.3: Evaluation of Competing Attenuation Processes for Mobile Contaminants in Hanford Sediments

FIU Year 3 Projected Scope

- Conduct column studies: U, Cr, and competitive U and Cr
- Develop competitive batch studies including U, Cr, and I-127
- Characterize post treated sediment via x-ray diffraction (XRD) and scanning electron microscopy-energy dispersive spectroscopy (SEM) analysis

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Subtask 1.4: Experimental Support of Lysimeter Testing

Site Needs:

This task provides support to the large-scale field experiments at the Hanford Field Lysimeter Test Facility (FLTF) located in the 200-W Area of the Hanford site. The FLTF study is being initiated as a long-term experiment to provide data on glass and cementitious waste form durability, contaminant release from waste forms, and resulting transport in the near-field environment anticipated to be present at the Hanford Site Integrated Disposal Facility (IDF). The findings of the FLTF will be used to validate model predictions of long-term waste form behavior upon safe disposal of immobilized low-activity waste (ILAW) in the IDF and used in the IDF Performance Assessment (PA) calculations.

One of the planned configurations of the lysimeter units described in the Implementation Plan (Bacon et. al., 2018) is to place grout waste forms above glass waste forms. This waste form arrangement has limited laboratory data regarding the dissolution of glass in the presence of grout-contacted water.

Objectives:

To investigate the impact of major elements, Ca, Si, and Al, present in the grout-contacted solution on the dissolution behavior of borosilicate glass at varying temperatures (25°C, 40°C, 70°C) using single-pass flow-through (SPFT) and static Product Consistency Test (PCT) (90°C).

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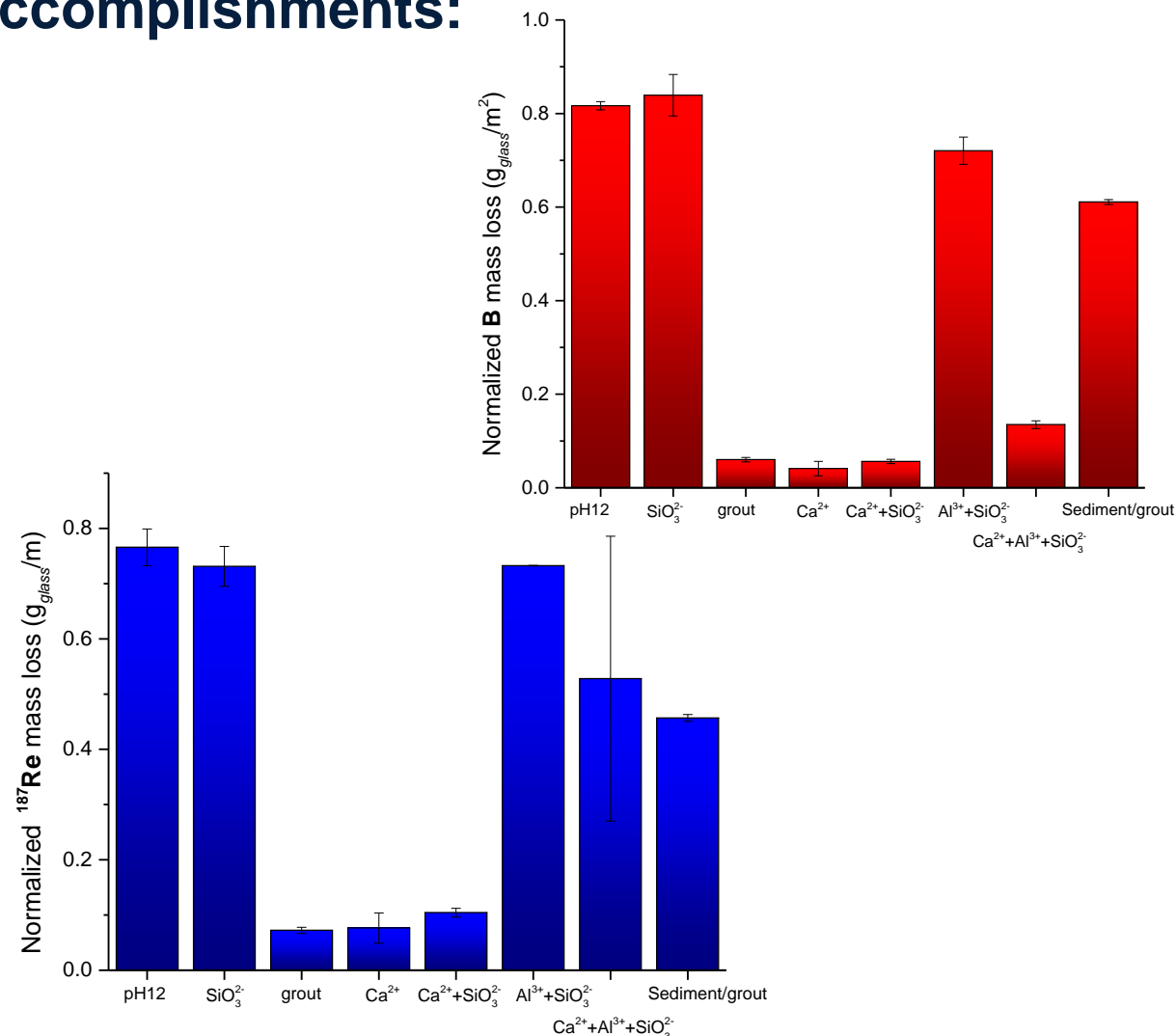
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Subtask 1.4: Experimental Support of Lysimeter Testing

FIU Year 2 Research Highlights & Accomplishments:

- Investigated impact of major elements on dissolution behavior of borosilicate ORLEC28 glass
 - Test matrix in SPFT: duplicated reactors with grout, Ca-amended, pH 12 buffered soln., flow rate 40 mL/day at 25°C, 40°C, and 70°C
 - Test matrix in PCT: triplicated reactors, pH 12 buffer, grout soln., grout/ sediment soln., Si (5 ppm), Ca (130 ppm) and Al (7 ppm) amended buffers at 90°C
- XRD analyses of treated glass and SEM/EDS measurements in cross-sections of glass coupons to study glass erosion
- Poster presentation at Waste Management Symposia (March 2022) - *“Effect of Grout-Contacted Solution on the Glass Dissolution Behavior”*



PCT results on the ¹⁸⁷Re and B release by ORLEC28 glass in different solutions at 90°C

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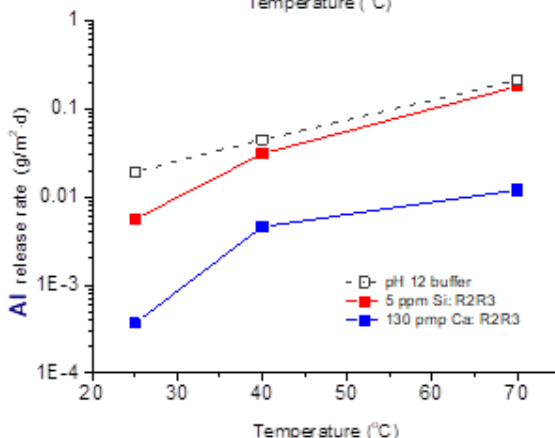
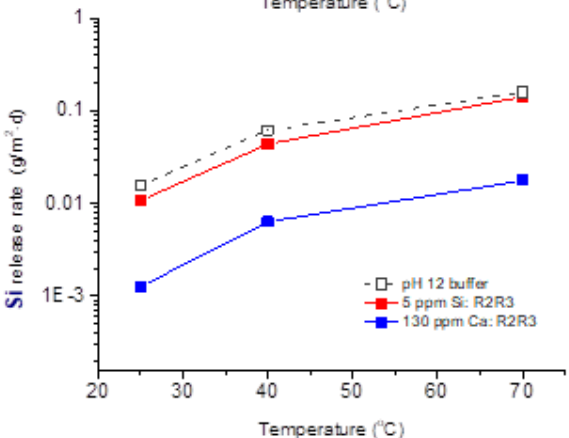
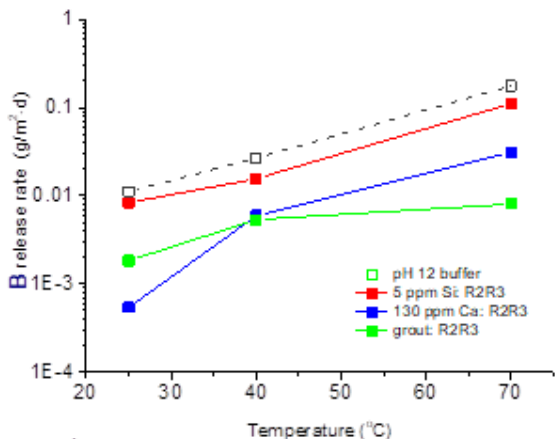
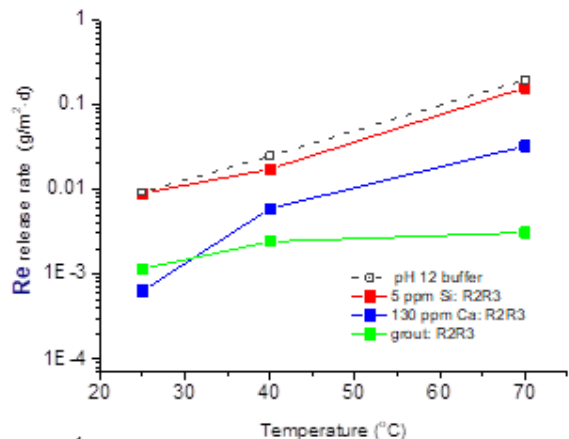
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Subtask 1.4: Experimental Testing

FIU Year 2 Research Highlights & Accomplishments:

SPFT experiments: Normalized release rates for Re, B, Si, and Al



BET surface area & cumulative volume of pores of glass powders used in duplicate static test at 90°C

Sample	BET surface area, m ² /g	BJH adsorption cumulative volume of pores (17.000 Å to 3000.000 Å width) cm ³ /g
Pristine glass	0.004(6)	0.0090 (9)
pH12	0.788(4)	0.891(8)
grout-contacted solution	0.075(5)	0.0003(4)
Si-amended solution	0.354(8)	0.417(8)
Ca ²⁺ -amended solution	0.121(7)	0.0004(6)

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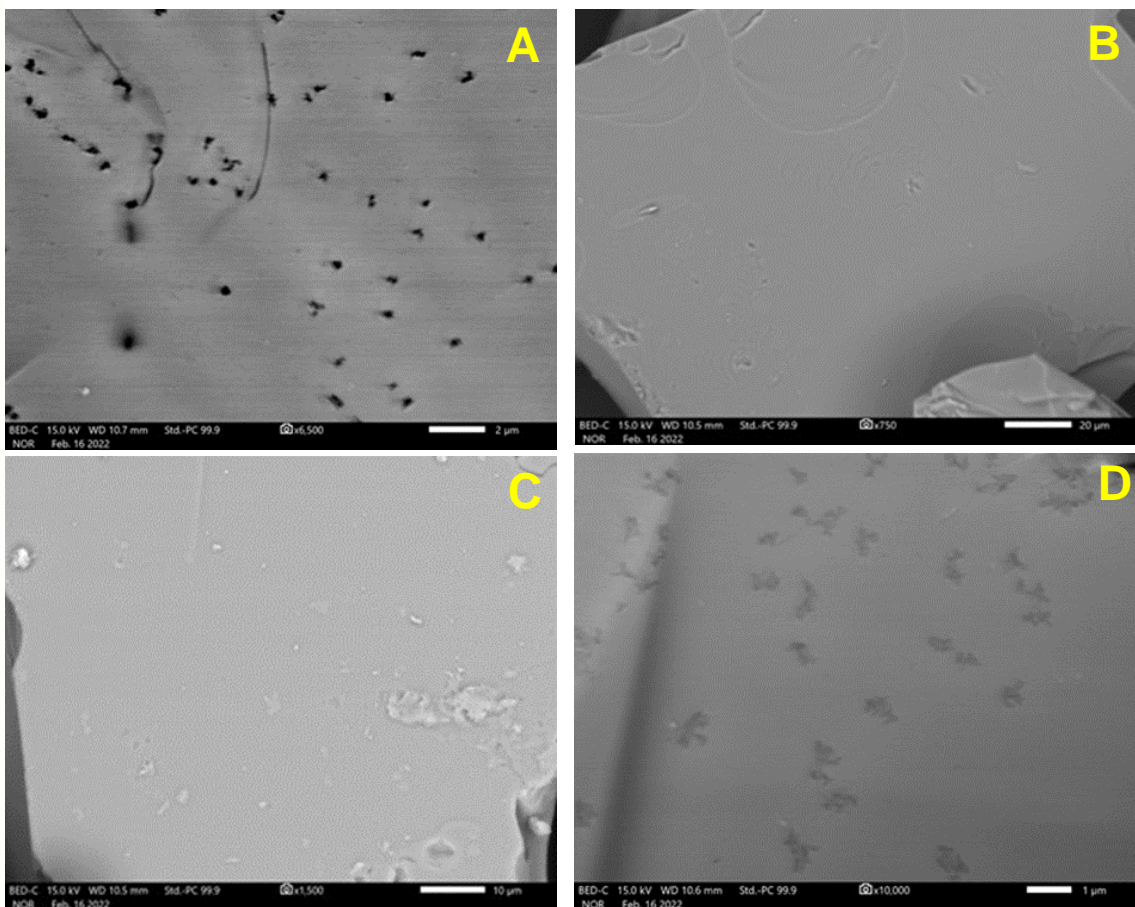
Leaching solutions: grout-contacted, Si- amended, Ca- amended at pH 12 as a function of temperature.



Subtask 1.4: Experimental Support of Lysimeter Testing

FIU Year 2 Research Highlights & Accomplishments:

SEM images of glass particles after PCT test



A) pH 12 buffer; B) Ca^{2+} amended buffer solution; C) grout-contacted soln.; D) glass surface defects after grout-contacted soln.

Alternation layer thickness for different elements in the static PCT test at 90°C

Solution	Na	K	Si	Al	Ca	Zn
Ca^{2+}	-4.05	-3.31	-1.84	-1.6	+3.3	+3.3
$\text{Ca}^{2+} + \text{SiO}_3^{2-}$	+0.85; -3.5	+0.72; -3.5	-0.91	-0.84	+2.05	+0.72
$\text{Al}^{3+} + \text{SiO}_3^{2-}$	-4.4	-3.8	-1.2	-0.71	0.0	0.0
$\text{Ca}^{2+} + \text{Al}^{3+} + \text{SiO}_3^{2-}$	-4.15	-3.36	0.0	0.0	+2.2	+2.2

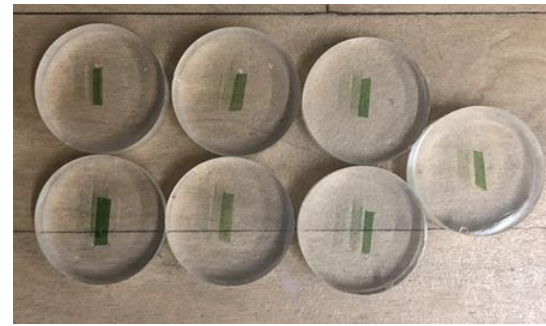
- **Negative** sign corresponds to decreased concentration of element compared to concentration in bulk glass.
- **Positive** sign corresponds to increased amount of element compared to concentration in bulk glass.



Subtask 1.4: Experimental Support of Lysimeter Testing

FIU Year 3 Projected Scope

- Investigate impact of Ca, Al, and grout/sediment-contacted solution on the dissolution behavior of borosilicate glass.
 - Varying Ca across a few orders of magnitude; pH 8, 12.
 - Al concentrations in leachate range from 0.3 ppm-30 ppm at different pHs (7, 9, 10, 11).
- Complete grout-sediment static experiment at variable temperature (25° C, 40° C, 70°C).
- Complete long-term static PCT experiment with three solutions:
 - pH 12 buffer
 - Ca^{2+} (130 ppm) in pH 12 buffer
 - Grout-contacted solutions(Samples to be collected after 2 weeks and 1 month in epoxy for SEM/EDS)
- Support glass characterization studies via microscopy, spectroscopy, and X-ray diffraction techniques.



Glass coupons in epoxy for SEM/EDS analysis.



Task 2

Remediation Research and Technical Support for the Savannah River Site

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Subtask 2.1: Environmental Factors Controlling the Attenuation and Release of Contaminants in the Wetland Sediments at Savannah River Site

Site Needs:

- **Iodine-129** poses a substantial clean-up problem at Savannah River Site due to its perceived high mobility in the environment, toxicity, and long half-life (~16 million years), as well as it having one of the lowest maximum contamination levels (1 pCi L^{-1}) of all radionuclides.
- Wetlands at the F-Area have been an important sink for I-129 and other contaminants. The complex and diverse physical and biogeochemical processes within the wetlands are mainly responsible for retaining these contaminants.
- However, these areas are sensitive to changing boundaries and geochemical conditions, resulting in the release of iodine-129 into surrounding areas.

Objectives:

- The sorption study of iodine on the wetland soils will improve understanding of the factors that contribute to the attenuation of iodine-129 at the F-Area wetlands and will provide SRS and the DOE with the ability to remediate I-129 from the F-Area more effectively.
- The removal study of iodine is to evaluate the efficacy in the use of amendments such as PM-199 and MRM that can be deployed in the subsurface to enhance the attenuation of I-129 and identify the optimal conditions for the amendment efficacy.

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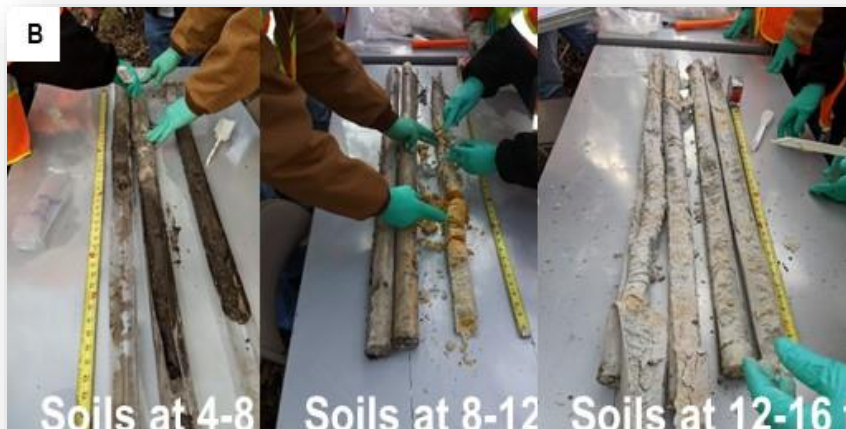
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Subtask 2.1: Environmental Factors Controlling the Attenuation and Release of Contaminants in the Wetland Sediments at Savannah River Site

FIU Year 2 Research Highlights & Accomplishments:

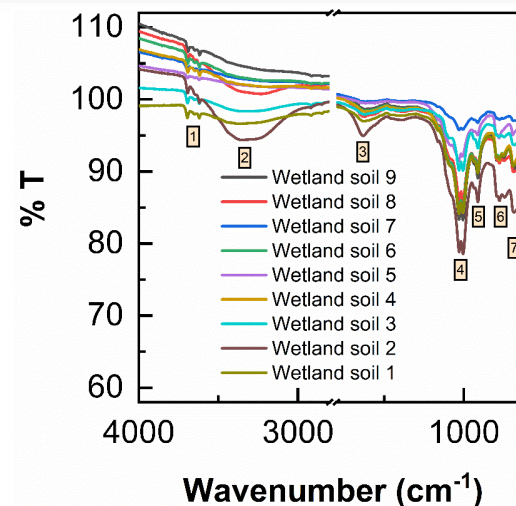
Soil Sampling:



Characterization of SRS wetland soil:



- Soil collected from background area
- Soil samples sorted into 3 fractions:
 - organic rich topsoil
 - intermediate soil
 - aquifer sediments
- Topsoil samples consist of kaolinite and quartz peaks

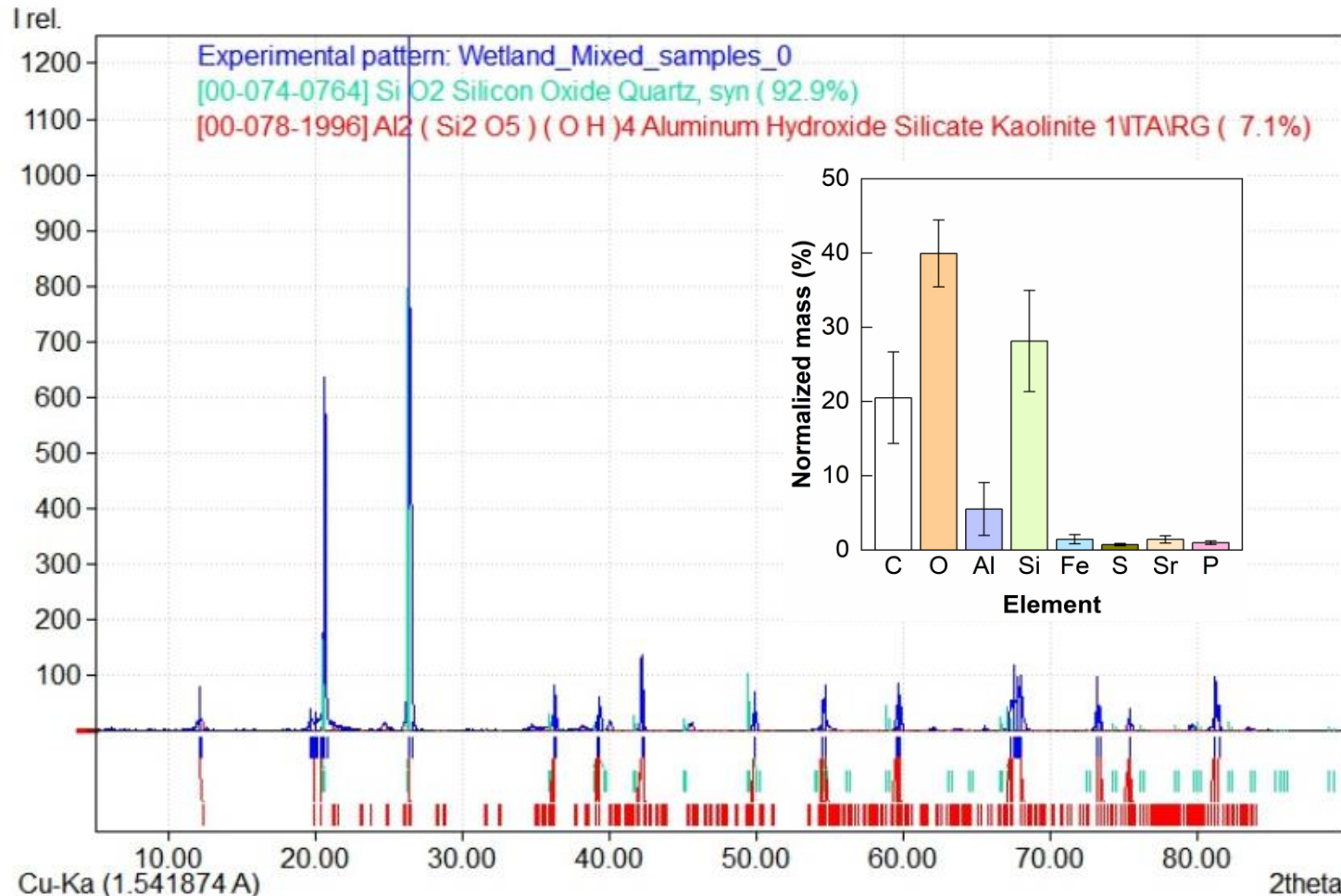




Subtask 2.1: Environmental Factors Controlling the Attenuation and Release of Contaminants in the Wetland Sediments at Savannah River Site

