PROJECT TECHNICAL PLAN

Project 3: Remediation and Treatment Technology Development and Support for DOE Oak Ridge Office

For the period September 17, 2013 to May 17, 2014

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INTRODUCTION

Approximately 75 to 150 metric tons of elemental mercury (used in a lithium-isotope separation process for production of nuclear fusion weapons), were released into East Fork Poplar Creek (EFPC) watershed from the Y-12 National Security Complex (Y-12 NSC) in eastern Tennessee, USA. Under typical environmental conditions, elemental mercury is oxidized to mercuric ion which has a greater solubility and mobility in groundwater and surface water. The increased mobility of the mercuric ion results in elevated concentrations of total mercury in soil, surface water and groundwater. The mercuric ion has high affinity to many organic ligands and in the water column the majority of the mercuric ions are bound to suspended and colloidal particles. Storm events increase the turbulence and velocity of river flow and may result in additional mobilization and transport of mercury downstream in the EFPC.

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In order to analyze the mercury cycle in the environment and to provide forecasting capabilities for the fate and transport of contamination within the watershed, an integrated surface and subsurface flow and transport model for the Y-12 NSC was developed. The model couples the hydrology of the watershed with mercury transport and provides a tool for analysis of changes of mercury load as function of changes in hydrology, including remediation scenarios which modify the hydrological cycle. The model couples the overland and subsurface flow module with the river flow and transport module. The model includes the main components of the hydrological cycle: groundwater flow (3D saturated and unsaturated), 2D overland flow, 1D flow in rivers, precipitation, and evapotranspiration. Furthermore, the model includes 57 outfalls along Upper East Fork Poplar Creek (UEFPC) which have been listed in the National Pollutant Discharge Elimination System (NPDES) permit from 2005. A sedimentation module was included to simulate the interactions between sediment particles, water and mercury species within the EFPC.

The numerical model was calibrated for the period of 1996-2009 using recorded stream flow and mercury concentrations measured in groundwater, surface water and soil. The model was subsequently applied to evaluate the effect of nine remediation strategies/scenarios in the UEFPC region on reducing the mercury concentrations. For each remediation scenario, flow duration curves and mercury load duration curves were compared at Station 17 for the computed and

recorded data. The remediation efficiency was determined by comparing the percent daily reduction of mercury discharges downstream of Station 17. The results of numerical simulations showed that exchange of mercury species between sediment, pore water, aqueous media and suspended solids significantly affects the mercury load detected at Station 17.

A series of laboratory studies were conducted to analyze the effect of various environmental factors (pH, pE) on methylation and demethylation processes in the water column. Experimental work was used to obtain critical mercury exchange parameters between pore water, colloidal and suspended particles, and streambed sediment, which were applied in the numerical model to study the effect of sediment transport on mercury mobilization.

For year 2010-2011, the model, which was developed for the Y-12 NSC, was extended to include the EFPC watershed and the creek between Y-12 NSC and Station EFK 6.4. The research focused on conducting additional simulations using the EFPC watershed model which extend the studies for Y-12 NSC. In addition, flow and transport studies were conducted for the Bear Creek watershed (a sub-watershed of the larger EFPC watershed). A geodatabase was also developed as a strategy for supporting hydrological model data input by creating a centralized data storage system to store model parameters instead of a collection of data layers, which provides a more stable foundation for building GIS-based water resources applications.

During FY 2012, FIU continued using the numerical model of EFPC to determine the impact of remediation alternatives on the complete hydrologic cycle, the transport overland and in surface water and rivers, sediment transport and reactions, and mercury exchange with sediments. Stochastic analysis was performed on measured hydrological and transport data including flow and pollutant concentrations at each outfall. A detailed mass balance was developed for the site for contaminants of concern, including inorganic (Hg) and organic contaminants. The work provides insight on the contribution of each outfall to the load at Station 17. The laboratory work included additional studies to determine experimental parameters related to cinnabar dissolution and contribution for mercury distribution between various phases (aqueous and soil) for different environmental factors including pH, dissolved oxygen, dissolved organic matter, organic and inorganic content of soils and pore water, on mercury fate and transport within the creek and for overland flow. The work will provide a better understanding of the mercury dynamics within the Oak Ridge Reservation watersheds (EFPC, Y-12 NSC, Bear Creek, White Oak Creek) for variable environmental conditions and for specified remediation alternatives. Student support was also provided for numerical modeling of subsurface flow and transport at Moab site.

The activities described in the Continuation Application for FIU Year 4 were planned for a period of performance from May 18, 2013 to May 17, 2014. However, two no cost extensions were executed by DOE-EM for FIU Year 3, which extended the end of the FIU Year 3 period of performance to September 16, 2013. Therefore, the period of performance for the FIU Year 4 activities described in this Project Technical Plan is shortened to 8 months, September 17, 2013 to May 17, 2014. The scope of some tasks has been affected/reduced due to the shortened period of performance and will be re-evaluated as FIU approaches the May 2014 timeframe. The affected scope may transfer to FIU Year 5.

The affected tasks from the CA for this project include the following:

- Subtask 3.5.1 – This scope will transfer to FIU Year 5.

- Subtask 3.5.2 – This scope will transfer to FIU Year.

OVERVIEW OF WORK ACCOMPLISHED DURING FY12 (FIU YEAR 3)

During FY2008-2012, FIU developed integrated flow and transport models of East Fork Poplar Creek (EFPC), Upper EFPC (Y-12 NSC) and White Oak Creek (WOC) watersheds at the Oak Ridge (OR) site, and conducted numerical modeling and reviews of monitoring data available from OREIS and related to mercury contamination and remediation within these watersheds. A surface water flow and transport model was developed to provide information about the quantities, frequencies and concentrations resulting from stormwater drainage and discharging through a number of outfalls in the upper section of the EFPC and WOC. The model showed excellent accuracy for the measured flow events in the drainage system. In addition, experimental studies provided experimental kinetic and equilibrium data about important parameters related to mercury transport, speciation and methylation/demethylation kinetics within the watershed. A variable density model, which was developed by site contractors for the Moab site, was used to provide simulations of several scenarios related to creating a hydraulic barrier between the mine tailings stored at the site and ecologically sensitive areas of the Colorado River. A geodatabase was developed for storing experimental and computed data for the OR and Moab sites. The following outlines the project-wide and individual task accomplishments for FY2012.

- A draft Project Technical Plan for FY2012 (FIU Year 3) was prepared and sent to DOE on June 25, 2012.
- Provided presentation overviews to DOE HQ and DOE ORO of the project progress and accomplishments (August 2012, April 2013 and June 2013).
- Finalized the XPSWMM model preliminary configuration parameters (September 2012) and completed a summary report on the results (November 2012).
- Developed the preliminary results summary of laboratory experiments (January 2013).
- Completed the development of sample Python scripts and Model Builder process workflow diagrams (February 2013).
- Completed a preliminary results summary for the Moab Model (October 2012).
- Technical Reports for all the tasks related to this project have been submitted to DOE as follows:
    - Technical report on “EFPC Model Update, Calibration and Uncertainty Analysis” submitted 3/1/2013
    - Technical report on “Simulation of NPDES and TMDL for EFPC and Y-12 NSC” wassubmitted with End of Year Report 8/17/2013.
    - Technical report on “Parameterization of Major Transport Processes of Mercury Species” submitted 2/18/2013.
    - Technical report on “Geodatabase Development for Hydrological Modeling Support” submitted 4/1/2013.

- Technical report on "Modeling of Groundwater and Flow and Transport at the Moab Site in Utah" submitted 3/19/2013.