FIU Year 2 Research Highlights & Accomplishments:

Characterization of SRS wetland soil:



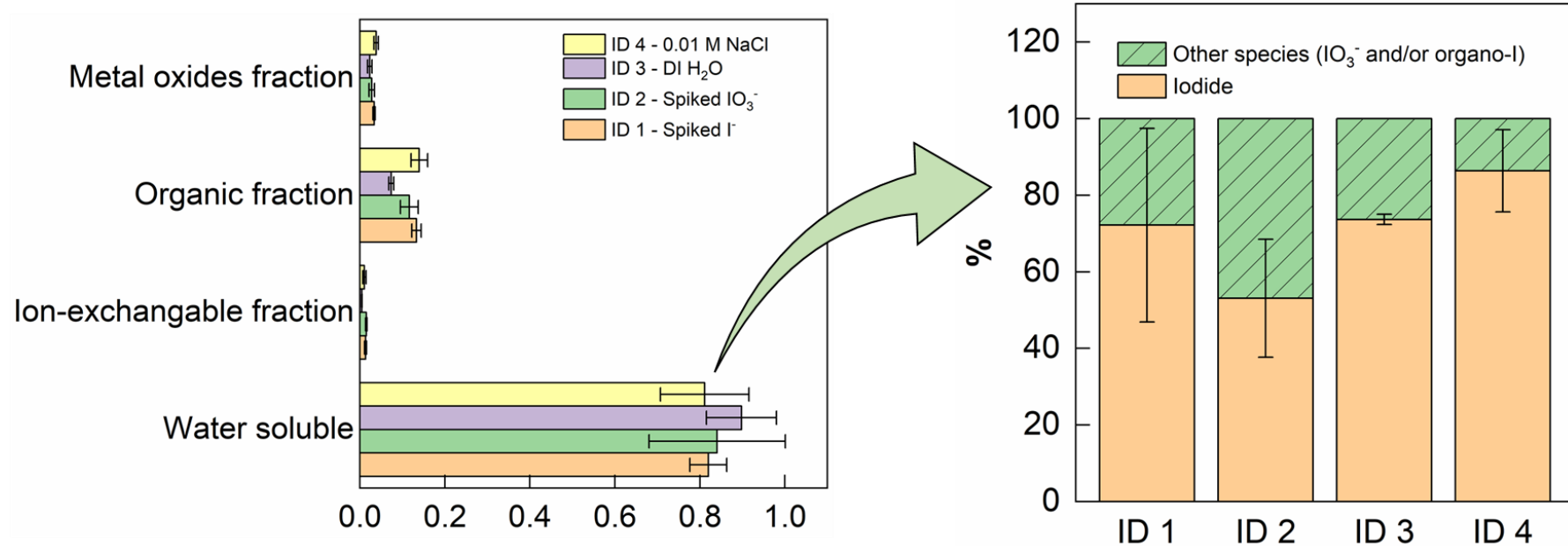
- Topsoil samples consist of kaolinite and quartz peaks
- Elemental analysis by EDS also confirm that observation



Subtask 2.1: Environmental Factors Controlling the Attenuation and Release of Contaminants in the Wetland Sediments at Savannah River Site

FIU Year 2 Research Highlights & Accomplishments:

Sequential Extraction:



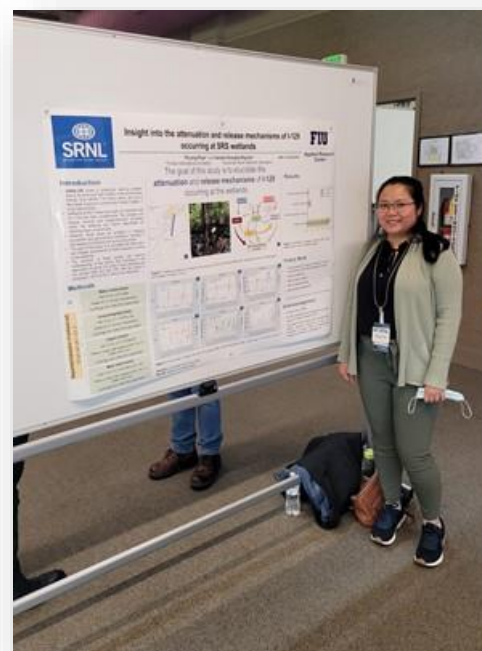
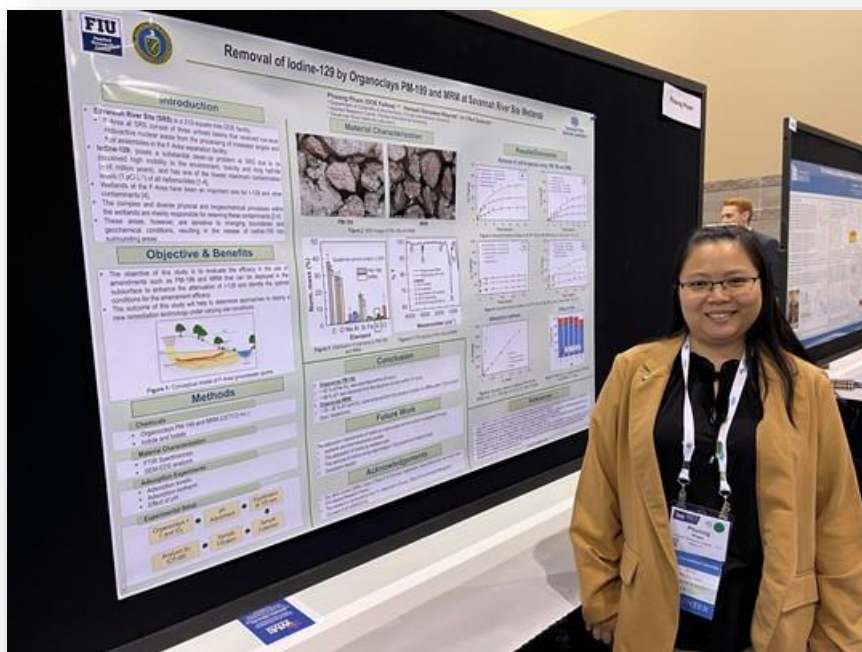
- ~ 80 % of iodine in SRS wetland's topsoil is water-soluble, within the soluble fraction
- ~ 50 – 80 % of Iodine is in the form of iodide
- ~ 20 % of iodine bounded to organic molecules
- ~ 5 % of iodine bounded to the metal oxides



Subtask 2.1: Environmental Factors Controlling the Attenuation and Release of Contaminants in the Wetland Sediments at Savannah River Site

FIU Year 2 Research Highlights & Accomplishments:

- Completion of SRS's wetland topsoil characterization.
- Summer internship at SRNL working on the attenuation/release of I-129 by wetland soils at different depth intervals and investigate the use of organoclays as potential remediation technology for I-129 under the mentorship of Dr. Hansell Gonzalez-Raymat.
- Student poster presentation at Waste Management Symposia 2022 meeting on: Removal of I-129 by organoclays PM-199 and MRM at Savannah River Site



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Subtask 2.1: Environmental Factors Controlling the Attenuation and Release of Contaminants in the Wetland Sediments at Savannah River Site

FIU Year 3 Projected Scope

- Iodine speciation batch adsorption studies using organoclays in presence of wetland soils.
- Investigation of sorption and release of iodine species on soils collected at different depth intervals.

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Subtask 2.2: Investigating the Effect of KW-30 (Humate Material) on the Removal of Uranium

Site Needs:

- Low-cost unrefined humic substances are potential amendments for treatment of uranium in groundwater associated with the F-Area Seepage Basin plume.
- These experiments will determine necessary parameters helping to simulate the creation of a sorbed humate treatment zone in the acidic groundwater contaminated with uranium.

Objectives:

- Investigate, via batch experiments, the sorption behavior of modified humic substances (KW-30) for groundwater remediation and the effect of sorbed humic substances on uranium removal.

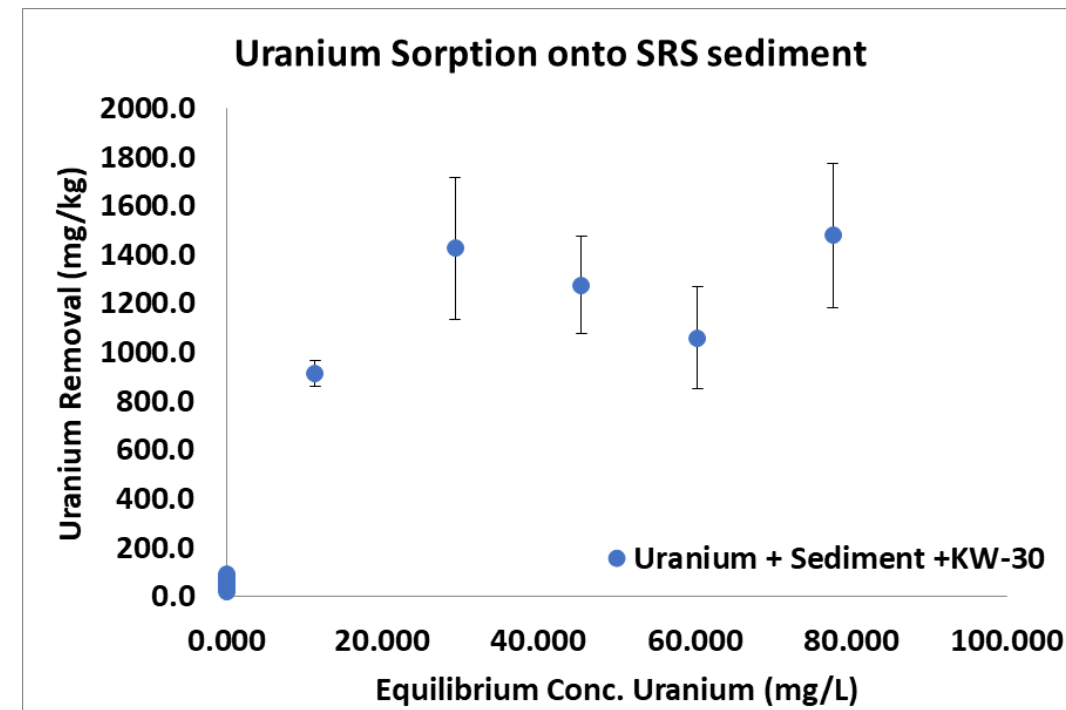
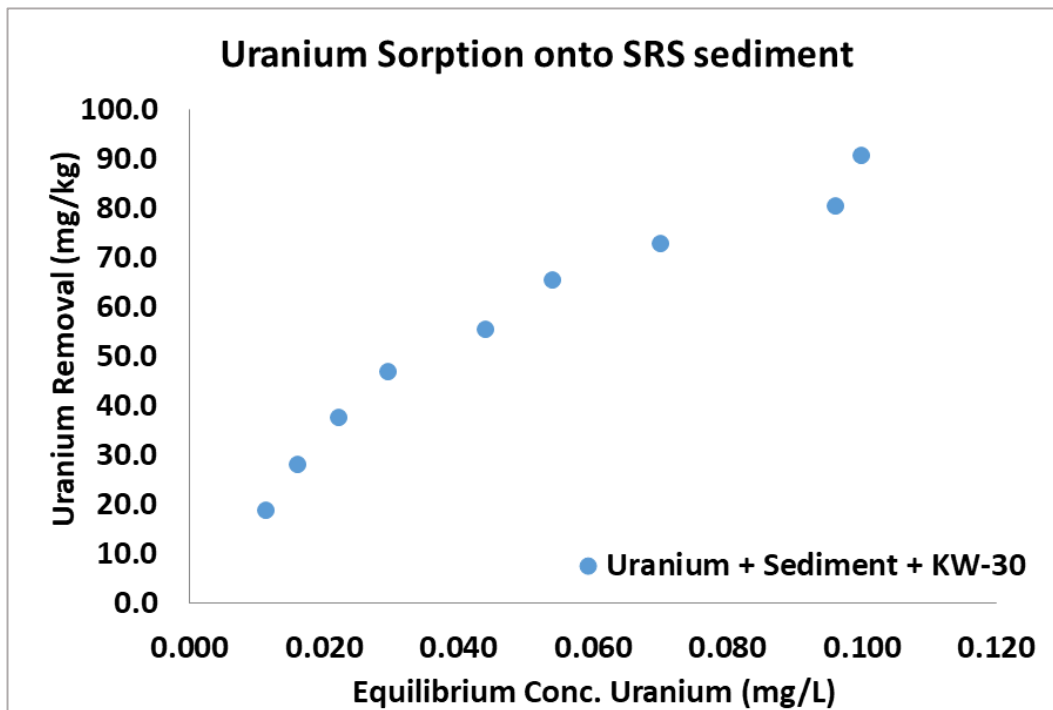
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Subtask 2.2: Investigating the Effect of KW-30 (Humate Material) on the Removal of Uranium

FIU Year 2 Research Highlights & Accomplishments:

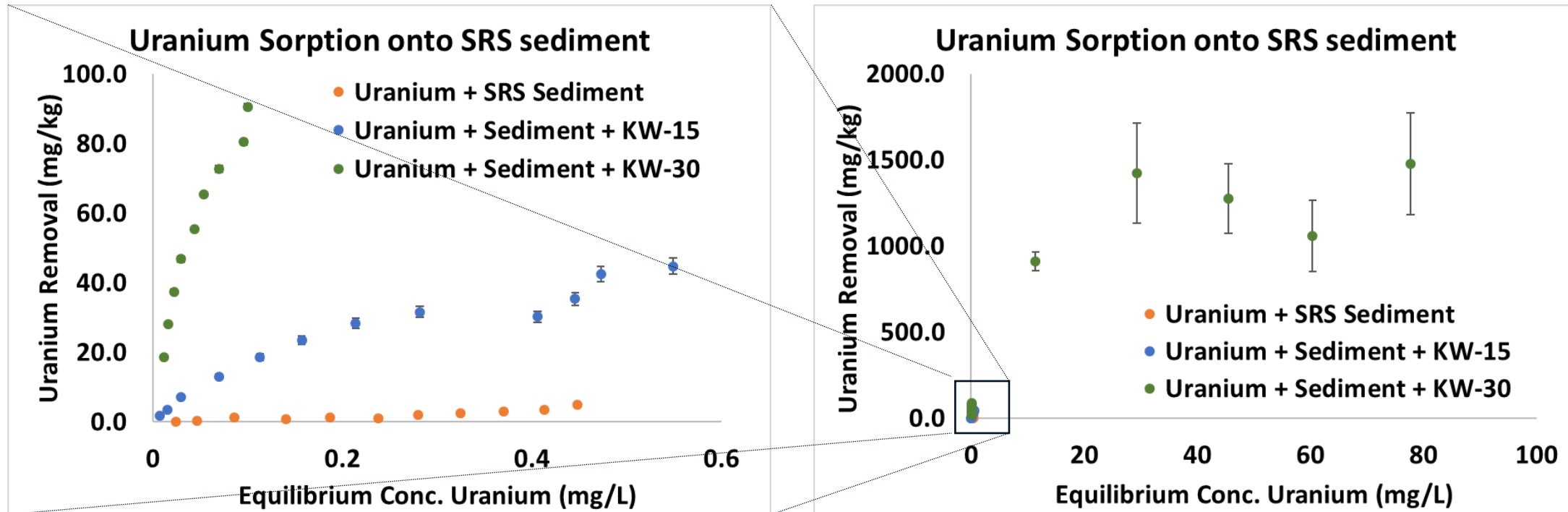


- Performed isotherm experiments to study influence of sorbed humate on uranium removal.
- Increased initial uranium concentration to 100 ppm to reach steady state.



Subtask 2.2: Investigating the Effect of KW-30 (Humate Material) on the Removal of Uranium

FIU Year 2 Research Highlights & Accomplishments:



- Compared KW-30 isotherm data with previous data.
- KW-30 shown to increase uranium removal compared to plain sediment and sediment coated with KW-15



Subtask 2.2: Investigating the Effect of KW-30 (Humate Material) on the Removal of Uranium

FIU Year 2 Research Highlights & Accomplishments:

	Average Humate Sorption (mg/kg)	Average U Removal (mg/kg)	Max U Removal (mg/kg)
Sediment	NA	1.9	5.00
Sediment + KW-15	393	24	44.82
Sediment + KW-30	2435	474	1478

- 6X more KW-30 was sorbed compared to KW-15
- 9X more uranium was removed by KW-15 compared to plain sediment
- 300X more uranium was removed by KW-30



Subtask 2.2: Investigating the Effect of KW-30 (Humate Material) on the Removal of Uranium

FIU Year 3 Projected Scope

- Investigation of the effect of pH on sorption and desorption of uranium with humate (KW-30)-coated sediment.
- Study the influence of KW-30 on other contaminants of concern such as Iodine and Strontium.

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Task 3

Contaminant Fate and Transport Modeling for the Savannah River Site

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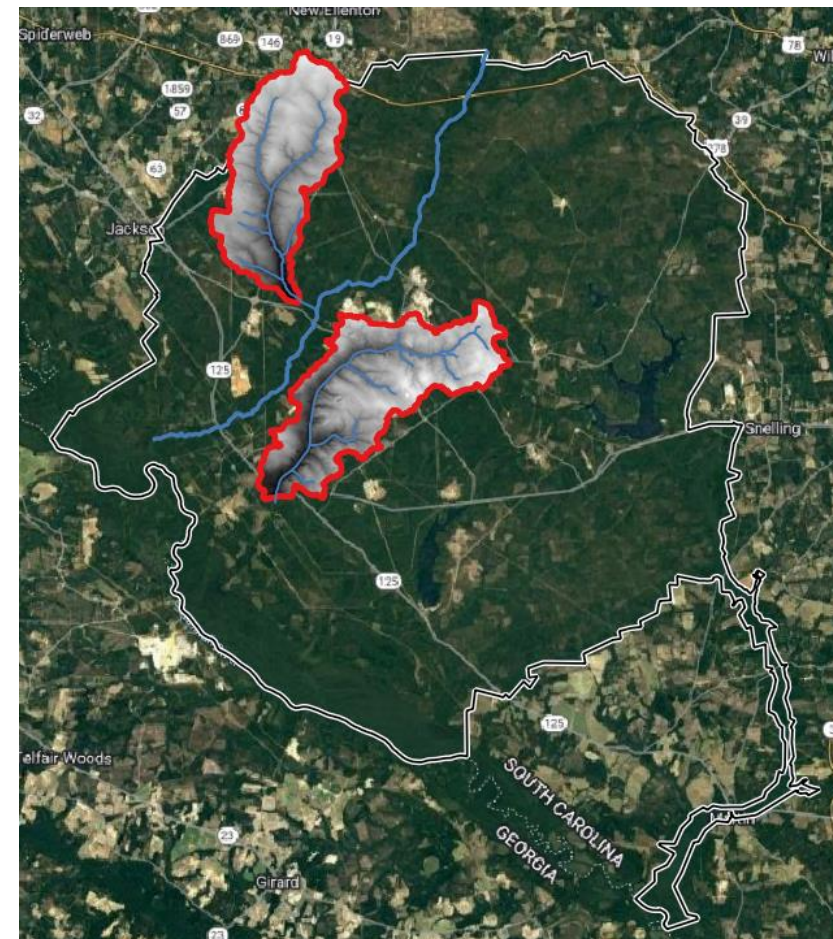
Contaminant Fate and Transport Modeling for the Savannah River Site

Site Needs:

- SRS and other DOE sites challenged with heavy metal and radionuclide contamination in surface/subsurface environments.
- With the push towards site closure, there is a need to:
 - Evaluate effectiveness of applied remediation technologies
 - Establish a long-term monitoring strategy
- Address knowledge gaps related to fate and transport of major contaminants of concern in SRS stream systems by developing numerical models to better understand the impact of hydrological extremes (i.e., heavy precipitation, floods, drought) due to climate change on contaminant transport.

Objectives:

- Develop numerical models to evaluate impact of extreme hydrological events and long-term hydrological changes on groundwater-surface water interactions as well as on fate and transport of major contaminants of concern in SRS streams.
- Focus on Tims Branch and Fourmile Branch watersheds.
- Collect field data to support model calibration and validation.
- Train FIU graduate and undergraduate students (DOE Fellows).



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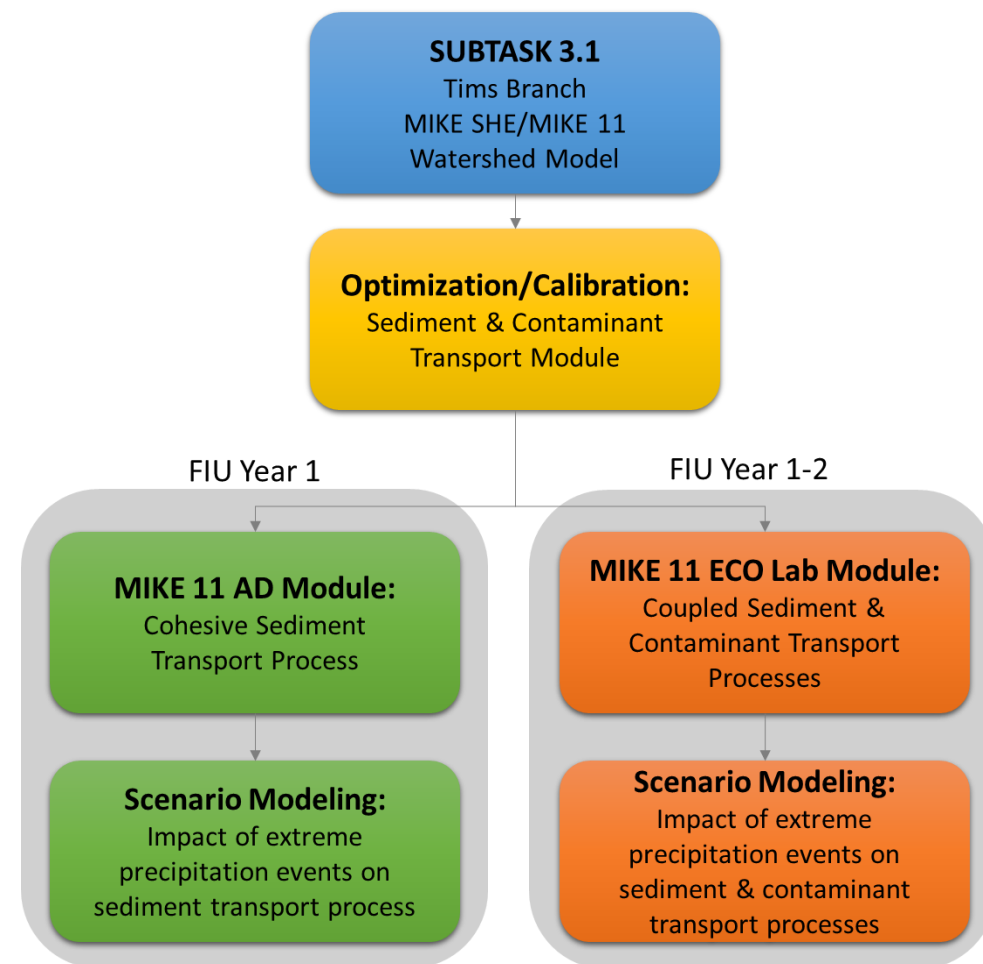
Subtask 3.1: Calibration of the Tims Branch Watershed Model and Scenario Analysis

Background:

A MIKE SHE/MIKE 11 contaminant fate and transport model was developed by FIU to better understand the impact of extreme atmospheric events on the remobilization, transport and redistribution of sediment-bound heavy metals and radionuclides in the Tims Branch watershed.

Objectives set for FIU Year 2:

- Develop and test comprehensive transport model for uranium, tin, and nickel using available hydrological modeling software and GIS tools.
- Examine response of Tims Branch to historical discharges and environmental management remediation actions.
- Study transport scenarios of heavy metal contaminants of concern under extreme hydrological conditions that provide information related to inter-compartmental transfers and the environmental conditions that result in mobilization of adsorbed heavy metals in sediment, and accumulation of priority contaminants of concern due to sedimentation.



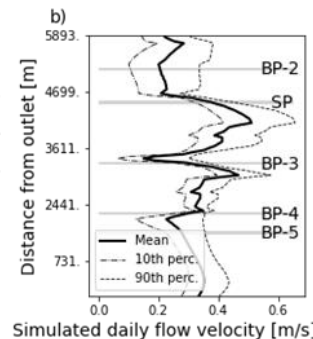
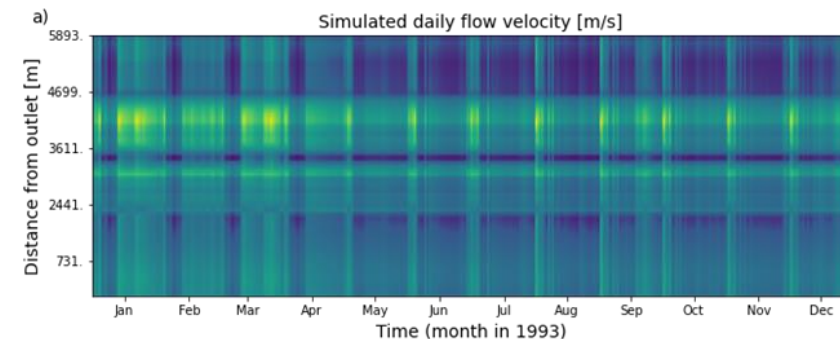
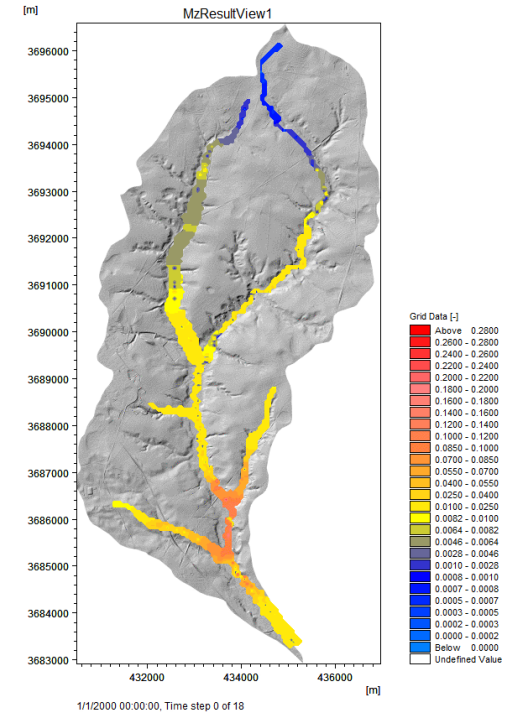


Subtask 3.1: Calibration of the Tims Branch Watershed Model and Scenario Analysis

FIU Year 2 Research Highlights & Accomplishments:

1. Identification of sediment and heavy metal transport parameters for uranium, tin and nickel.
2. Calibration of MIKE 11 sediment & contaminant transport modules (AD & ECO Lab) for simulation of **uranium transport** in Tims Branch with focus on storm events observed in the 1990s that had both temporally varying flow & uranium concentrations available.
3. Transformation of event-based MIKE SHE/MIKE 11 hydrological model to continuous model that allows for long-term simulations to assess the role of climate change on heavy metal transport.
4. Development of scripts using GIS and Python to automate and accelerate hydrological model development
 - Fast-tracks MIKE model development for ANY basin of interest
 - Uses publicly available info to generate 1st version model in days
 - Performance can be enhanced with site specific information
 - Provides DOE with complex-wide support as needed within a relatively short timeframe.

Velocity*Flow Depth (U*D) for a 100-year 24-hour design storm event.



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Subtask 3.1: Calibration of the Tims Branch Watershed Model and Scenario Analysis

1. Identification of sediment and heavy metal transport parameters for uranium, tin and nickel from literature, historical data and field observations

Literature review

Example: Distribution coefficient, K_d [ml/g]:

$$K_d = \frac{\text{Amount of element sorbed on solid/solid mass}}{\text{Amount of element dissolved in solution /solution volume}}$$

Historical data analysis



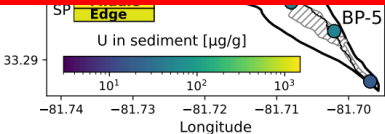
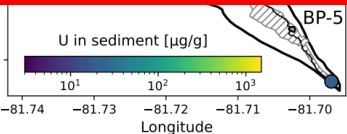
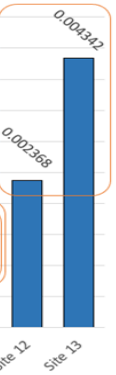
pH	pH ≥ 9			pH 5 – 9			pH ≤ 5		
Total percent-by-weight composition of 1. Clay 2. Iron 3. Aluminum oxyhydroxide 4. Organic matter contents	Sandy soils	Loamy soils	Clayey soils	Sandy soils	Loamy soils	Clayey soils	Sandy soils	Loamy soils	Clayey soils
	< 10%	10-30%	≥30%	< 10%	10-30%	≥30%	< 10%	10-30%	≥30%
Nickel	1.22	5.86	65.0	12.2	58.6	650.0	1.2	5.86	65.0
Tin	2.5	5.0	5.0	5.0	10.0	10.0	2.5	5.0	5.0
U	0.0	5.0	50.0	0.0	50.0	500.0	0.0	5.0	50.0

Calculated K_d from in situ observations within Tims Branch

Class	K_d in (L/Kg)	$\log K_d$ in (L/Kg)	Area classification
Min	ND	ND	Control site (BP1)
Max	2,586	3.41	
Min	130,750	5.12	Low contaminated
Max	35,000^a	4.54	
Min	54,515	4.74	Mid contaminated
Max	88,362	4.95	
Min	113,070	5.05	High contaminated
Max	120,278	5.08	

1989

ions



concentration variability in 1980s, 2002 and 2011

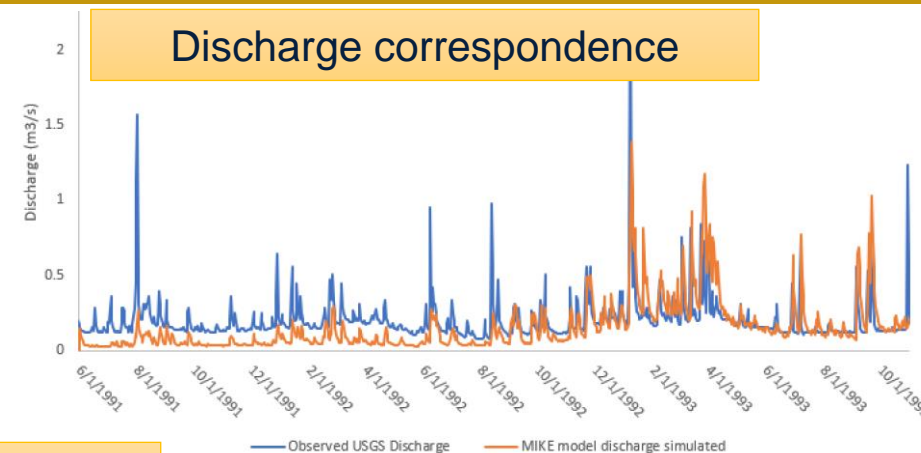
Aqueous U conc. in (mg/L). Data extracted by Morales, ARC, 2016; 2017)



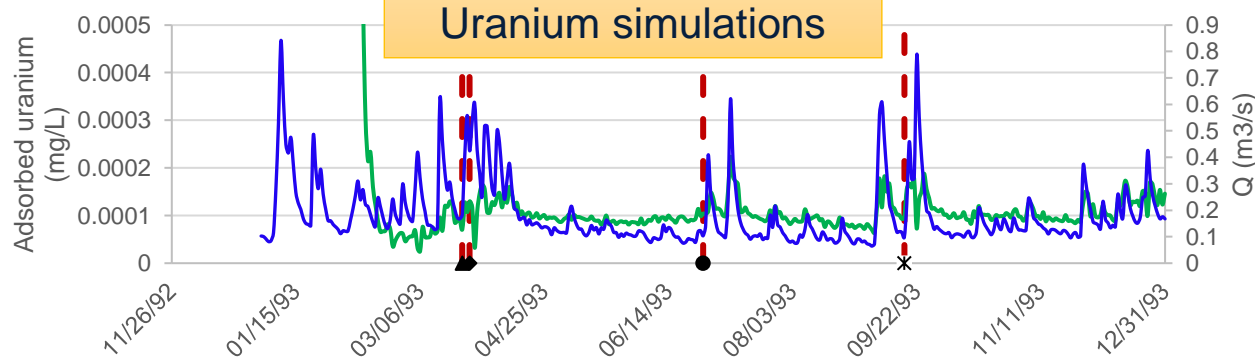
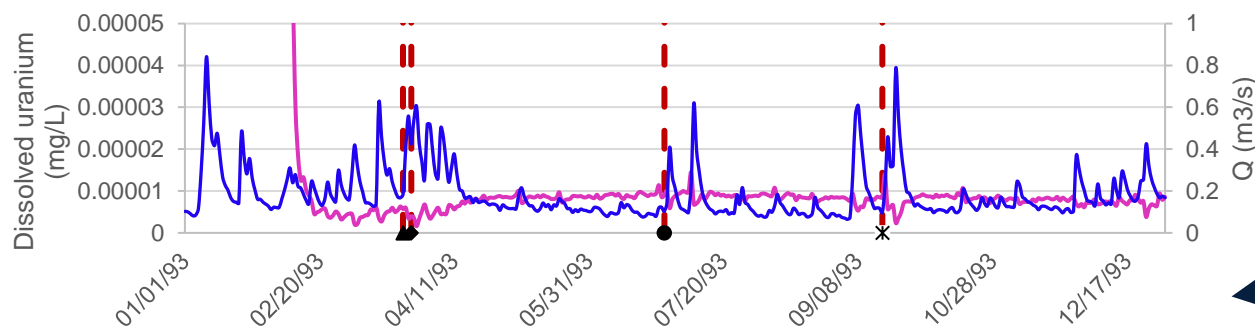
Subtask 3.1: Calibration of the Tims Branch Watershed Model and Scenario Analysis

2. Calibration of MIKE 11 sediment & contaminant transport modules (AD & ECO Lab) for simulation of **uranium transport** in Tims Branch with focus on storm events observed in the 1990s that had both temporally varying flow & uranium concentrations available.

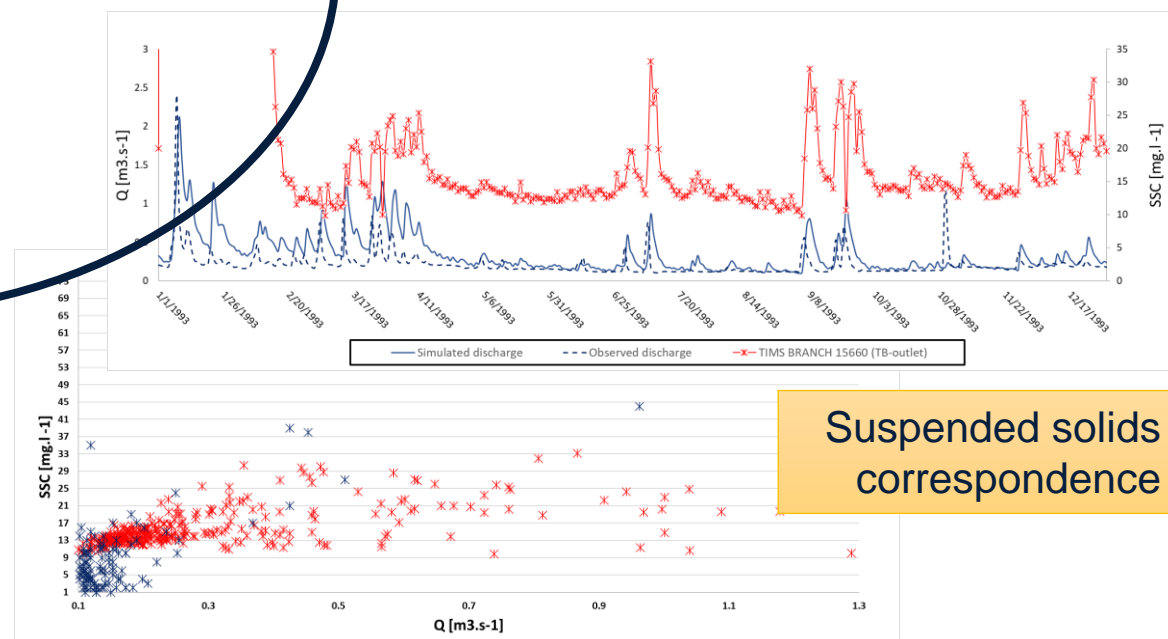
Discharge correspondence



Stepwise development and calibration



Uranium simulations



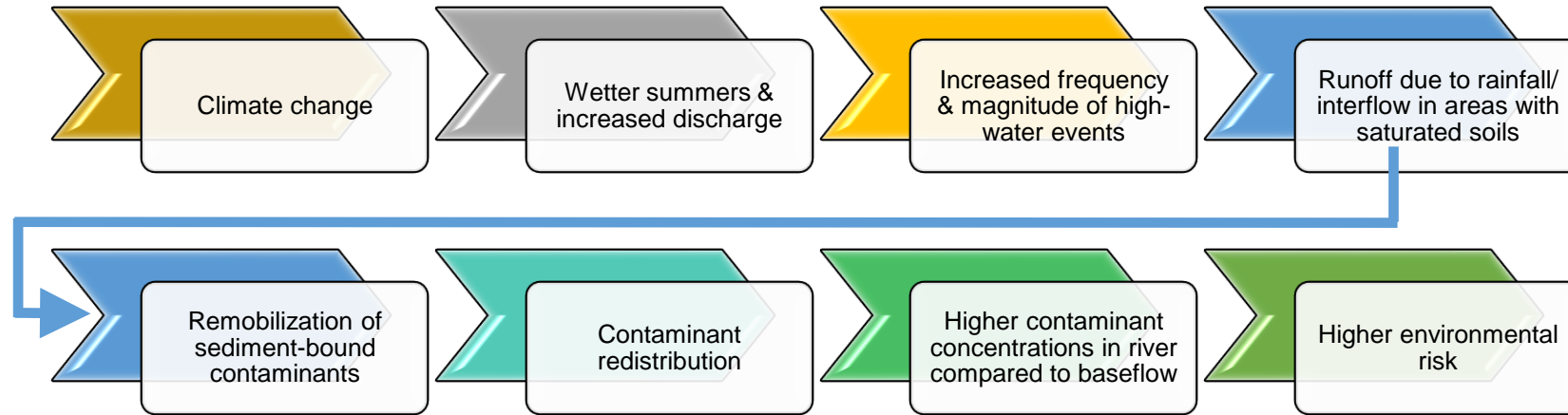
Suspended solids correspondence

Next step: Evaluate role of model parameter uncertainty

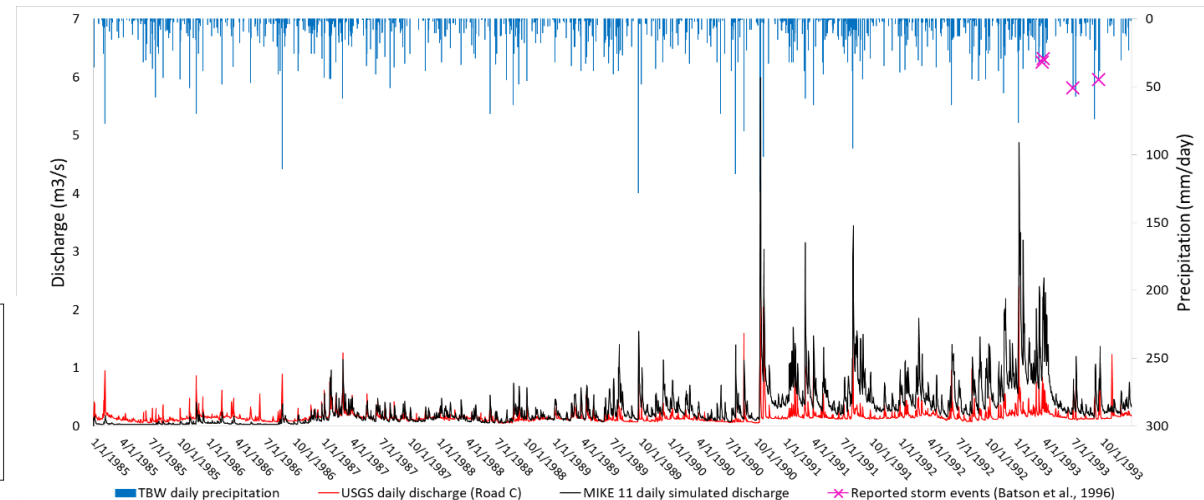
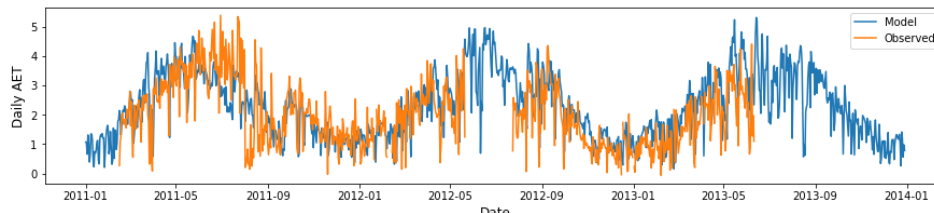


Subtask 3.1: Calibration of the Tims Branch Watershed Model and Scenario Analysis

3. Transformation of event-based MIKE SHE/MIKE 11 hydrological model to continuous model that allows for long-term simulations to assess the role of climate change on heavy metal transport.