- Published 4 journal articles based on work conducted within the project:
  - Malek-Mohammadi, S., Tachiev, G., Cabrejo, E., and Lawrence, A. (2012). "Simulation of flow and mercury transport in Upper East Fork Poplar Creek, Oak Ridge, Tennessee." *Remediation*, 22(2), 119–131.
  - Li, Y., Yin, Y., Liu, G., Tachiev, G., Roelant, D., Jiang, G., and Cai, Y. (2012). "Estimation of the Major Source and Sink of Methylmercury in the Florida Everglades." *Environmental. Science & Technology*, 46(11), 5885–5893.
  - Dickson, D., Liu, G., Lib, C., Tachiev, G., and Cai, Y. (2012). "Dispersion and Stability of Bare Hematite Nanoparticles: Effect of Dispersion Tools, Nanoparticle Concentration, Humic Acid and Ionic Strength." *Science of the Total Environment*. 419(1), 170–177.
  - Malek-Mohammadi, S., and Tachiev, G. (Winter 2013). "Migration of VOC Plume in the Subsurface Domain at the Y-12 National Security Site." *Remediation*, 23(1), 139-153.
- Presented results of research accomplishments at the following conferences:
  - "Hydrologic and Kinetic Parameters Impacting the Total Mercury Transport within the EFPC Watershed of Oak Ridge Reservation", Lilian Marrero, Georgio Tachiev, Nantaporn Noosai. The 9th International Symposium on Persistent Toxic Substances, October 2012, Miami, FL.
  - "Estimation of the Major Source and Sink of Methylmercury in the Florida Everglades", Yanbin Li, Yongguang Yin, Guangliang Liu, Georgio Tachiev, David Roelant, Guibin Jiang, Yong Cai, The 9th International Symposium on Persistent Toxic Substances, October 2012, Miami, FL.
  - "Dissolution of Mercury Sulfide in the Presence of Thiol-containing Substances", Guangliang Liu, Guidi Yang, Yanbin Li, Sen Chen, Yong Cai, Georgio Tachiev, Leonel Lagos, The 11th International Conference on Mercury as a Global Pollutant (ICMGP), Miami, FL.
  - "Long-Term Performance of Uranium Tailings Disposal Cells (13340)", Georgio Tachiev, Kent Bostic (P2S), Anamary Daniel (P2S), Ken Pill (P2S), Viviana Villamizar, Nantaporn Noosai. WM2013 Conference, February 2013, Phoenix, AZ.
  - "Coupling and Testing the Fate and Transport of Heavy Metals and Other Ionic Species in a Groundwater Setting at Oak Ridge, Tennessee (13498)", Nantaporn Noosai, Hector Fuentes. WM2013 Conference, February 2013, Phoenix, AZ.
  - "Recent Approaches to Modeling Transport of Mercury in Surface Water and Groundwater – Case Study in Upper East Fork Poplar Creek, Oak Ridge, TN (13349)", Georgio Tachiev, Anamary Daniel (P2S), Kent Bostick (P2S). WM2013 Conference, February 2013, Phoenix, AZ.

        - "XPSWMM Analysis of the Oak Ridge Stormwater Collection System Up To Outfall 211 (Student Poster)", Heidi Henderson (DOE Fellow), Georgio Tachiev, Leonel E. Lagos. WM2013 Conference, February 2013, Phoenix, AZ.
        - "Improvements and Modifications of an Integrated Flow and Mercury Transport Model for East Fork Poplar Creek, Oak Ridge, Tennessee (Student Poster)", Lilian Marrero, (DOE Fellow). WM2013 Conference, February 2013, Phoenix, AZ.
    - Two Master's theses and two PhD dissertations are being pursued based on this project work, specifically Task 3.1 "EFPC Model Update, Calibration, and Uncertainty Analysis" and Task 3.5 "Student Support for Modeling of Groundwater Flow and Transport at the Moab Site, Utah".
        - Lilian Marrero, an MS Candidate and DOE Fellow, working with the surface and groundwater model analyzing fate and transport of mercury in the EFPC watershed. Thesis completed in Spring 2013.
        - Heidi Henderson, an MS Candidate and DOE Fellow, a thesis using a surface water model analyzing the drainage flows and mercury transport within the ORNL site. Thesis work completed in Summer 2013.
        - Viviana Villamizar, an MS candidate, developed a surface and groundwater model for analysis of tailings at the Moab and Shiprock sites, supporting the work at ORNL.
        - Nantaporn Noosai, a PhD candidate, developing the thermodynamic database of mercury species and integrating the interactions within a flow and transport model.
    - This project overall has provided training for 5 DOE Fellows during FIU Year 3

TECHNOLOGY NEEDS

Conventional hydrologic and remediation methodologies provide limited understanding of the interactions between the hydrological cycle, contaminant mobilization and environmental impacts. This project uses conventional hydrologic and remediation analytical tools (accepted by the EPA, USACE, and USGS) in combination with latest scientific software (2D and 3D numerical flow and transport models integrated with reaction kinetics and thermodynamic software) to provide an integrated solution for understanding the mobility and the impacts of contaminants within DOE sites. In addition, state of the practice tools for analysis of sustainable and green remediation alternatives (developed for DOD sites) are needed to address long term sustainability in terms of reduced environmental and energy footprints of the remedial actions.