- Storage in saturated zone becomes stable after 7-10 year (increases initially)
- Discharge simulations increase during this 7-10 year period
- Need to recalibrate hydrological model for long-term simulations





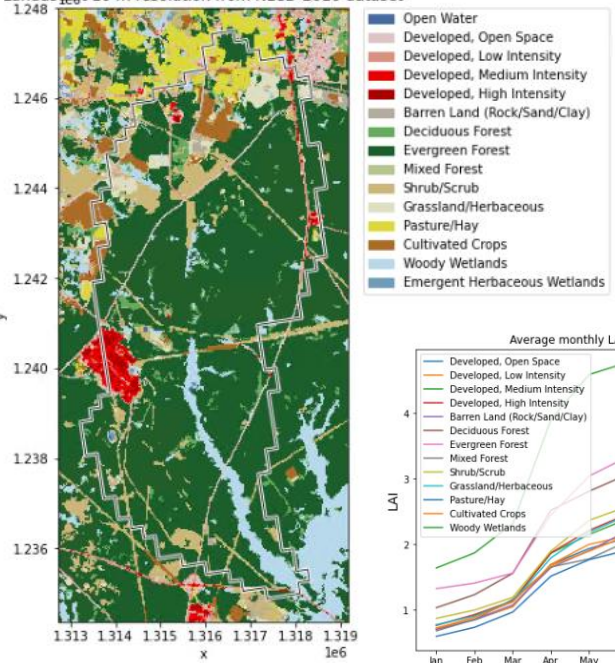
Subtask 3.1: Calibration of the Tims Branch Watershed Model and Scenario Analysis

4. Development of scripts using GIS and Python to automate and accelerate hydrological model development

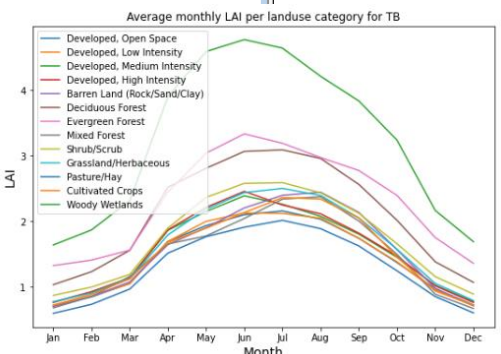
Initial version of a MIKE SHE/MIKE 11 model can be developed within day(s)

Land use information (NLCD, MODIS)

Landuse at 10 m resolution from NLCD-2016 dataset



- Open Water
- Developed, Open Space
- Developed, Low Intensity
- Developed, Medium Intensity
- Developed, High Intensity
- Barren Land (Rock/Sand/Clay)
- Deciduous Forest
- Evergreen Forest
- Mixed Forest
- Shrub/Scrub
- Grassland/Herbaceous
- Pasture/Hay
- Cultivated Crops
- Woody Wetlands
- Emergent Herbaceous Wetlands

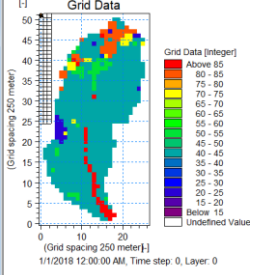


MIKE SHE Flow Model Description

- Display
- Simulation specification
- Model Domain and Grid
- Topography
- Climate
 - Precipitation Rate
 - Reference Evapotranspiration
- Land Use
 - Vegetation
 - Grid code = 21
 - Grid code = 22
 - Grid code = 23
 - Grid code = 24
 - Grid code = 31
 - Grid code = 41
 - Grid code = 42
 - Grid code = 43
 - Grid code = 52
 - Grid code = 71
 - Grid code = 81
 - Grid code = 82
 - Grid code = 90
 - Paved Runoff Coefficient
- Rivers and Lakes
- Overland Flow
 - Manning Number
 - Detention Storage
 - Initial Water Depth
- Unsaturated Flow
 - Soil Profile Definitions
 - Grid code = 1
 - Grid code = 2
 - Grid code = 3
 - Grid code = 4
 - Grid code = 5
 - Grid code = 6
 - Grid code = 7
 - Grid code = 8
 - Grid code = 9
 - Grid code = 10

User Defined Vegetation Development

	End day	LAI	Root	Kc
1	0	0.721219	457	0.9
2	31	0.716186	457	0.9
3	59	0.844139	457	0.9
4	90	1.04942	457	0.9
5	120	1.69097	457	0.9
6	151	1.93229	457	0.9
7	181	2.09936	457	0.9
8	212	2.15582	457	0.9
9	243	2.0307	457	0.9
10	273	1.74013	457	0.9
11	304	1.3681	457	0.9

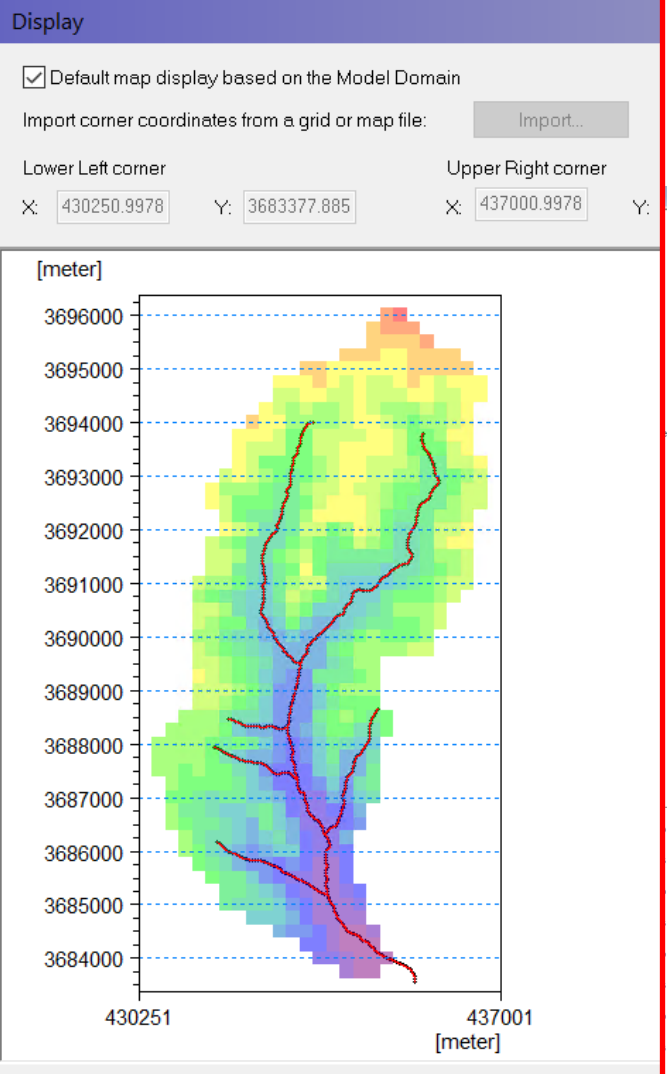


MIKE Zero - [MIKE_model_TB]

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MIKE SHE Flow Model Description

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 - Grid code = 8
 - Grid code = 9
 - Grid code = 10





Subtask 3.1: Calibration of the Tims Branch Watershed Model and Scenario Analysis

FIU Year 3 Projected Scope

- Complete FIU Year 3 Project Technical Plan.
- Deliver calibrated/validated MIKE 11 model for uranium to DOE and perform scenario modeling using Tims Branch MIKE 11 ECO Lab sediment & contaminant transport models for uranium.
- Complete calibration of Tims Branch sediment & contaminant transport model for tin and nickel including optimization of the ECO Lab module.
- Continue scenario analyses using calibrated coupled hydrology and contaminant transport model of Tims Branch by running long-term as well as event-based simulations aimed at evaluating the potential impact of seasonal and annual climate variability as well as extreme storm events (e.g., 500-yr Average Recurrence Interval (ARI)) on the transport of uranium in Tims Branch.
- Continue automation development by further optimizing Python scripts to accelerate hydrological model development.
- Complete FIU Year 3 Year End Report

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Subtask 3.2: Model Development for Fourmile Branch with Specific Focus on the F-Area Wetlands

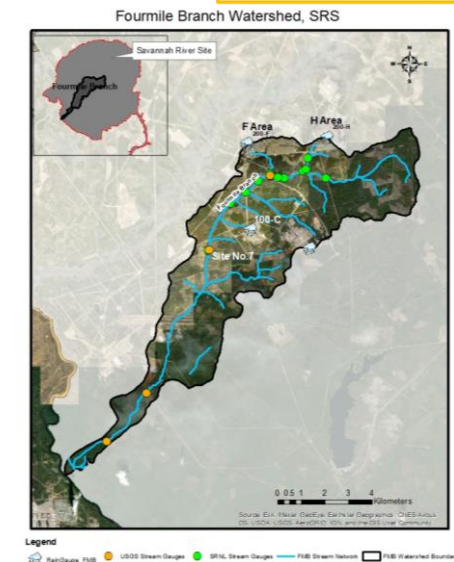
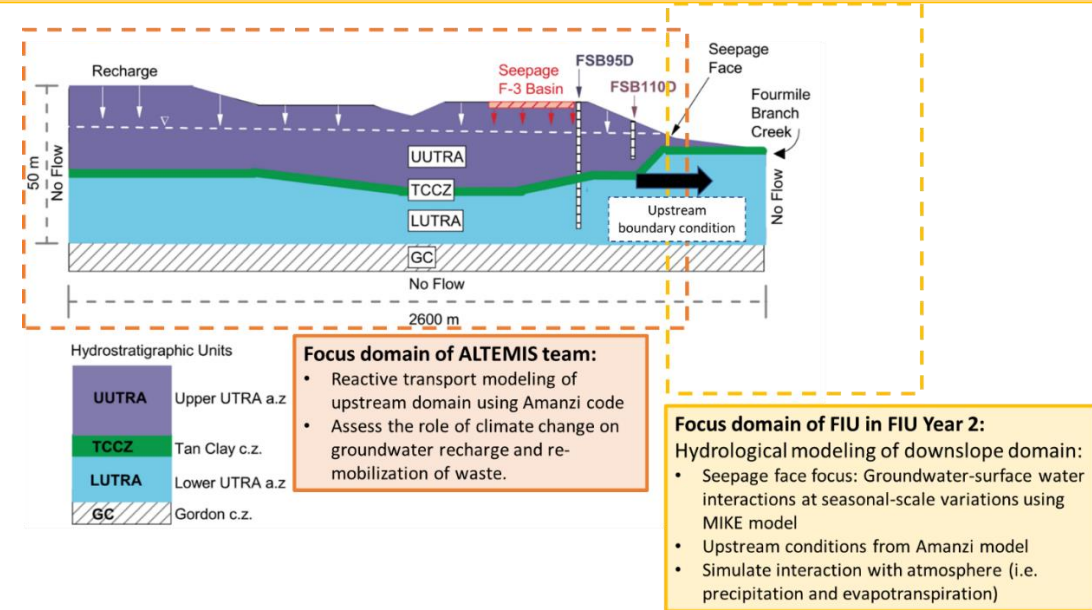
NOTE: This subtask revised to provide support to current research in SRS F-Area under ALTEMIS project.

Background:

- Fourmile Branch stream contaminated by historical release of radionuclides (e.g., ^{129}I , ^{137}Cs)
- Site environmental reports indicate contaminants bound to sediment and soil along wetland riparian forests downstream from reactor discharge points.
- Potential exists for remobilization and redistribution of sediment-bound contaminants during frequent or heavy rainfall or storm events.

Objectives:

- Develop conceptual model of hydrological flow processes within seepage line over time in response to precipitation as well as seasonally [lateral (shallow) surface flow vs groundwater seepage] via detailed assessment of in situ observations.
- Build hydrological model focused on flow of GW downslope through funnel & gate system and entering seepage line—riparian zone—river network using MIKE model.
- Create 2D model for improved understanding of flow dynamics in study area.
- Develop 3D model of GW-seepage-line-river network system and role of funnel and gate system.
- Incorporate biogeochemistry focusing on fate and transport of I-129 (and possibly other radionuclides) in F-Area.



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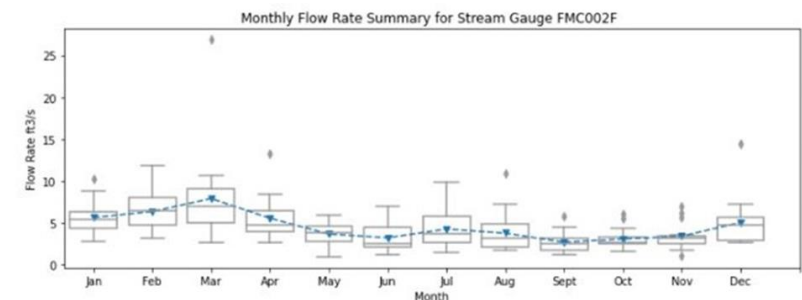
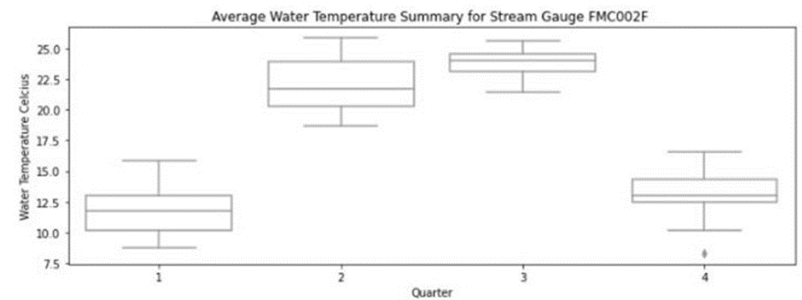
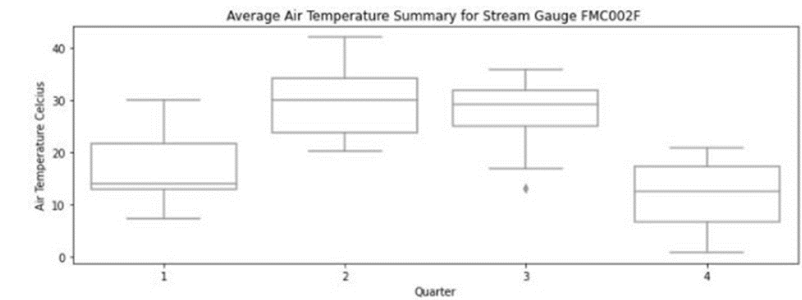
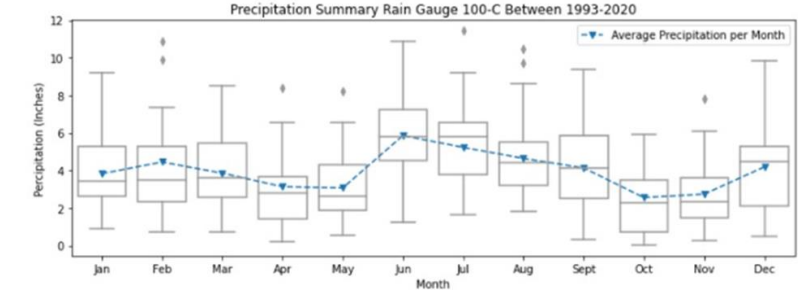
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Subtask 3.2: Model Development for Fourmile Branch with Specific Focus on the F-Area Wetlands

FIU Year 2 Research Highlights & Accomplishments:

1. Performed analysis of F-Area GW & SW variability from precipitation gauges, wells and surface water data using Python as part of site characterization to:
 - Better understand how different physical fluxes and chemical properties vary at a single location.
 - Enable comparison of observations at multiple locations within the landscape and generate a perceptual model of seasonal variations in atmospheric forcing (precipitation, temperature and evapotranspiration) that trigger lateral variations in groundwater and river flow, which in turn impact chemical variations.
2. Developed an initial version of a MIKE SHE / MIKE 11 model to enable simulations of intra-year and inter-year variations of groundwater-river network interaction and flow variability.



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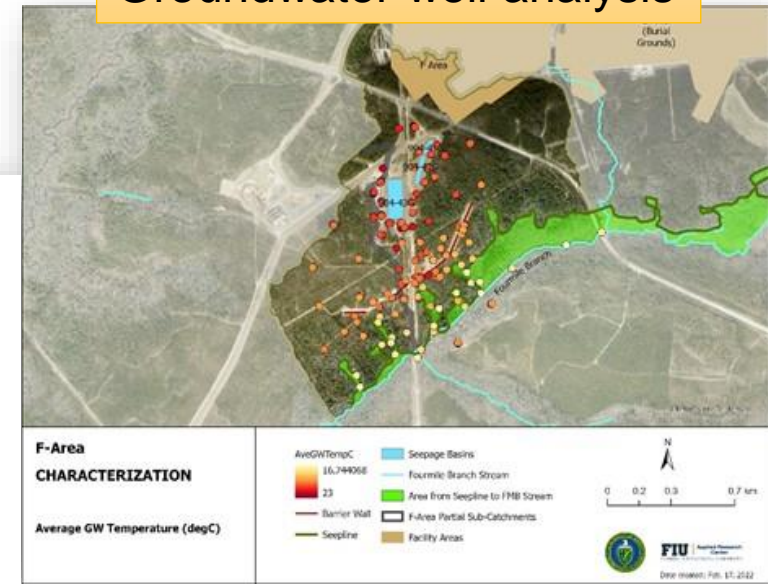
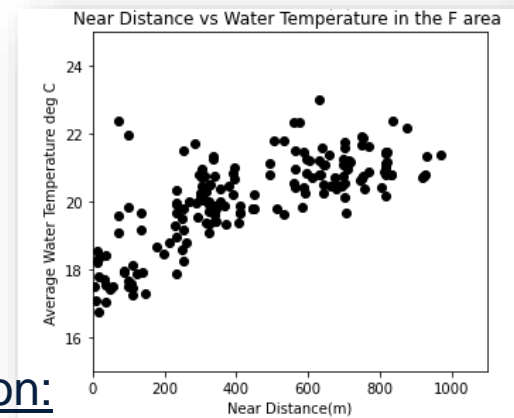
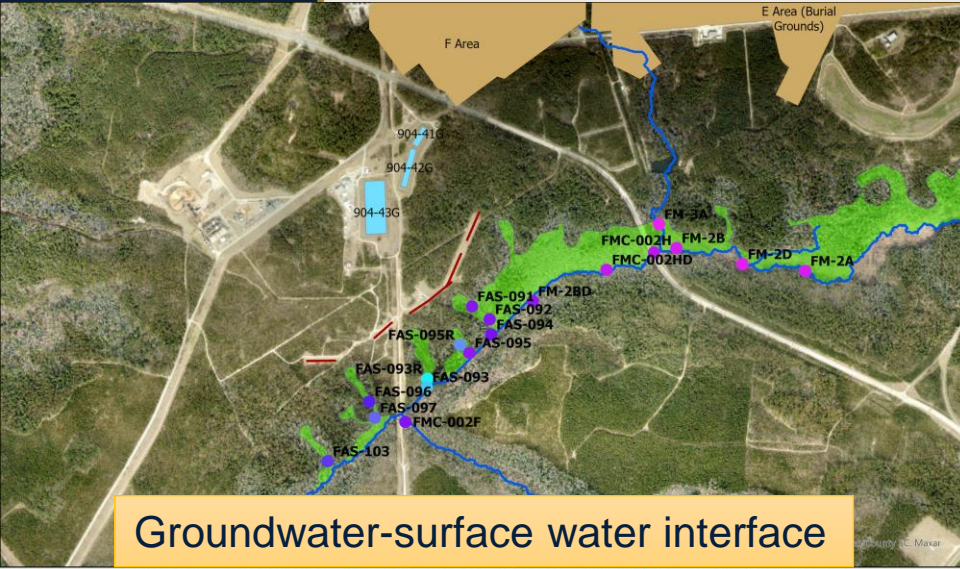
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Subtask 3.2: Model Development for Fourmile Branch with Specific Focus on the F-Area Wetlands

1. Performed analysis of F-Area GW & SW variability from precipitation gauges, wells and SW data using Python.

Groundwater well analysis



1. Focus on:

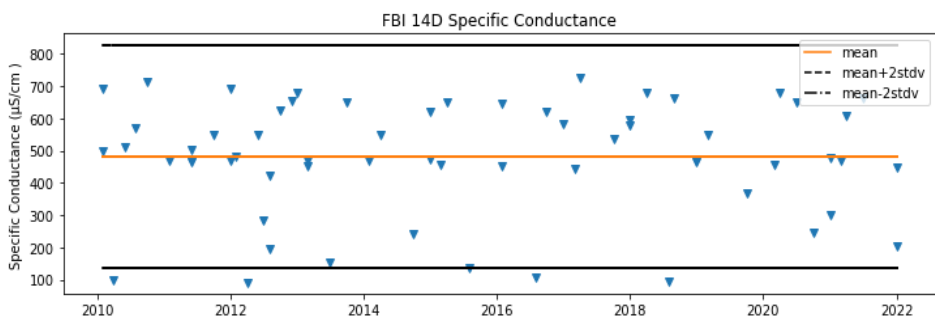
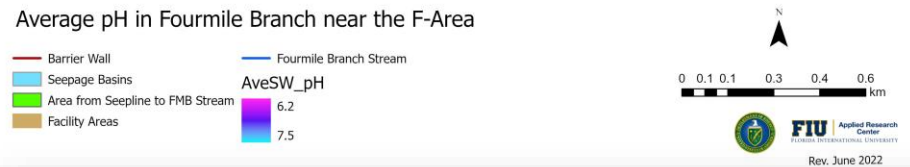
Physical properties

- Precipitation
- GW levels
- Temperature

Chemical properties

- pH
- Specific conductance

Area	Average pH of Multiple Gauges	Average of the pH Variance at multiple gauges	Average Temp of Multiple Stream Gauges	Average of the Temp Variance
Upper Aquifer Zone	4.709	0.756	19.975	2.1
Lower Aquifer Zone	5.216	0.887	20.368	0.416
Gordan Aquifer	7.316	1.387	20.44	0.16
Within Seepines	6.019	1.275	17.978	0.538
UAZ (Outside Seepines)	4.578	0.645	20.274	1.719
LAZ (Outside Seepines)	5.176	0.878	20.376	0.4309



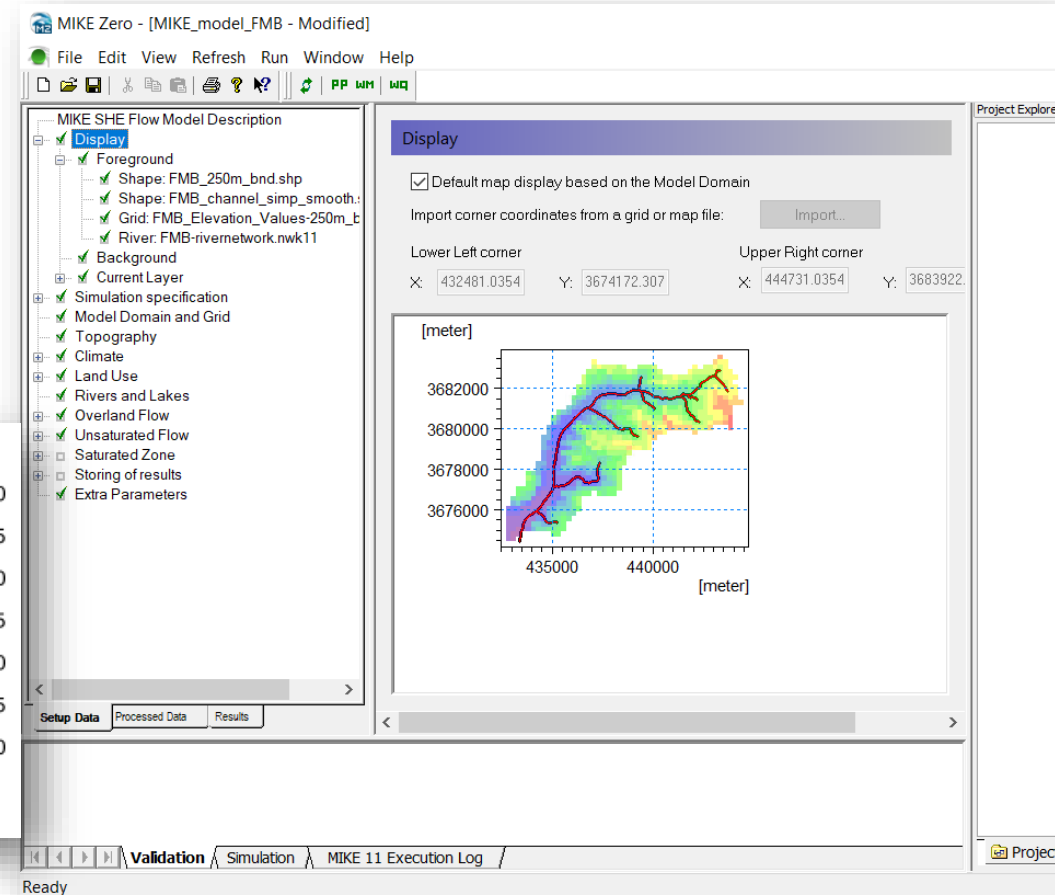
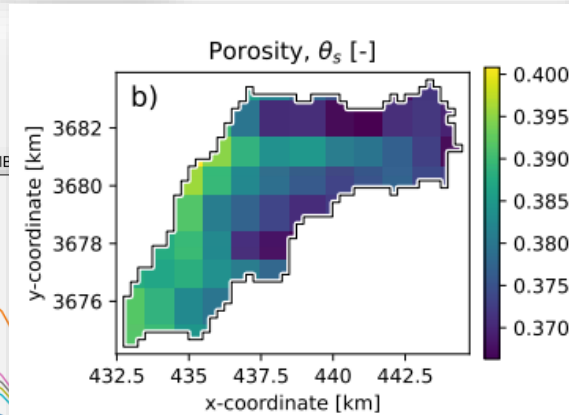
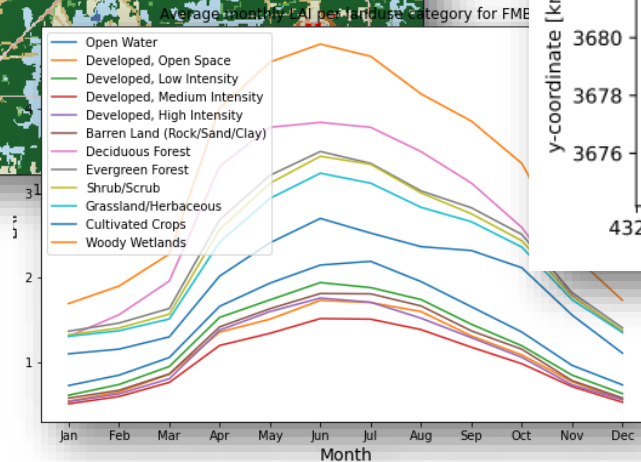
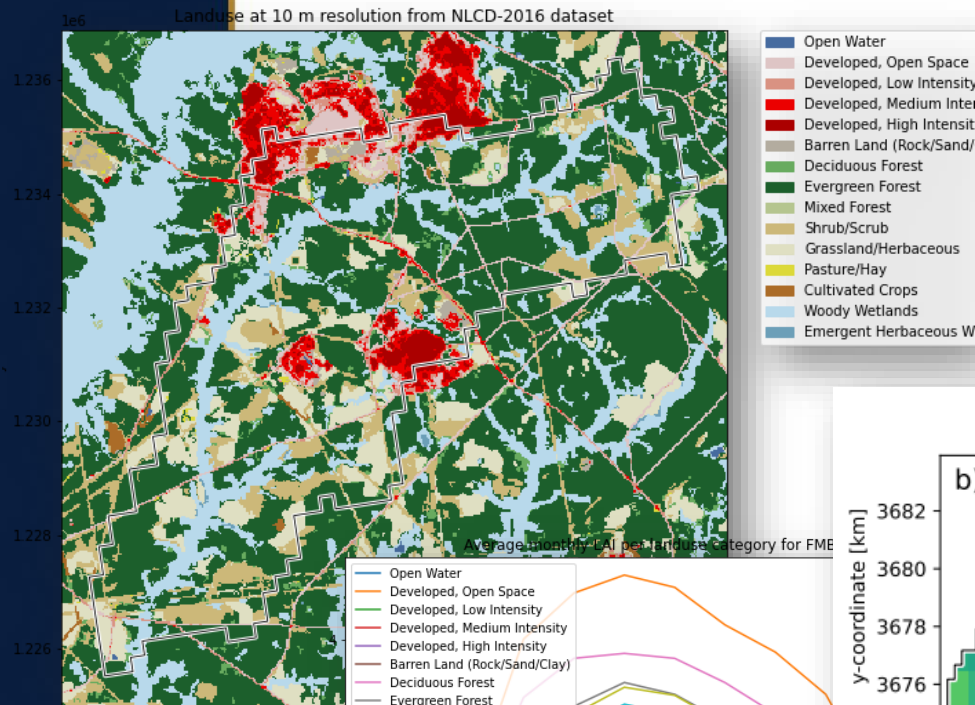
2. Data evaluation and outlier removal
3. Evaluation of both average behavior and variability

Conceptual analysis for different hydrological components



Subtask 3.2: Model Development for Fourmile Branch with Specific Focus on the F-Area Wetlands

2. Developed an initial version of a MIKE SHE / MIKE 11 model to enable simulations of intra-year and inter-year variations of groundwater-river network interaction and flow variability.



Allowed for testing of automation procedure
Next step: Calibration of model to historical observations

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Subtask 3.2: Model Development for Fourmile Branch with Specific Focus on the F-Area Wetlands

FIU Year 3 Projected Scope

- Calibration of hydrological model of Fourmile Branch riparian stream system.
- Long-term simulation of GW-SW interactions within FMB to:
 - Examine impact of seasonal changes in precipitation on hydrological variability in SW & GW.
 - Assess impact of climate change by examining yearly variations in precipitation over 30-yr period.
 - Examine SW-GW interaction, zooming in on SRS F-Area seepage face.
- Extend model by adding contaminant fate and transport simulations at FMB watershed scale.
- Literature review and collection of SRS site characterization data required for model development.
 - Acquire timeseries data being analyzed using PyLEnM package developed under ALTEMIS project by FIU-ARC's IT team.
 - Process observed timeseries data for evaluation within MIKE modeling results.
 - Fieldwork required will be conducted in collaboration with SRNL scientists and members of the ALTEMIS team (e.g., surface water as well as soil/sediment samples at a downstream location in FMB to assess suspended solids and contaminant (e.g., I-129, Sr-90) concentrations).
- Train FIU graduate and/or undergraduate students on GIS data processing, model development using MIKE, and data generation and model evaluation using Python.

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Task 5

Research and Technical Support for WIPP

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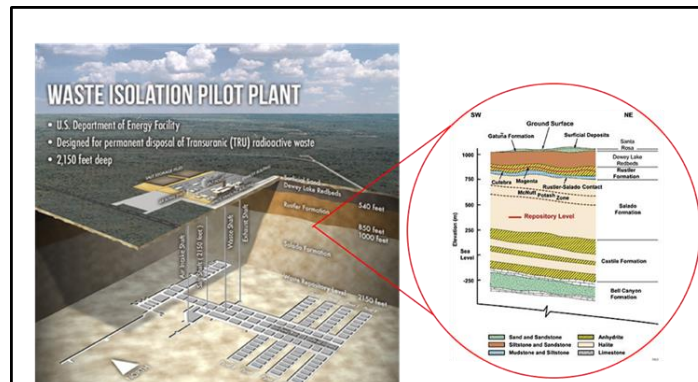
Subtask 5.1: The Fate of Actinide in the Presence of Ligands in High Ionic-Strength System

Site Needs:

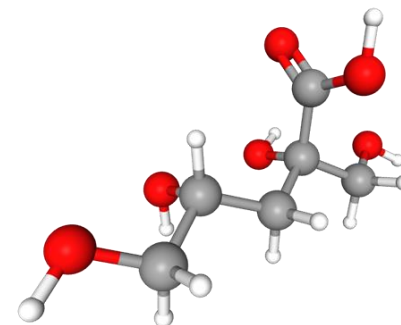
- Safety Assessment is required for recertification of the Waste Isolation Pilot Plant (WIPP) every 5 yrs.
- There is a critical need to understand the safety ramification of the long-term storage of TRU waste.
- A better understanding of the fate and transport of actinide in a high ionic-strength brine environment is important to addressing the low-probability scenario of potential brine inundation and contaminants' release due to human intrusions.

Objectives:

- The role of corrosion products—iron oxide minerals (e.g., magnetite) and cement additive (gluconate [GLU])—that may enhance actinide solubility is poorly understood:
 - Sorption retards migration of radionuclides to the environment by allowing longer transport time and decay of larger portions of nuclide inventory
- Investigate, via batch sorption experiments, actinide interaction with brines in environments expected at the WIPP.



A rendered layout of the WIPP, Carlsbad NM

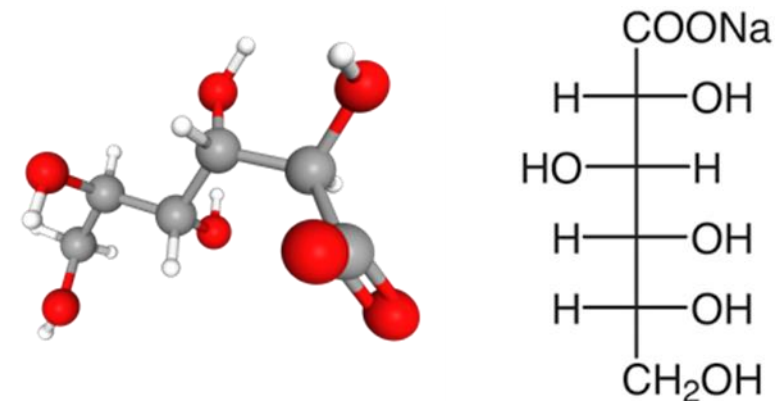
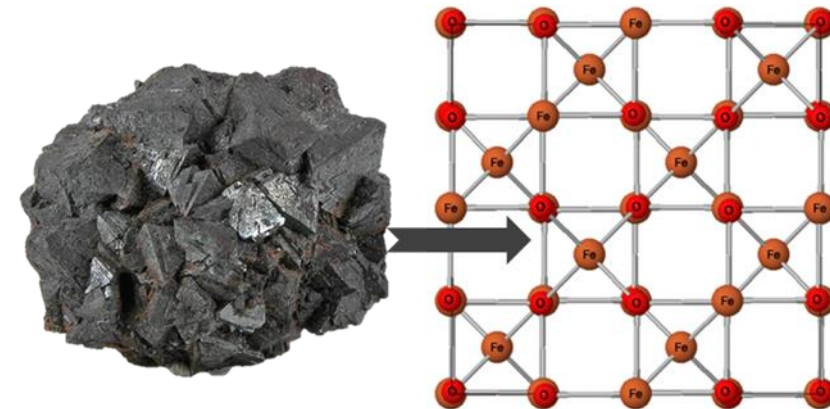




Subtask 5.1: The Fate of Actinide in the Presence of Ligands in High Ionic-Strength System

FIU Year 2 Research Highlights & Accomplishments:

- Studied the impact of GLU on adsorption of actinide onto iron oxide mineral (magnetite) under anaerobic conditions.
- Magnetite - BET surface area & pore size: 8.1 m²/g & ~11.5 nm
- UO₂²⁺ and, Nd³⁺, Th⁴⁺, were used as stable chemical analogs for americium and plutonium.
- An actinide concentration used in these studies ranged from 10⁻⁸ to 10⁻⁶ M.
- Brines concentration & type: 0.1, 1.0 and 5.0 mol/L NaCl, MgCl₂ and CaCl₂.
- Batch experiments:
 - 1 g/L magnetite and GLU 10⁻⁶ mol/L GLU, (NaC₆H₁₁O₇).
 - Spiked samples were pH adjusted to pH 8 ±0.5.
 - Centrifuged at 8,000 RPM for 20 min.
 - All batch experiments were performed in triplicates with standard deviations <10%.
- Samples were collected at various time intervals and analyzed on the ICP-MS.



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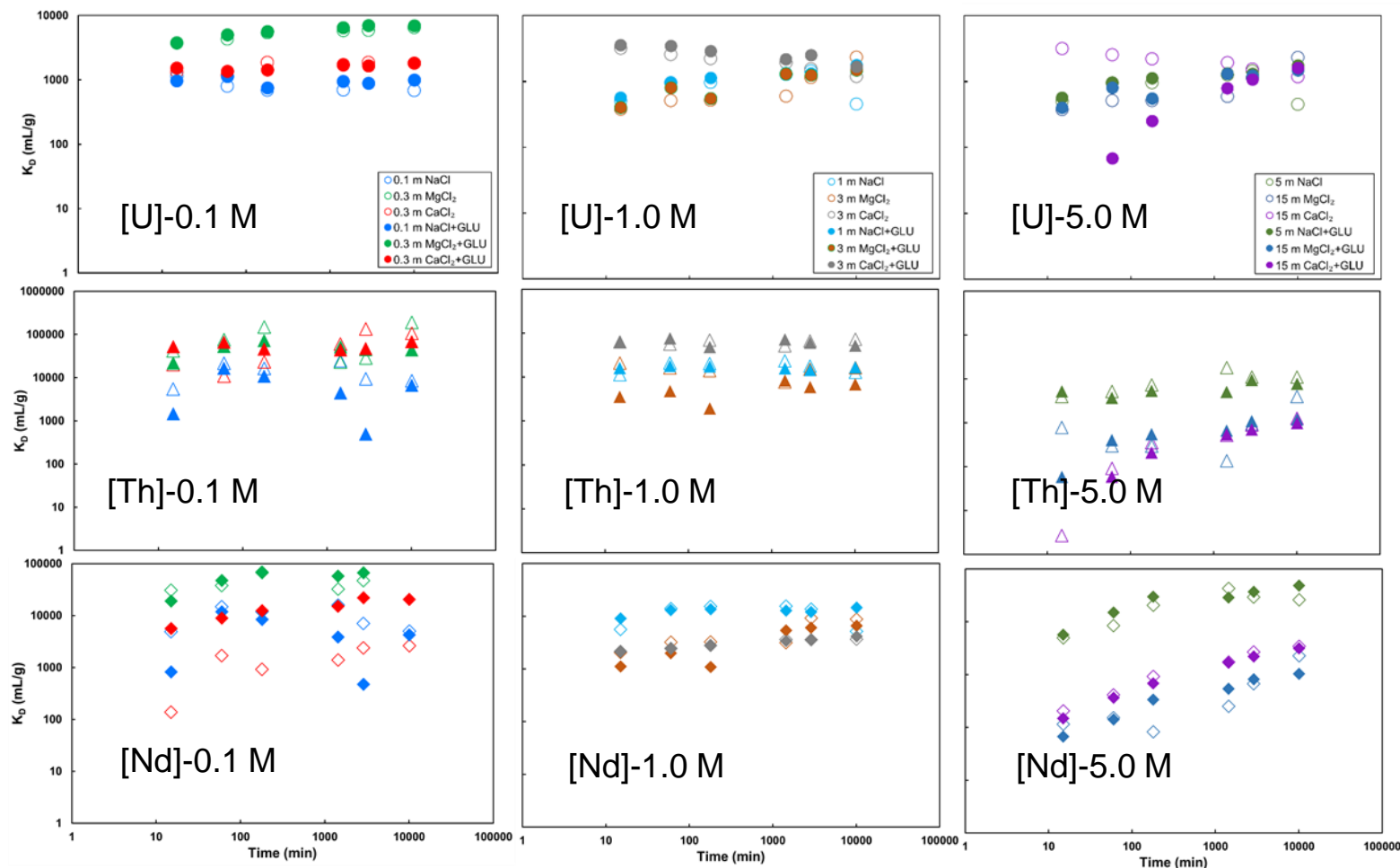
Subtask 5.1: The Fate of Actinide in the Presence of Ligands in High Ionic-Strength System

FIU Year 2 Research Highlights & Accomplishments:

- Sorption quantified in terms of distribution coefficient (K_d)
- $K_d(\text{mL g}^{-1}) = \frac{[\text{An}]_{\text{solid}}}{[\text{An}]_{\text{solution}}}$
- GLU addition has little impact on adsorption of contaminants onto magnetite.
- GLU did not enhance solubility of UO_2^{2+} and, Nd^{3+} , Th^{4+} .
- Sorption trends for the GLU-free brines were similar to that for GLU-amended brines.
- Brine types had a significant influence on actinide solubility in the following order:

$\text{CaCl}_2 \approx \text{MgCl}_2 > \text{NaCl}$
with increasing ionic strength.

Increasing ionic strength →



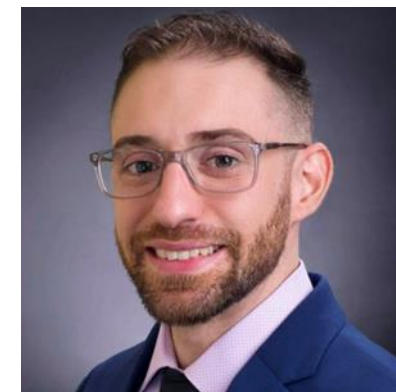
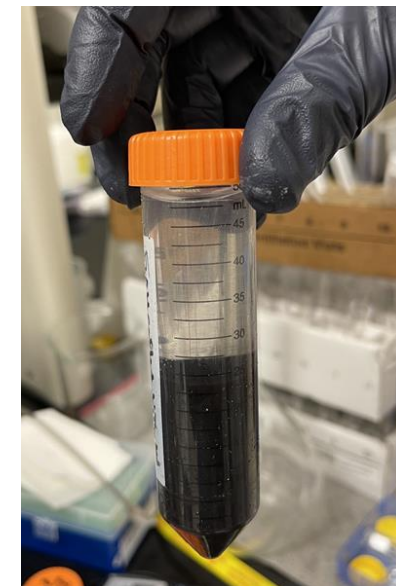
FIU



Subtask 5.1: The Fate of Actinide in the Presence of Ligands in High Ionic-Strength System

FIU Year 2 Research Highlights & Accomplishments:

- Alexis Vento, DOE fellow supporting this Subtask graduated with a Masters degree in Environmental Engineering (July 2021). Alexis currently works at Stearns, Conrad & Schmidt, Consulting Engineers, Inc.
- Completed batch sorption experiments investigating the impact of GLU on actinide sorption onto magnetite in WIPP-relevant brines such as NaCl, MgCl_2 , CaCl_2 , the U.S. Energy Research and Development Administration Well 6 brine (ERDA-6, low Mg) and generic weep brine (GWB, high Mg) using higher An concentration of 1,000 $\mu\text{g/L}$.
- Conference presentation at the International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP-19).



**DOE Fellow Alexis Vento,
Class of 2017.**

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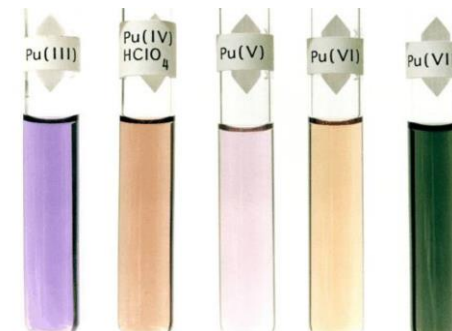
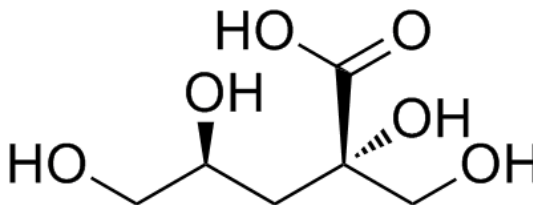
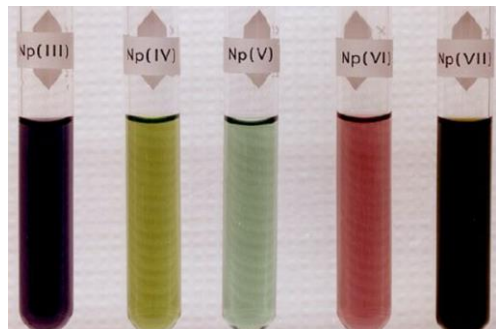
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Subtask 5.1: The Fate of Actinide in the Presence of Ligands in High Ionic-Strength System

FIU Year 3 Projected Scope

- Undertake modeling of collected sorption data by SIT or Pitzer models to obtain pertinent interaction parameters (virial coefficients) required for high salt systems.
 - TOUGHREACT
- Study the impact of citrate or isosaccharinate (ISA), an important byproduct of alkaline degradation of cellulose on sorption of actinide onto iron (II) hydroxide in WIPP-relevant brines and conditions.
- Characterization of treated solid phases employing microscopy, spectroscopy and x-ray diffraction techniques.



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Task 6

Hydrology Modeling of Basin 6 of the Nash Draw Near the WIPP

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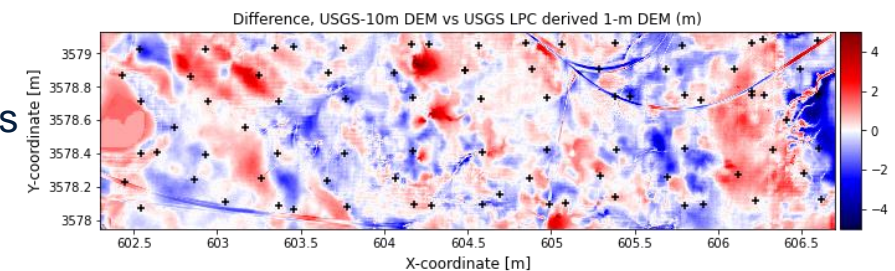
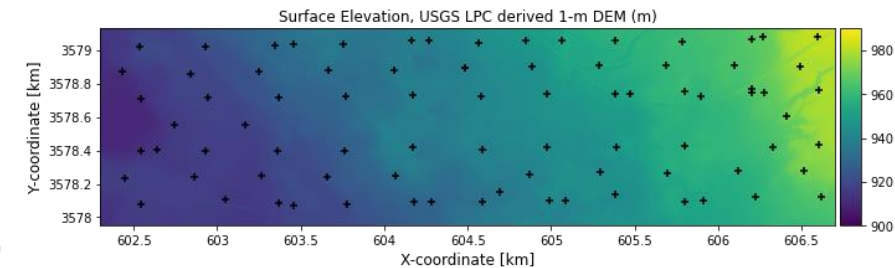
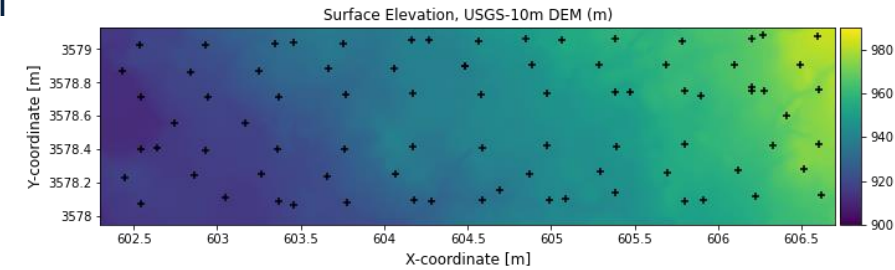
Hydrology Modeling of Basin 6 of the Nash Draw Near the WIPP

Site Needs:

- Improve current understanding of regional and local GW flow near WIPP to compute water balance and derive more accurate estimates of GW recharge to better predict propagation rate of shallow dissolution front and potential long-term impact on repository performance.