Regulatory requirements: The Clean Water Act and associated regulations require each state to determine which waters do not meet applicable water quality standards according to their uses. Computation of contaminant distribution within a watershed domain requires an integrated surface and subsurface flow model, which includes sedimentation processes along the creek. In order to extend the development of TMDLs onto other locations in the watershed, and provide a better understanding of the discharges and Hg concentrations along the stream reaches (EFPC

and Bear Creek) of the EFPC watershed, hydrological and transport simulations are needed. The computer simulations use the historical data to develop a calibrated numerical model, which is subsequently used to provide a forecasting capability and estimate load changes as a function of hydrological events.

Contaminant interactions and complexities: Sequestered mercury species in solid matrices, which are often known to be relatively stable, could be released as dissolved and/or colloidal species into the solution phase and thus contribute to the aquatic cycling of mercury. The redox potential and presence of organic ligands may affect the stability of elemental mercury beads and the distribution of released mercury species. The role of mercury migration from solid to solution in the mercury cycle, and the correlation between mercury mobilization and environmental chemical processes, needs to be better understood.

Data storage and integration: Sites have accumulated years of data and millions of spatial and temporal records related to the hydrological cycle, contaminant transport, and parameters of remediation technologies. In addition, numerical models produce gigabytes of computed spatial and temporal data for each computation node. Data management, storage, processing, retrieval and integration can be accomplished using a geodatabase. The development of an ArcSDE geodatabase will facilitate the centralized storage, backup, accessibility, organization, and management of model configuration and computed simulation data, and will put it into a structured, coherent, and logical computer-supported system. The hydrologic geodatabase model used in this project possesses a structure that enables linkage with scalable hydrologic modeling tools, applications to model hydrologic systems, and in this case, enables the testing of the potential impacts of various D&D scenarios on the ORR watersheds. The ArcSDE geodatabase can be used to automate and simplify the process of calling stored GIS and timeseries data. This geodatabase can also serve as a tool for contaminant flow and transport analyses which require large amounts of high-quality spatial and temporal data in order to ensure reliability and validity of modeling results.

PROJECT EXECUTION PLAN

The project execution plan is divided into two sections:

- Project execution for FIU Year 4, the period of September 17, 2013 to May 17 2014, will be the main work scope of the project which will cover the eight month period.
- The optional project scope will be transferred to FIU Year 5, provided that there will be no adjustments to budget and priorities.

The division of main and optional work scope is based on site priorities and efforts to provide continuity of the work developed for the past few years and available funds. The tasks which are part of the main scope and optional/delayed scope are identified in the table below:

Table 1 Project Work Scope for this Period of Performance

Task No	Task	Period	Workscope
Task 3.1:	**EFPC Model Update, Calibration and Uncertainty Analysis**		
Subtask 3.1.1:	Review of the existing Hg thermodynamic database and update for EFPC environmental conditions.	09/18/13-05/17/14	Main scope
Subtask 3.1.2:	Integration of the Hg thermodynamic database into the existing EFPC model.	09/18/13-05/17/14	Main scope
Subtask 3.1.3:	Provide a series of simulations using the EFPC model and the thermodynamic and kinetic interactions.	09/18/13-05/17/14	Main scope
Task 3.2:	**Simulation of NPDES- and TMDL-Regulated Discharges from Non-Point Sources for the EFPC and Y-12 NSC**		
Subtask 3.2.1:	Use of the observed outfall discharges to provide simulations of the entire EFPC watershed and the load discharge at Station 17	09/18/13-05/17/14	Main scope
Task 3.3:	**Sustainable Remediation and Optimization: Cost Savings, Footprint Reductions, and Sustainability Benchmarked at EM Sites**		
Subtask 3.3.1:	Benchmarking of current methodology using SITEWISE™	09/18/13-05/17/14	Main scope
Subtask 3.3.2:	Implementation of a SITEWISE™ module for sustainable analysis and optimization of monitoring programs.	09/18/13-05/17/14	Main scope
Subtask 3.3.3:	Calibration and Verification of the SITEWISE™ monitoring program module.	09/18/13-05/17/14	Main scope
Task 3.4:	**Geodatabase Development for Hydrological Modeling Support**		
Subtask 3.4.1:	Update of existing EFPC geodatabase	09/18/13-05/17/14	Main scope

Subtask 3.4.2:	Development of customized Python scripts to enhance database querying capabilities.	09/18/13-05/17/14	Main scope
Subtask 3.4.3:	Use the existing geodatabase structure developed for the EFPC modeling work at OR to create similar databases	09/18/13-05/17/14	Main scope

A detailed description is provided for each project task.

PROJECT TASKS

For FIU Year 4, FIU is proposing a scope which builds upon previously developed models to analyze flow, fate and transport of site contamination and remedial activities at the OR and Moab sites. This work is synergistic with the work ORNL is performing and will involve the integrated surface/subsurface flow and transport model developed for the EFPC, the surface model developed to study the drainage discharges from the outfalls along EFPC, and the variable density model for the Moab site. This work will involve the integrated surface/subsurface flow and transport model developed for the EFPC; the surface model developed to study the drainage discharges from the outfalls along EFPC; and the variable density model for the Moab site. A series of simulations, coordinated with the site, will be developed to provide better understanding of the mercury dynamics within the OR watersheds (i.e., EFPC, Y-12 NSC, Bear Creek, and WOC) for variable environmental conditions and for specified remediation alternatives. In addition, the XPSWMM modeling work conducted for White Oak Creek will be conducted on the premise that this smaller system could be modeled at ORNL to prove the concept and then expanded to a larger area at Y-12. However, security issues at Y-12 will need to be addressed. The overarching geodatabase at FIU will be updated with recent monitoring and simulation data to provide remote access, storage and retrieval of the data for analytical and reporting purposes.

FIU proposes to add new scope in FIU Year 4, focused on EM pilot studies and software use to evaluate the benefit of sustainable remediation practices; quantify the environmental footprint of remedial and other alternatives; and develop a sustainable optimization module for monitoring program analysis on EM sites. Sustainability evaluation, integrated into existing 5-year regulatory reviews is a common industry and federal practice to assess footprint impact, as well as to improve system design performance and efficiency.

Task 3.1: EFPC Model Update, Calibration and Uncertainty Analysis

Background

An integrated surface/subsurface flow and transport model of EFPC watershed was developed to analyze the mercury transport patterns within the ORR domain. For the development of the hydrology model, historical measurement records including the timeseries for precipitation, evapotranspiration, groundwater levels, and river discharges were obtained from the OREIS and ORNL databases and incorporated into the MIKE model as boundary conditions. The hydrological model was calibrated and then validated by comparing the computed discharges and water levels with the historical records at selected monitoring stations (the outfalls listed in the NPDES document for Y-12 NSC). Uncertainty and sensitivity analyses were performed for critical hydrological parameters such as the Manning number, and the vertical and horizontal hydraulic conductivities of each of the five geologic layers.

During FY11, the focus was on extending the sedimentation module to include the entire EFPC and Bear Creek. This research has also provided stochastic modeling of the system and has included an analysis of the spatial and temporal patterns as a result of the stochastic variations of selected properties of the sub domain. In FY12, FIU continued using the numerical model of EFPC to determine the impact of remediation alternatives on the complete hydrologic cycle, the transport overland and in surface water and rivers, sediment transport and reactions, and mercury exchange with sediments. The research was coordinated with the site and ORNL personnel.

Technical Approach

The objective of this task is to provide analysis of the coupling between hydrology and mercury transport within the context of decreasing the risk of decontamination and decommissioning (D&D) activities. The major deliverable is numerical and stochastic analysis of observed and computed timeseries for flow and contaminant concentration for National Pollutant Discharge Elimination System (NPDES)-regulated outfalls within the watershed. To solve the challenges related to analysis of contaminants within the EFPC domain, FIU developed a numerical model of the entire EFPC watershed to determine the impact of remediation alternatives on the complete hydrologic cycle, the transport overland and in surface water and rivers, sediment transport and reactions, and mercury exchange with sediments. The model simulations accounted for a range of hydrological impacts related to planned remediation alternatives. Data resulting from this task will be integrated into the geodatabase and will be prepared for web publishing.