Objectives:

- Develop GW-basin model for Basin 6/Nash Draw west of WIPP using DOE-developed open-source Advanced Simulation Capability for Environmental Management (ASCEM): Amanzi Simulator to improve current understanding of regional and local GW flow.
- Currently, ASCEM toolset unable to account for land surface hydrology, which is essential for computing water balance across multiple scales.
- Use Advanced Terrestrial Simulator (ATS) code for solving ecosystem-based, integrated, distributed hydrology. ATS builds on the multi-physics framework and toolsets (such as mesh infrastructure, discretizations, solvers) provided by Amanzi.
- ATS will provide surface process parameters (e.g., infiltration rate) for incorporation into the GW models within ASCEM toolbox to facilitate sensitivity and uncertainty analysis of GW and SW flows.





Subtask 6.1: Basin 6 DEM Development and Delineation of Surface Hydrological Features

FIU Year 2 Research Highlights:

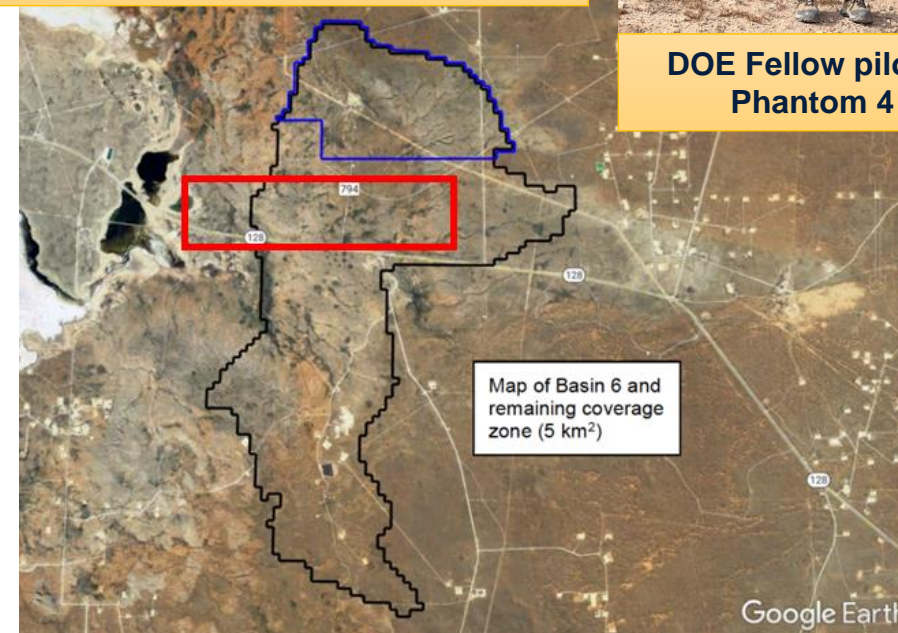
1. FIU team traveled to Carlsbad, NM (Dec 2021) to complete aerial survey and finish collecting images of remaining area in Basin 6 (~5 km²). Total of 22 km² surveyed.
2. Established photogrammetry workflow and developed a multitude of approaches to clean UAV drone observations from 'non-ground' targets.
3. Evaluated various approaches to identify and process 'non-ground' targets focused on Basin 6 Pilot Study Area (DSM & point cloud generation).
4. Final data set to be processed as per established photogrammetry workflow.



FIU Research Team: Mackenson Telusma and DOE Fellows (Gisselle Gutierrez-Zuniga and Eduardo Rojas)



DOE Fellow piloting DJI Phantom 4 Pro.



Basin 6 study area (area surveyed in Dec 2021 in blue, pilot study area in red).

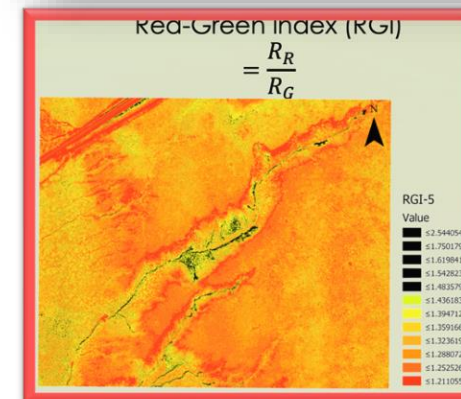
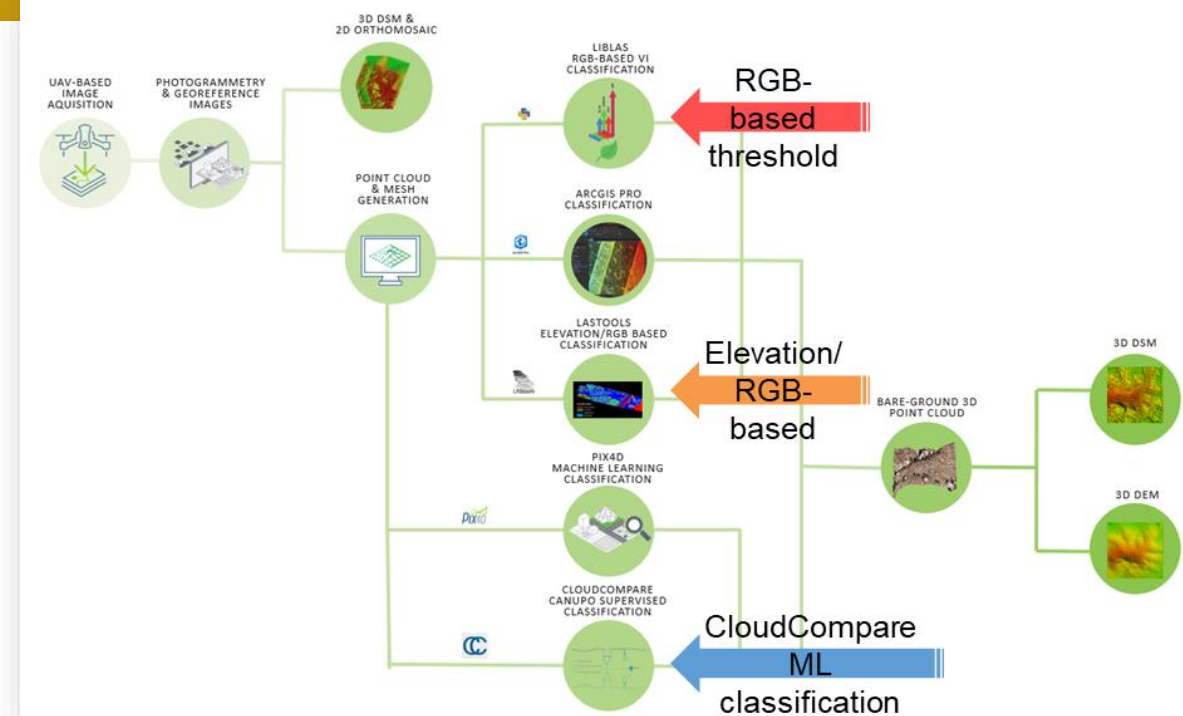
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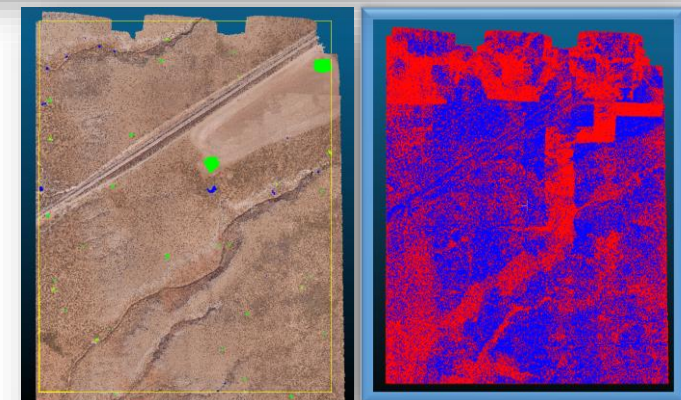


Subtask 6.1: Basin 6 DEM Development and Delineation of Surface Hydrological Features

2. Established photogrammetry workflow and developed a multitude of approaches to clean UAV drone observations from 'non-ground' targets.
 - Previously tested RGB-based vegetation indices derived from lit. review were applied to refine high-res DEM developed from drone imagery collected during pilot study in Basin 6 in 2020.
 - RGI, GLI, RGBVI, NGRDI, VARI
 - Supervised machine learning (ML) classification developed using CloudCompare to generate bare ground point cloud/DEM.
 - Elevation & RGB-based classification using LAStools Python package used to develop bare ground point cloud.



RGI-VI map with threshold values displayed to distinguish vegetation and ground.



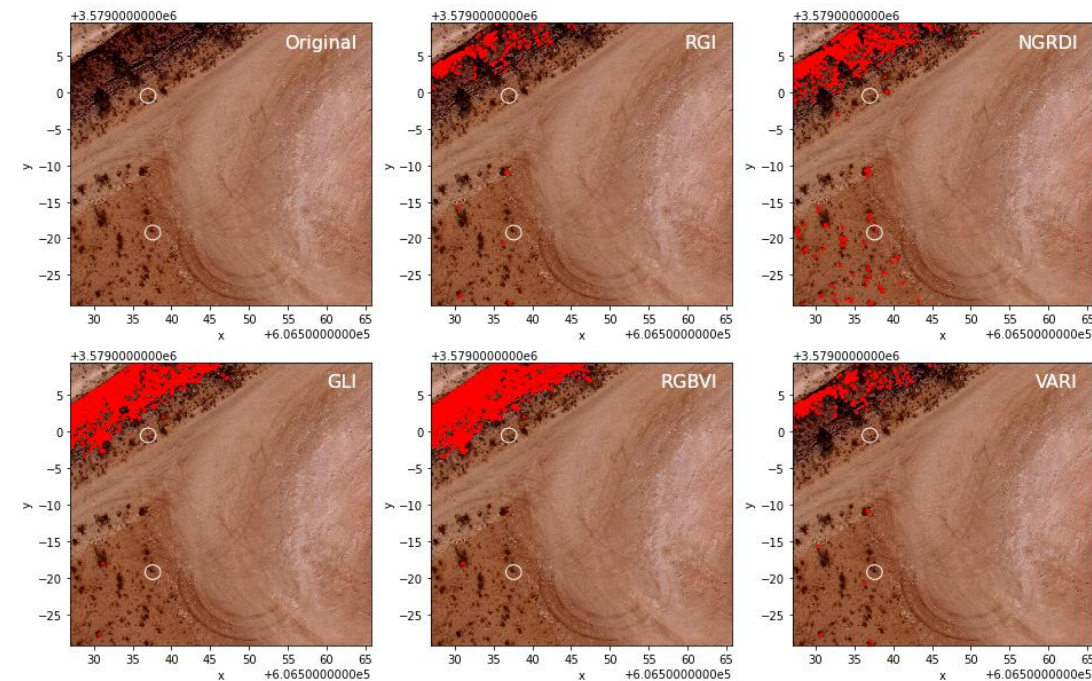
CloudCompare used to create supervised classification of ground and vegetation and applied to study area.



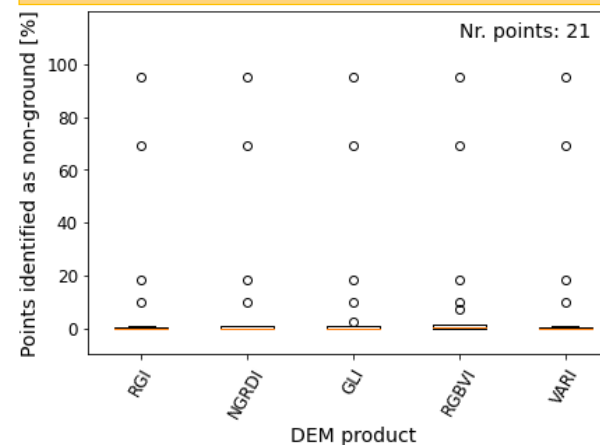
Subtask 6.1: Basin 6 DEM Development and Delineation of Surface Hydrological Features

3. Evaluated various approaches to identify and process 'non-ground' targets focused on Basin 6 Pilot Study Area (DSM & point cloud generation).

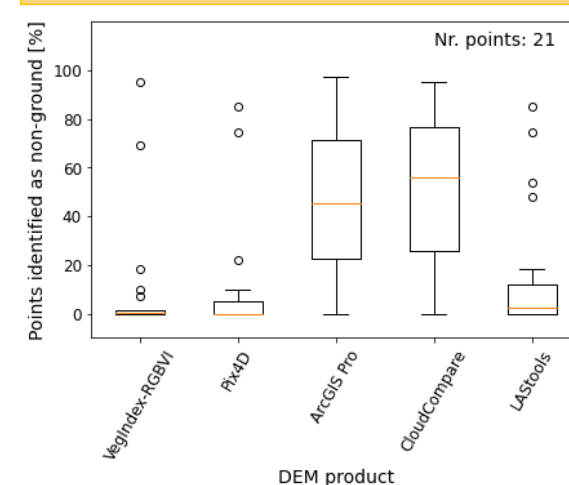
- With each vegetation removal method, a bare ground point cloud was generated using the Phantom 3 Pro and DEMs were created.
- Various method evaluated for their ability to identify ground surface from 'non-ground' (e.g., vegetation) points.
- Traditional Vegetation Index based approaches underestimate amount of point identified as 'non-ground'.
- Combined methods and ML-based approaches do better job identifying 'non-ground' points.
- Completed DEM development for Basin 6.



Vegetation Index methods:



Combined/ML methods:



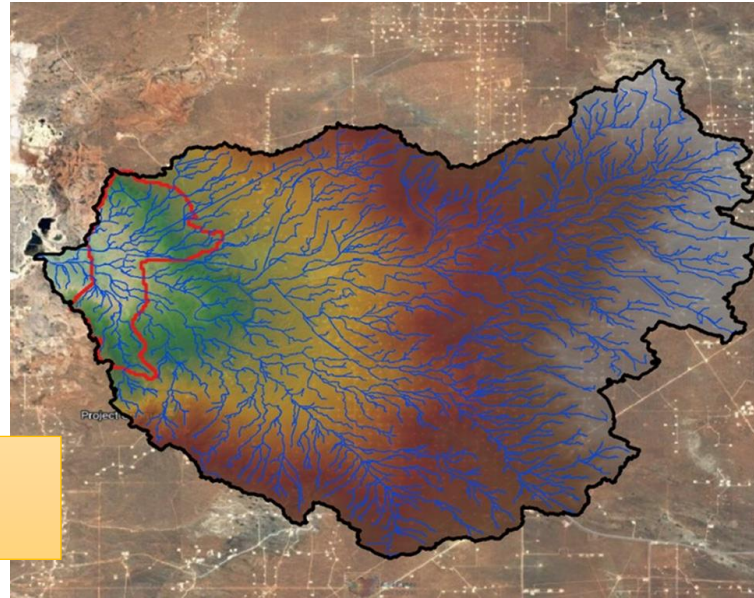


Subtask 6.1: Basin 6 DEM Development and Delineation of Surface Hydrological Features

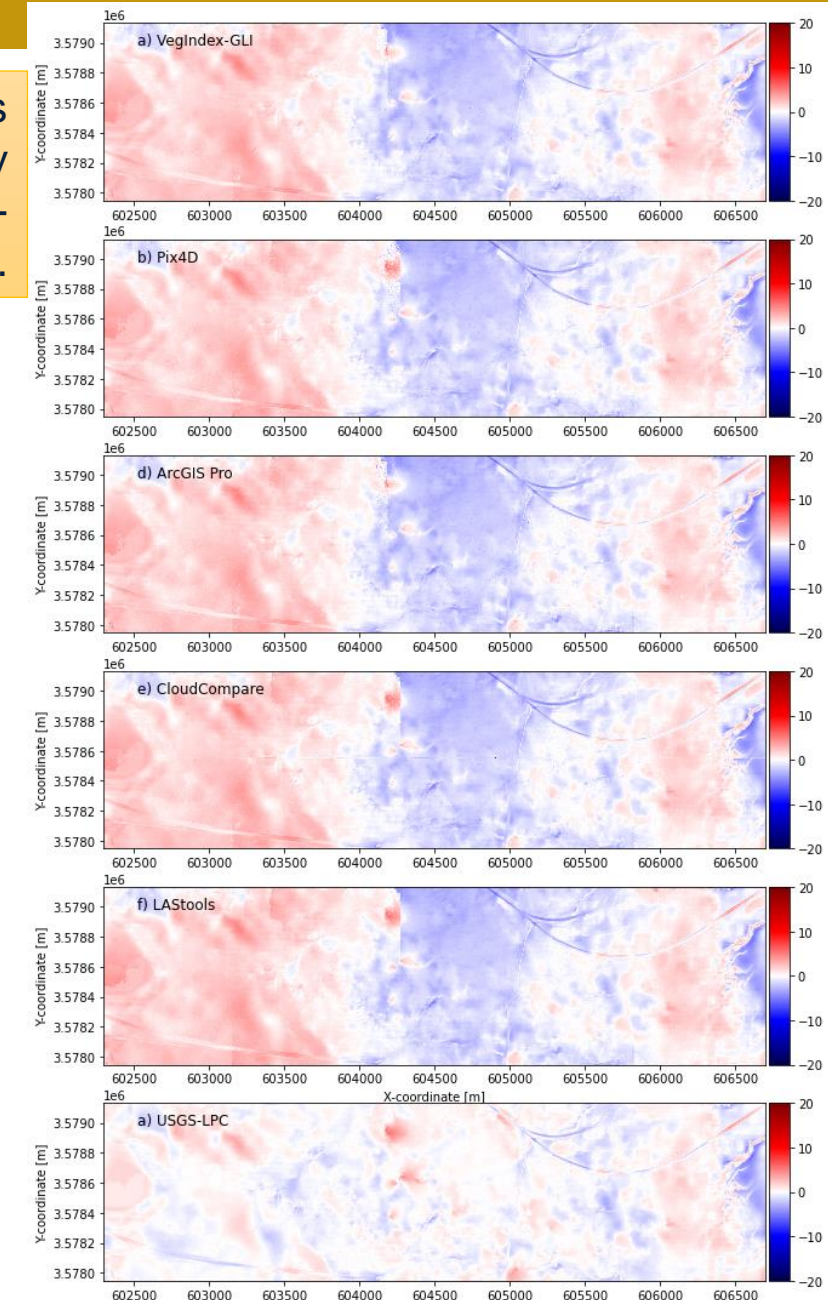
4. Final data set to be processed as per the established photogrammetry workflow.

Evaluation of various approaches by comparing with 10-meter USGS DEM.

- Elevation discrepancies discovered when compared with USGS 1 m DEM for Phantom 3 observations from February 2020.
- Phantom 4 observations from August and December 2021 currently being evaluated.
- Decided to generate DEM at 1-meter pixel resolution using USGS laser point cloud observations that became recently available.



1-meter DEM of Basin 6 and upstream area



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Subtask 6.1: Basin 6 DEM Development and Delineation of Surface Hydrological Features

FIU Year 3 Projected Scope

- FIU anticipates completing Subtask 6.1 in FIU Year 2 and no new scope will be incorporated in FIU Year 3 under this subtask.



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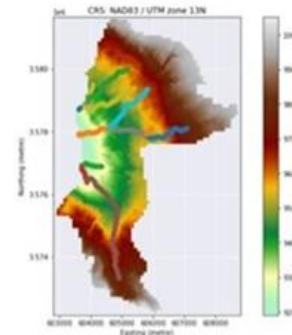
Subtask 6.2: Model Development

FIU Year 2 Research Highlights:

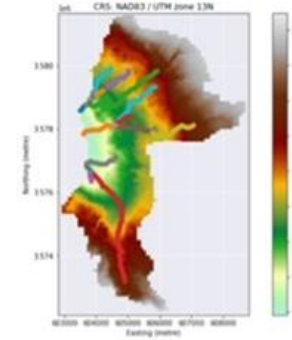
ARC Research

- Initiated training of DOE Fellow Aubrey Litzinger on ATS model development.
- Fellow worked on ATS-Basin 6 Docker image containing scripts generated during DOE Fellow Gisselle Gutierrez-Zuniga's Summer 2021 internship with LANL.
- 3 different DEMs of varying resolution (10m, 30m & 90m) used to test script created for generating the Basin 6 mesh that will be used for ATS model development.
- 3 different resolution meshes (10m, 30m & 90m) were generated using TINerator for comparison.
- Used 1-meter DEM developed under Subtask 6.1 to delineate smaller sub-basins to support further training of DOE Fellow on ATS model development and reduce simulation run time during Summer 2022 internship at LANL.

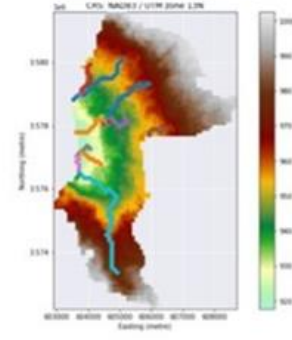
10-meter DEM
(Threshold Value: 10,000)



30-meter DEM
(Threshold Value: 1,000)

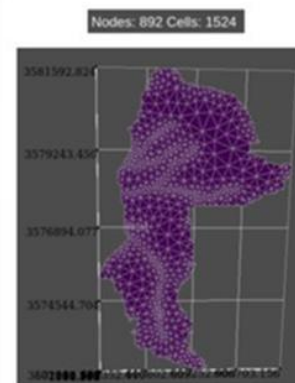


90-meter DEM
(Threshold Value: 140)

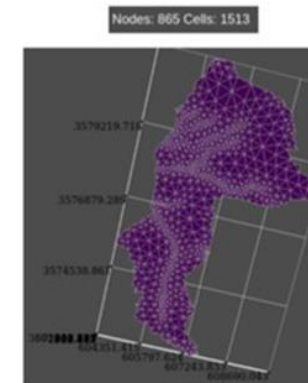


DEMs of Basin 6 of varying spatial resolution (10m, 30m and 90m).

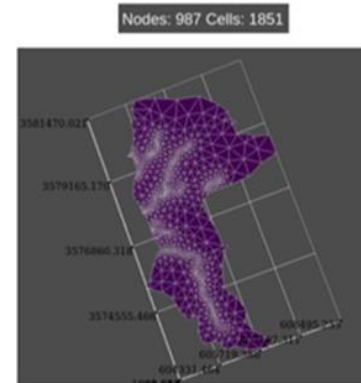
10-meter DEM
(Min = 0.01, Max = 0.5)



30-meter DEM
(Min = 0.01, Max = 0.5)



90-meter DEM
(Min = 0.005, Max = 0.5)



Meshes generated in TINerator from DEMs of Basin 6 of varying spatial resolution (10m, 30m and 90m).

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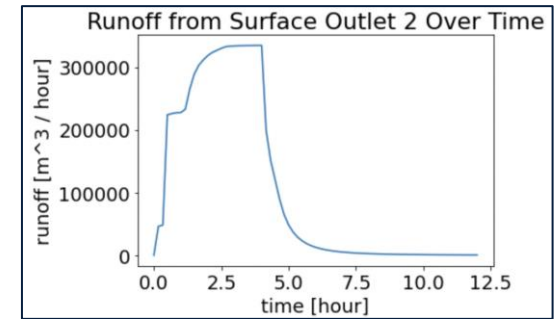
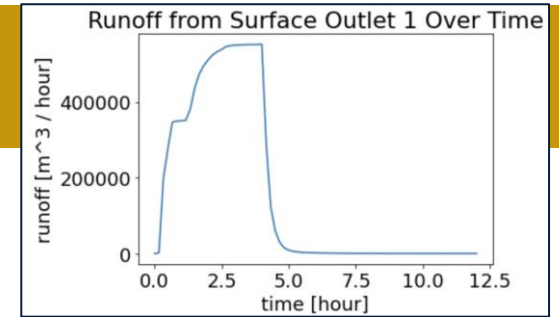
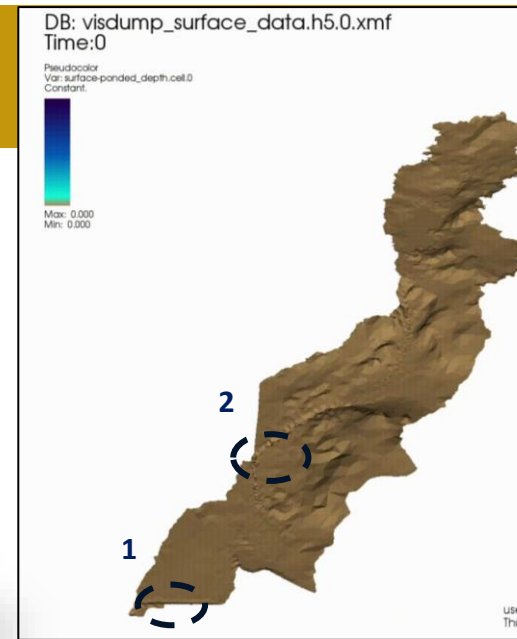
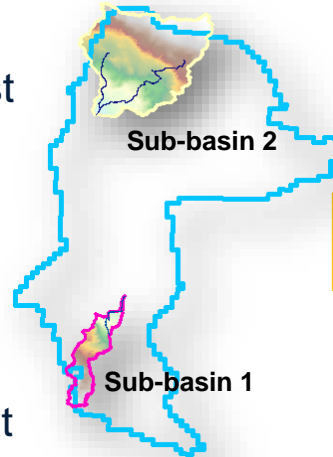


Subtask 6.2: Model Development

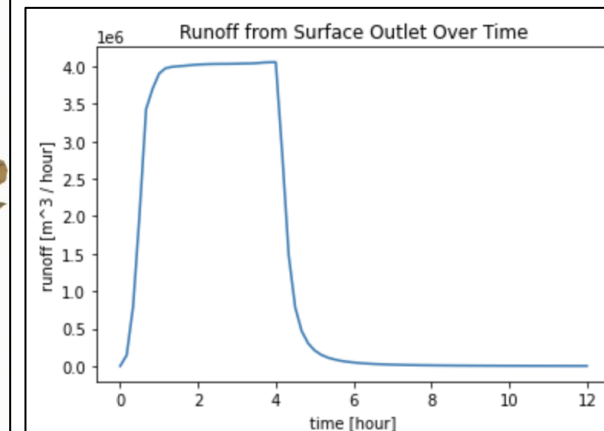
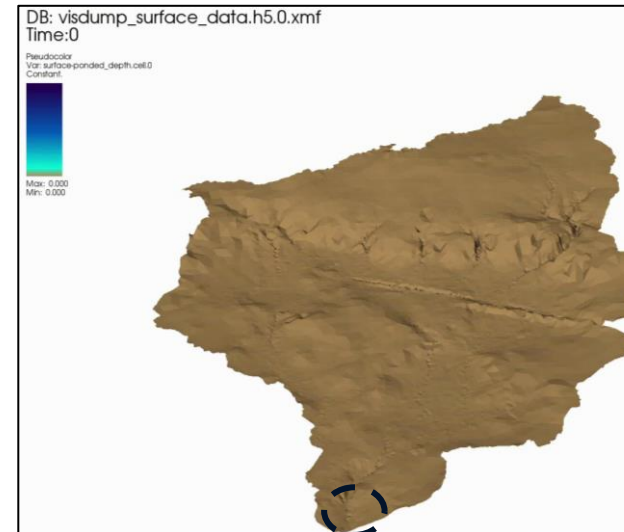
FIU Year 2 Research Highlights:

Summer 2022 Internship

- Used mesh created for small delineated sub-basins of Basin 6 and performed 12-hr simulation with rainfall for first 4 hrs across entire surface with outlet at the bottom of the basin to analyze the surface ponded depth.
- For Sub-basin 1, more runoff occurs at the outlet located at the bottom of the subbasin (outlet 1).
- For Sub-basin 2, water accumulates towards the outlet after 6 hours and runoff (plotted in ATS) decreases once the rain stops as there is less ponded water on the surface to drain.



Visualization of 12-hr simulation of Basin 6 Sub-basin 1 with rainfall for the first 4 hours across entire surface (left) and graph of associated runoff (right).



Visualization of 12-hr simulation of Basin 6 Sub-basin 2 with rainfall for the first 4 hours across entire surface (left) and graph of associated runoff (right).

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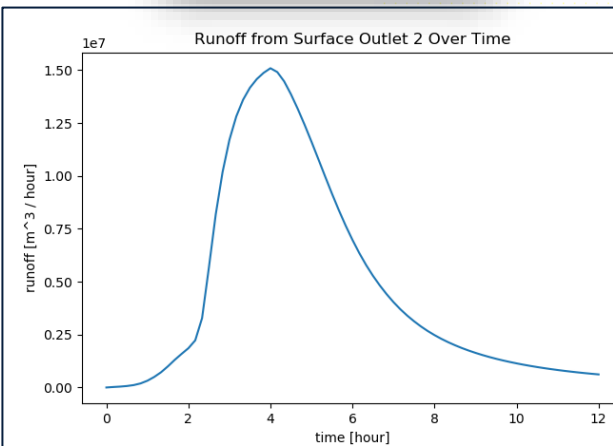
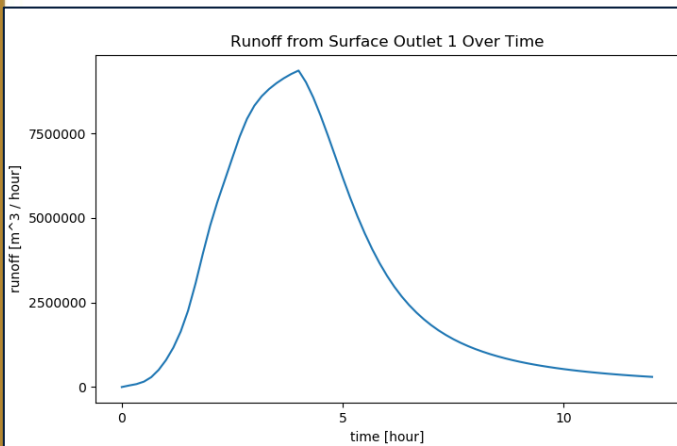
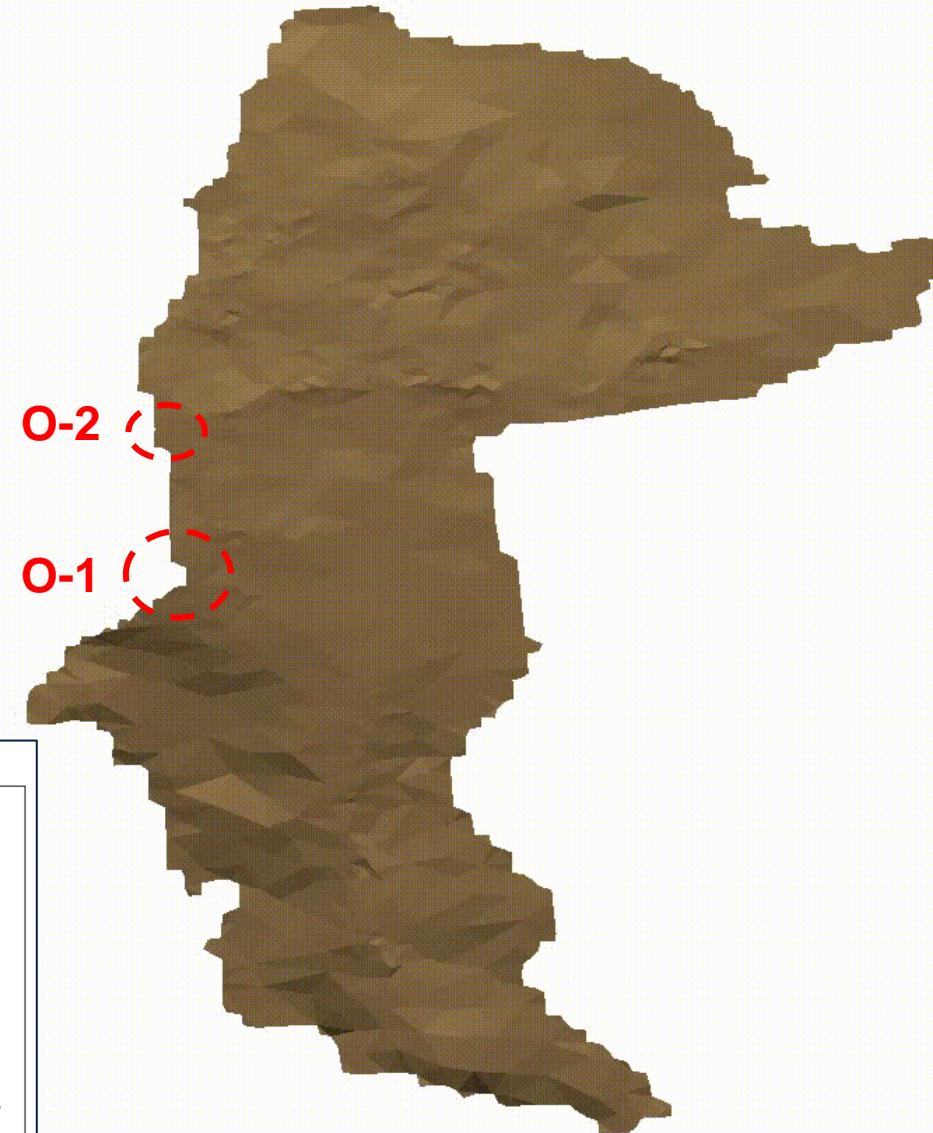
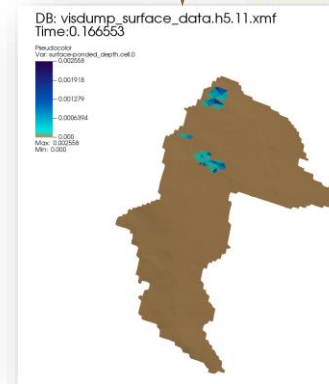
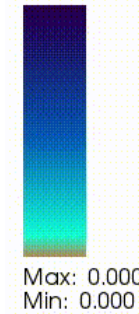
Subtask 6.2: Model Development

Implementation at ARC

- Final test on 10-meter DEM of Basin 6
- Two outlets (**O-1**, **O-2**)
- 12 hours with 4 hours of heavy rain
- Sinkholes present
- Sinkholes have a different manning coefficient than rest of surface domain
 - Surface domain = 0.07
 - Sinkholes = 0.03
 - Not based on Basin 6 data
- Surface ONLY - **not** integrated
- Does not include soil data from FIU

DB: visdump_surface_data.h5.0.xmf
Time:0

Pseudocolor
Var: surface-ponded_depth.cell.0
Constant.





Subtask 6.2: Model Development

FIU Year 3 Projected Scope

- Perform ATS simulations, including generation of meshes from DEM data, setting up of meteorological forcing data, development of input files for the ATS, executing simulations on local or remote systems, and analyzing the output. Jupyter notebooks will be utilized to detail each of the steps in this workflow.
- Collect soil samples in Basin 6 to evaluate soil physical properties for incorporation in ATS for model validation (soil particle size distribution, bulk density, porosity, organic content, etc.) at different depths that affect processes such as infiltration, erosion, nutrient cycling, and biologic activity. Compare collected soil data with national and global soil databases for additional validation (STATSGO2, SSURGO, SoilGrids2.0™).
- Identify location of any sinkholes and groundwater-surface seeps observed during field work to assist with ATS model validation.
- Field work will be incorporated as part of DOE Fellow summer internship in collaboration with LANL and CBFO scientists during which training on the relevant field sampling and measurement techniques will be conducted. FIU undergraduate/graduate students will also gain experience in laboratory sample analysis.
- FIU will work in close collaboration with the LANL scientists to extend model development using ATS and using Python develop approaches to acquire model forcing (i.e., weather, soil properties, land use) from available datasets.

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Task 7

Engineered Multi-Layer Amendment Technology for Hg Remediation on Oak Ridge Reservation

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Task 7: Engineered Multi-Layer Amendment Technology for Hg Remediation on Oak Ridge Reservation

Site Needs:

- Due to the range of phase(s) and redox transformations and toxicity, cleanup of mercury contamination is a challenging and costly endeavor for increasing numbers of mercury-contaminated sites globally.
- Widespread uses of Hg have led to diffuse sources that further complicate remediation efforts for Hg in freshwater systems, such as the East Fork Poplar Creek (EFPC) in Oak Ridge, Tennessee.
- EFPC is a 26-kilometer low gradient stream contaminated with Hg from past weapon development efforts at the Y-12 (National Security Complex) during the 1950s. Mercury releases persist from point and diffuse sources.

Objectives:

- Evaluate the effectiveness of a suite of sustainable sorbents for mercury removal in a freshwater system of EFPC. Formation of Hg–DOM complexes is problematic for remedial technology.
- Develop cost-effective, sorbent-based technology consisting of Hg-sequestering sorbents stacked between layers of porous geotextile mats.



Conundrum:

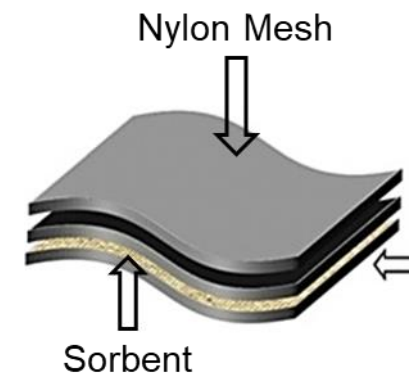
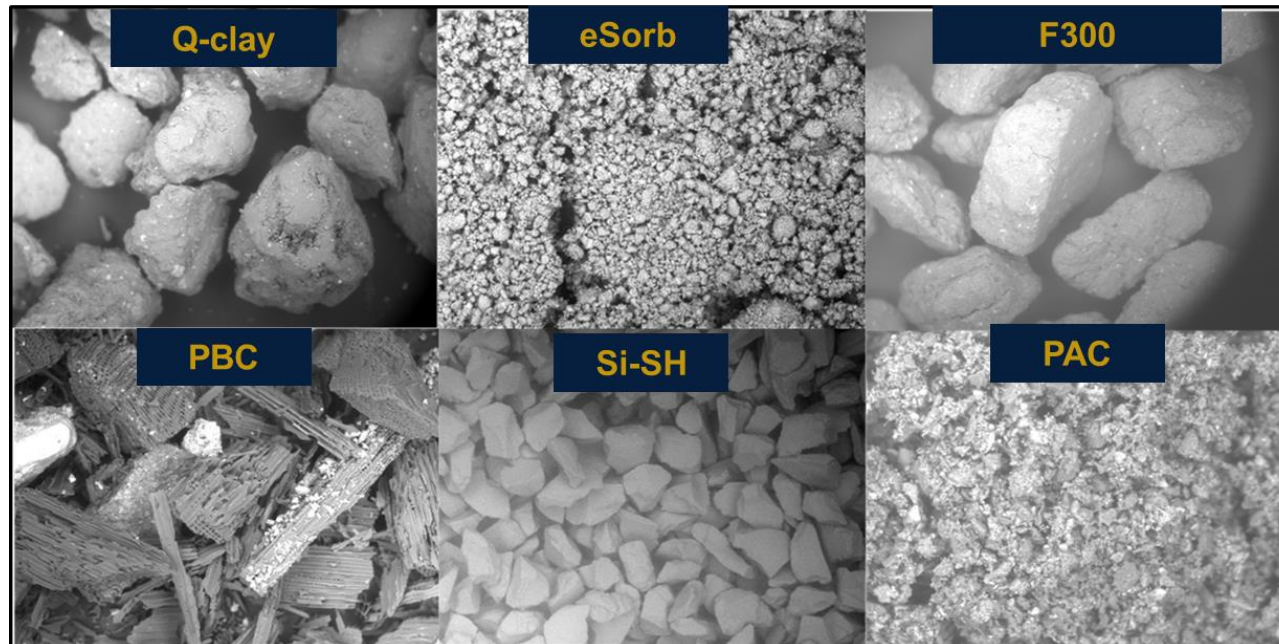
Hg fate and transport within EFPC ecosystem are controlled by its strong interaction with dissolved organic matter (~3 mg/L DOM at baseflow), which renders its sorption to sorbents and removal from the water column by strong reductants problematic.



Task 7: Engineered Multi-Layer Amendment Technology for Hg Remediation on Oak Ridge Reservation

FIU Year 2 Research Highlights & Accomplishments:

- Eight low-cost and environmentally friendly sorbents were studied as potential sorbents for in-situ remediation of mercury species in EFPC ecosystem.
 - Sorbent media were mostly carbon-based materials or functionalized silica/clays.
 - All batch experiments were performed in triplicates with standard deviations <10%.
- Evaluated materials: *Biochar; Sorbster; Si-thiol; Mackinawite blended powdered activated carbon; Powdered activated carbon; Organoclay PM-199; Filtrasorb 300 and RemBind.*



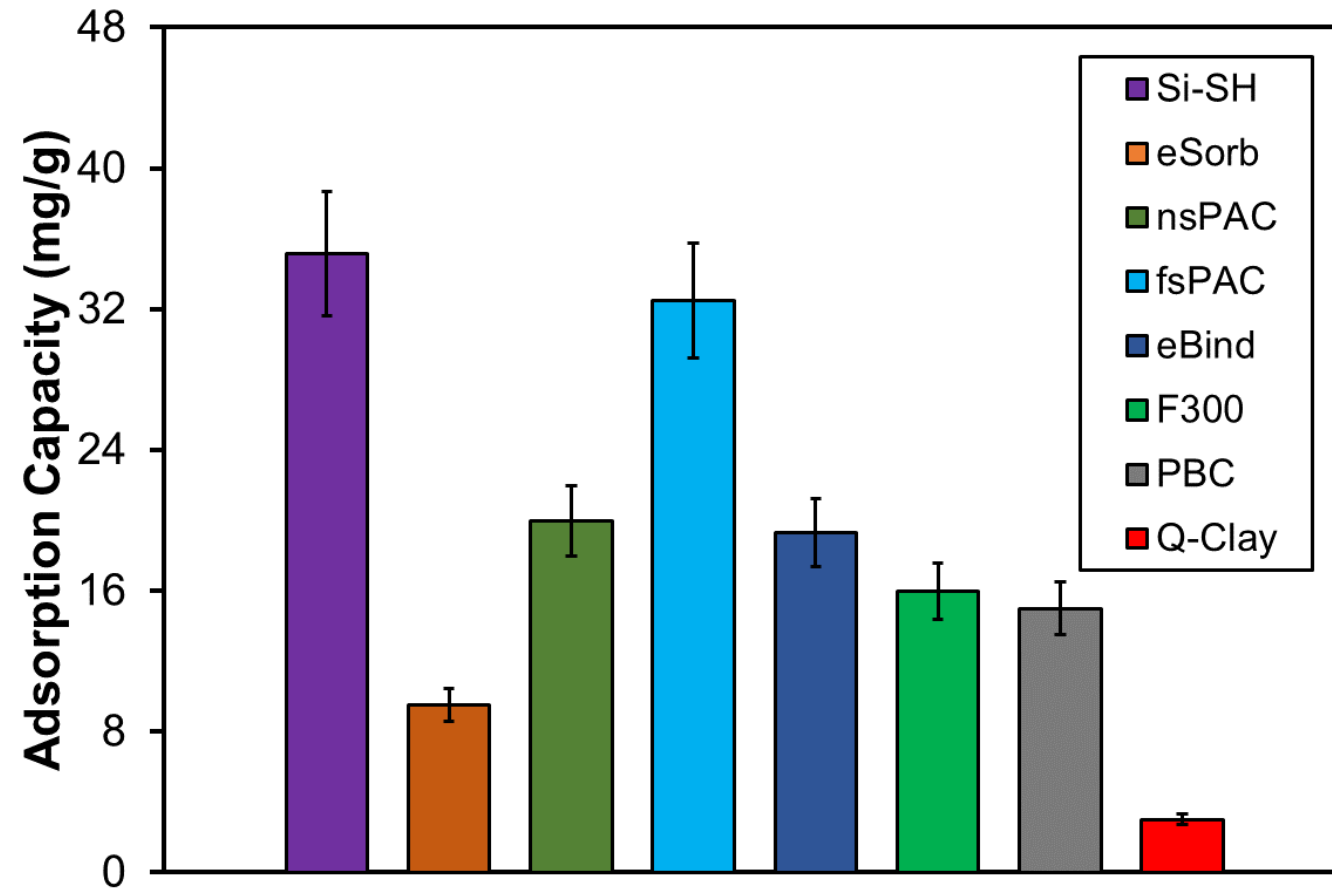
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Task 7: Engineered Multi-Layer Amendment Technology for Hg Remediation on Oak Ridge Reservation

FIU Year 2 Research Highlights & Accomplishments:



- Hg^{2+} adsorption capacity decreased as follows:

Si-thiol > FeS+PAC > PAC \geq RemBind > Filtrasorb \geq Biochar > Sorbster > Organoclay

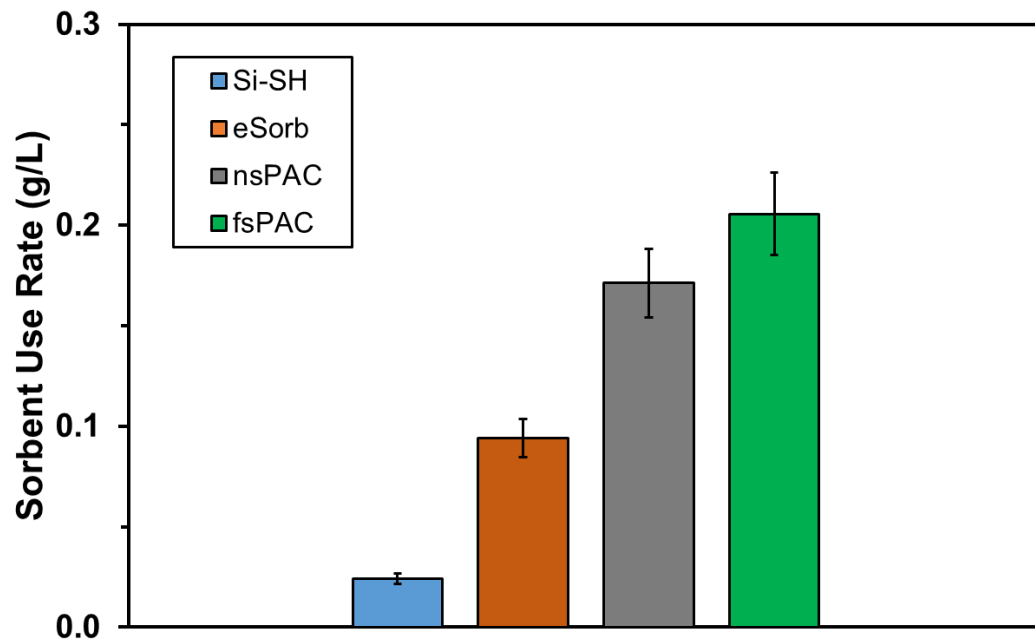
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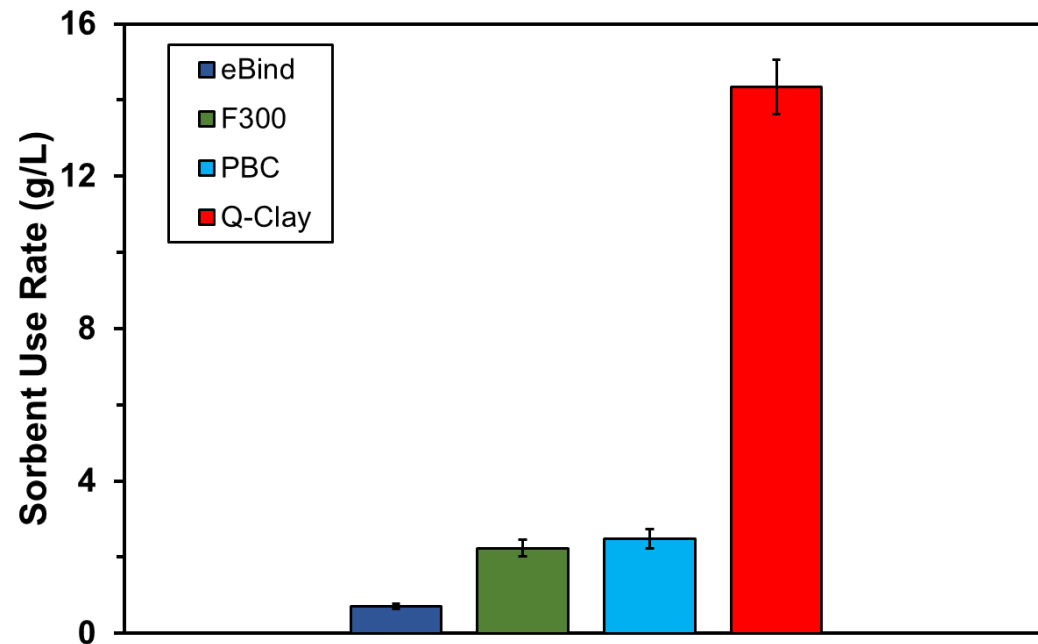
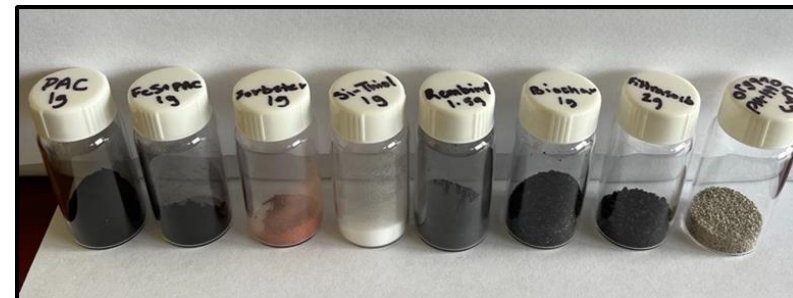


Task 7: Engineered Multi-Layer Amendment Technology for Hg Remediation on Oak Ridge Reservation

FIU Year 2 Research Highlights & Accomplishments:



$$K_d(\text{mL g}^{-1}) = \frac{[\text{Hg}]_{\text{solid}}}{[\text{Hg}]_{\text{solution}}}$$
$$\text{Use rate (g L}^{-1}\text{)} = \frac{1}{K_d}$$



- Hg-DOM adsorption capacity decreased as follows:

Si-thiol > Sorbster > FeS+PAC > PAC > RemBind > Filtrasorb > Biochar > Organoclay

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Task 7: Engineered Multi-Layer Amendment Technology for Hg Remediation on Oak Ridge Reservation

FIU Year 2 Research Highlights & Accomplishments:

- Oral presentations at the annual FIU MARC-U*STAR (Maximizing Access to Research Careers - Undergraduate Student Training for Academic Research) symposium.
- Recipient of the Roy G. Post scholarship.
- American Geophysical Union Conference and Waste Management Symposia 2022: “*Sorbent-Based Technology for Mercury Remediation in a Freshwater Aquatic System*” (Oral & posters)
- Summer Internship at Oak Ridge National Laboratory with Drs. Alexander Johs, Melanie Mayes and Eric Pierce.



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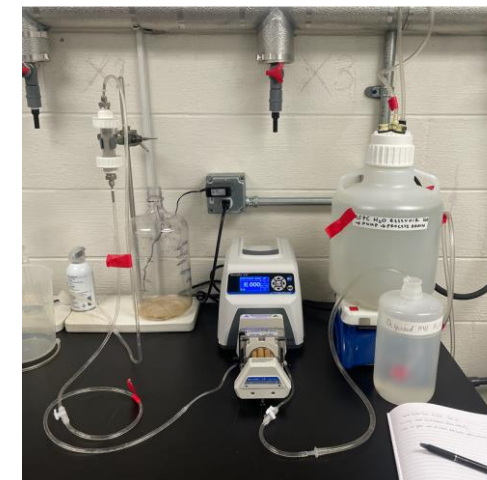
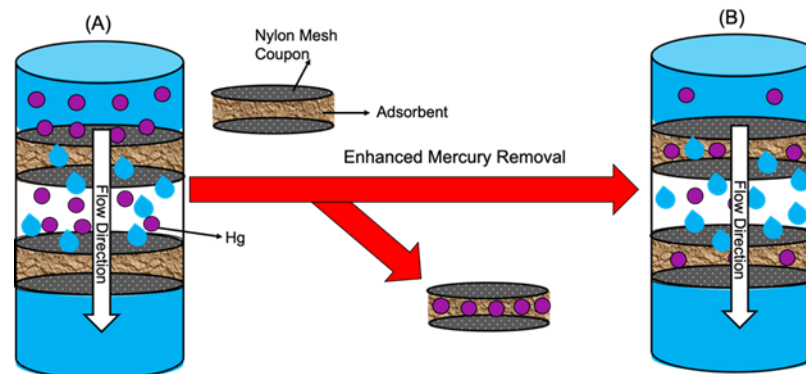
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Task 7: Engineered Multi-Layer Amendment Technology for Hg Remediation on Oak Ridge Reservation

FIU Year 3 Projected Scope

- Evaluate mercury species dynamics under conditions representative of EFPC using Geochemist Workbench and/or MINTEQA programs.
- Perform stability evaluation of sorbents via EPA's Toxicity Characteristic Leaching procedure (TCLP), SW-846 Test Method 1311.
- Determine physiochemical properties of Hg sorbents upon contact with environmental media (DI Water, ACW, EFPC water) and characterize pristine and treated sorbents using microscopy and spectroscopy techniques.
- Conduct column studies to elucidate mercury sorption under conditions representative of EFPC site.





FIU Year 2 Overall Accomplishments

Highlights

- Undergraduate DOE Fellow Aubrey Litzinger successfully graduated in Environmental Engineering.
- Graduate DOE Fellows successfully migrated into professional workforce: Juan Morales and Phuong Pham (SRNL) and Gisselle Gutierrez (Kimley-Horn).

WM22 papers & oral presentations:

Student Track (DOE Fellows)

- Re-oxidation of Technetium (^{99}Tc) Comingled with Uranium (^{238}U) and Nitrate (NO_3^-) Immobilized by Strong Reductants – Angel Almaguer
- Impact of Major Groundwater Components on the Adsorption of Uranium (VI) to Hanford Formation Sediment – Mariah Doughman
- Evaluation of a Suite of Sorbents for Cost-Effective Mercury Remediation in a Freshwater Stream Ecosystem – Caridad Estrada
- Utilization of Amanzi-ATS to Develop an Integrated Hydrology Model of the Nash Draw Basin West of the Waste Isolation Pilot Plant (WIPP) – Gisselle Gutierrez-Zuniga
- Removal of Iodine-129 by Organoclays PM-199 and MRM at Savannah River Site Wetlands – Phuong Pham
- Surface Water Dynamics within the F-Area of Savannah River Site and its Linkages with Groundwater and I-129 Geochemistry – Stevens Charles



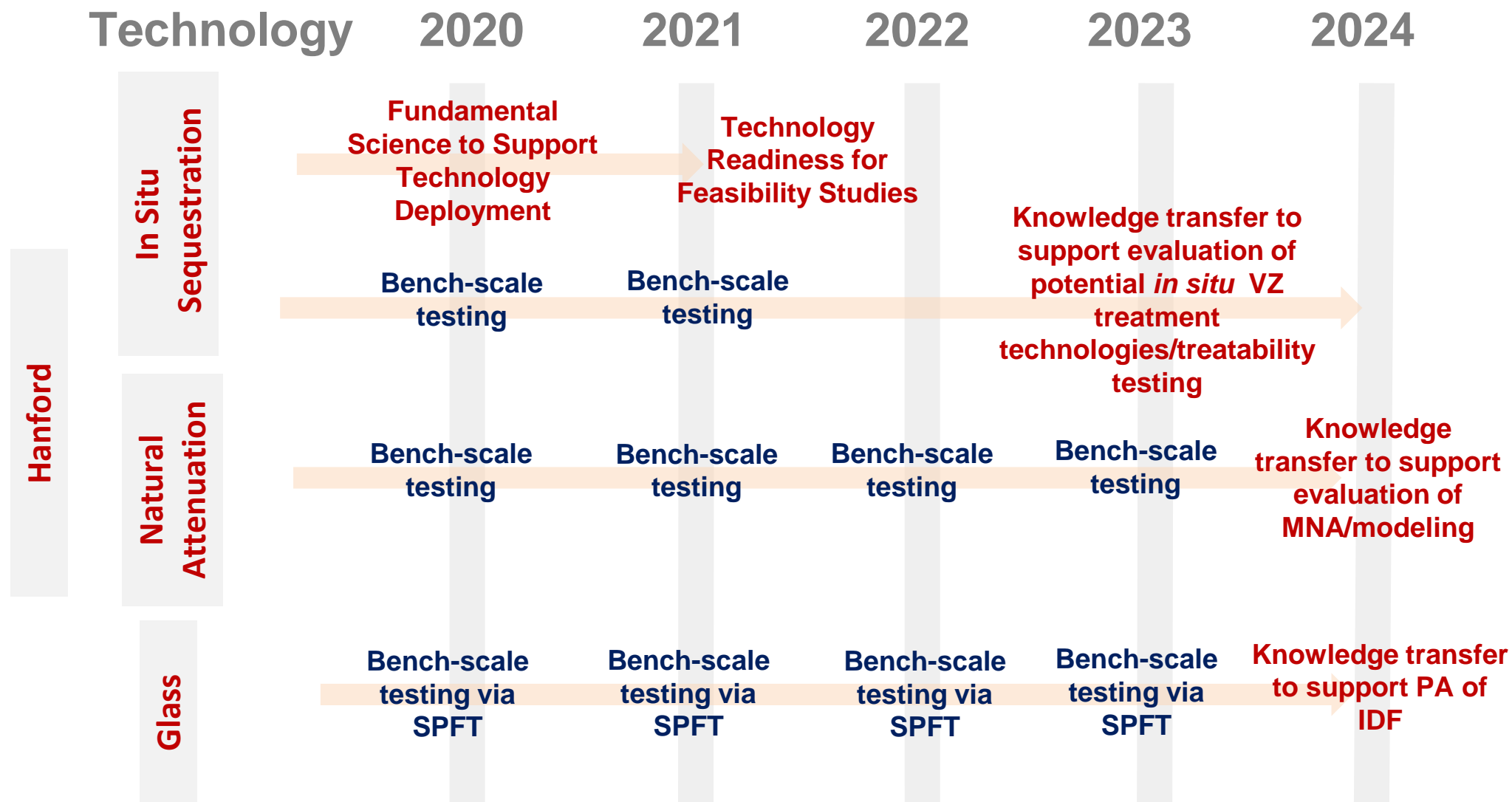
DOE Fellow, Aubrey Litzinger, receiving the “Outstanding Graduate Award in Environmental Engineering” at the Spring 2022 commencement ceremony.

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Technology Development and Deployment Road Map

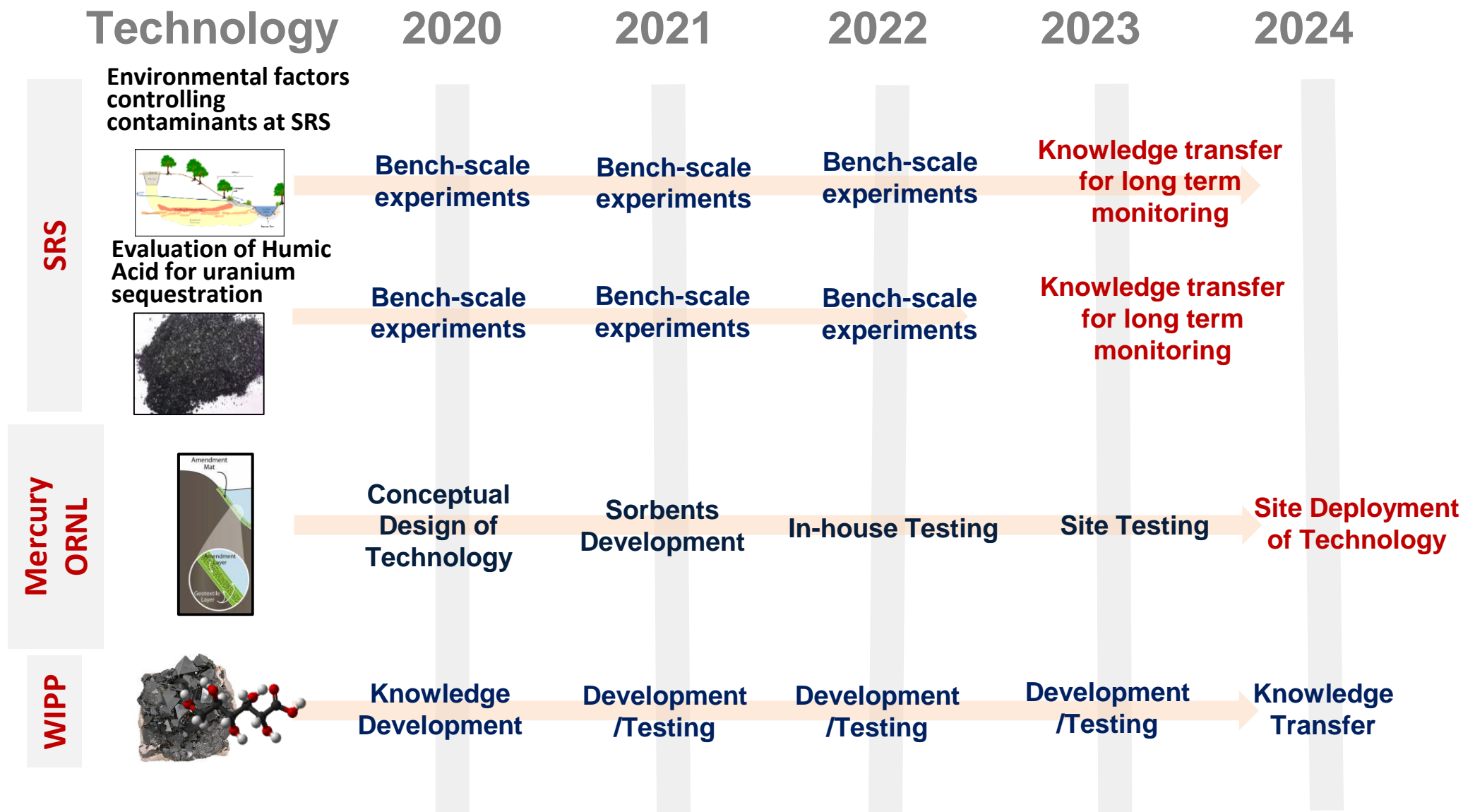


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Technology Development and Deployment Road Map

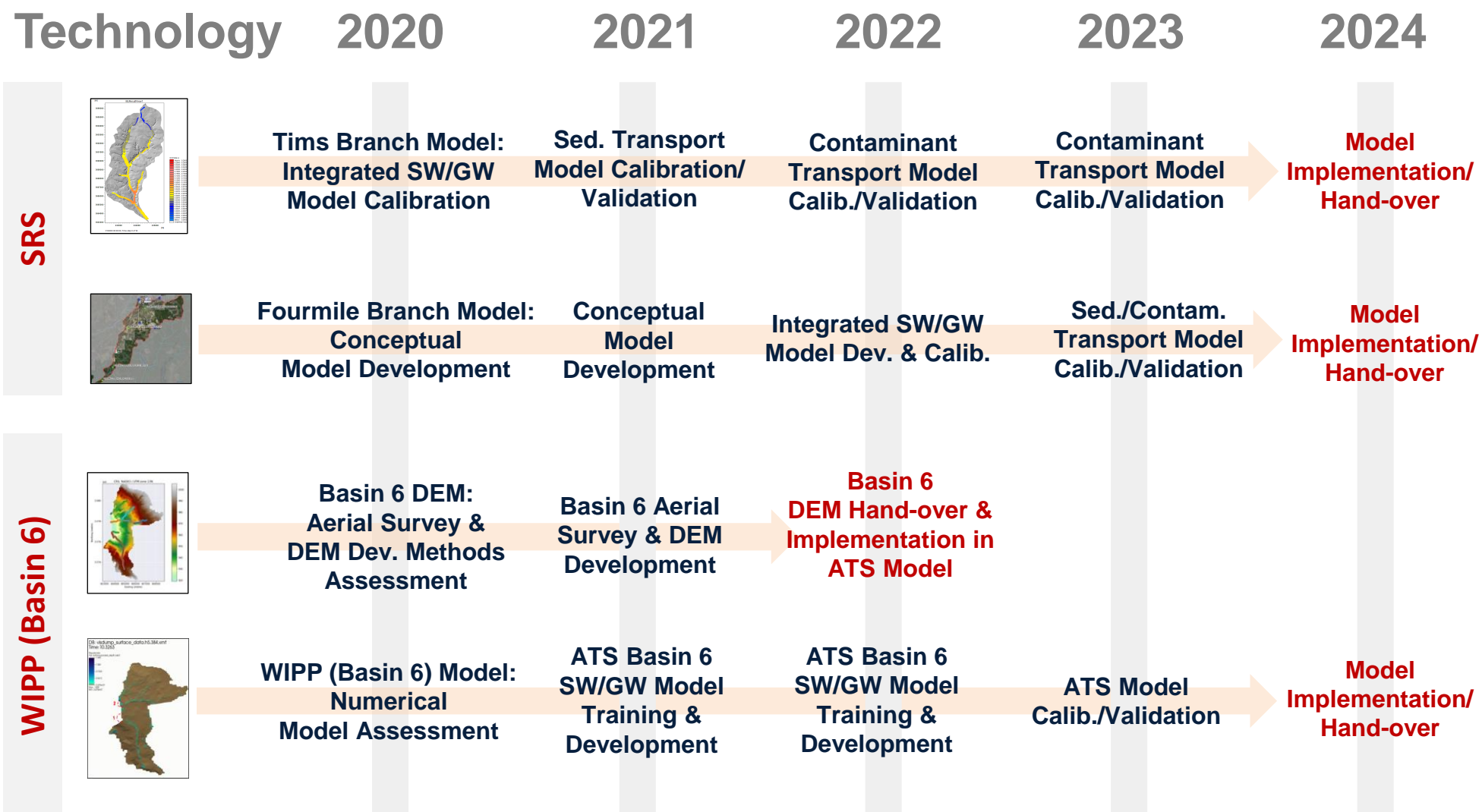


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Technology Development and Deployment Road Map



*DEM: Digital Elevation Model, SW: Surface water, GW: Groundwater

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DOE-FIU Cooperative Agreement

Upcoming Events Announcement



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DOE Fellows Poster Exhibition



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16th Annual

DOE FELLOWS POSTER EXHIBITION

NOVEMBER 7, 2022

1 pm – 4 pm

FIU ENGINEERING CENTER

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A STEM WORKFORCE DEVELOPMENT PROGRAM
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Save the Date

DOE-FIU Science & Technology Workforce Development Program's

16th DOE Fellows Induction Ceremony
Annual (Class of 2022)

Host: Applied Research Center, Florida International University

When: Tuesday, November 8, 2022 at 12:00 pm

Where: FIU Modesto Maidique Campus
Graham Center (GC) Ballroom
11200 SW 8th St, Miami, FL 33174



*A collaboration between the U.S. Department of Energy's Office of Environmental Management
and Florida International University's Applied Research Center*





Thank You. Questions?