The work proposed for FIU Year 4 will support a PhD student and will include using the model to provide simulations that implement selected main thermodynamic equilibria and reactions. The proposed scope under this task for FIU Year 4 will have a 20% allocation and involves the following subtasks:

> **Subtask 3.1.1: Review of the existing Hg thermodynamic database and update for EFPC environmental conditions.** The dissolution mechanism of the mercury beads within the EFPC watersheds which will be reviewed and the competitive absorption on the EFPC sediment between the major cations contained in EFPC water ($Ca^{2+,}$ $Mg^{2+,}$ etc.) and Hg^{2+} will be investigated. The deliverable from this task will include the Hg thermodynamic database relevant to EFPC environmental conditions that will be further utilized for and

integrate into the integrated flow and transport models already developed for the site (PHREEQC, XPSWMM, MIKE). The task will rely on a thermodynamic equilibrium software and reaction kinetic software to characterize the most dominant species and processes for the environmental conditions of ORR.

Subtask 3.1.2: Integration of the Hg thermodynamic database into the existing EFPC model. The integrated model will have improved capability to simulate the exchange of Hg between the creek and river, the distribution of mercury species within pore water, sorbed mercury within pores, sorbed mercury on suspended particles and "free" mercury (dissolved and chelated mercury species). The deliverables from this task will include the analysis of different remediation scenarios including hydrological and geochemical methods, tools that can be utilized to investigate the best remediation methods to address these issues. Variation of geochemical conditions (presence of naturally occuring strong chelating agents) will be investigated to determine the changes of reaction kinetics and equilibrium.

Subtask 3.1.3: Provide a series of simulations using the EFPC model and the thermodynamic and kinetic interactions. For these simulations, provide statistical analysis of observed data and development of timeseries, probability exceedance curves, and probability distribution models of flow, concentration and load data that integrate already downloaded data and new data as it becomes available. The data will include groundwater well monitoring, concentrations in groundwater wells, outfall flow, and concentration and load data. The deliverable of this subtask will include timeseries, probability exceedance curves, load exceedance curves, probability distribution models for each monitoring point and a report. The subtask will provide improved estimates for the stochastic nature of mercury fluxes within the EFPC domain.

Task 3.2: Simulation of NPDES- and TMDL-Regulated Discharges from Non-Point Sources for the EFPC and Y-12 NSC

Background

During FY11, the numerical model of UEFPC watershed which was developed by FIU-ARC to simulate fate and transport of mercury, conservative tracers and VOC plumes within the watershed based on several remediation scenarios was extended and applied to the entire EFPC watershed to determine the contribution of each subdomain component to the overall contaminant loads of the watershed streams, and to assist in analyzing the NPDES and TMDL requirements for surface water and groundwater within the EFPC watershed. In FY12, FIU used the EFPC model to provide numerical analysis of contaminant flow and transport within the EFPC and Y-12 NSC watershed and to determine the impact of model parameters on the TMDL. A major focus was placed on ecosystem responses to variations in contaminant loading (changes in external and internal loading in time and space), and how imminent ecosystem restoration may affect existing contaminant pools. Data resulting from this task will be integrated into the geodatabase and will be prepared for web publishing.

Technical Approach

During FIU Year 4, a surface flow model for Y-12 NSC, similar to the model developed for ORNL, will be developed. The purpose of the model will be to determine the discharges from the

stormwater drainage system and for each of the outfalls along EFPC. Subsequently the discharges will be implemented in the surface and groundwater model which was developed for the entire EFPC. A series of simulations will provide numerical analysis of contaminant flow and transport within the EFPC watershed and will determine the impact of model parameters on NPDES and TMDL regulations. The task will support an MS student. The proposed scope under this task for FIU Year 4 will have a 10% allocation and involves the following subtasks:

Subtask 3.2.1: Use of the observed outfall discharges to provide simulations of the entire EFPC watershed and the load discharge at Station 17 using the EFPC model previously developed with MIKE SHE and 11. During FY12 a series of simulations were executed to determine the significance of mercury reaction kinetic parameters on flow and transport within EFPC using a simulation period of one year. Additional work will be conducted for available data (starting from 1991-present). The additional simulations will provide the long term trends. Two periods will be considered, prior to flow augmentation of Upper EFPC and after flow augmentation. The results will be analyzed to determine the long term trends within each period. The deliverable of this subtask will include development of probability exceedance curves for each scenario; this data will provide additional insight of the effect for the entire range of hydrologic regimes (very wet to very dry conditions). The task will study the effects on diversion of clean water away from contaminated soils and storm water drains and possible positive impacts downstream through reducing the flood potential (by modifying the river bed) , and limit the infiltration of rainwater through areas with underlying mercury contamination.

Task 3.3: Sustainable Remediation and Optimization: Cost Savings, Footprint Reductions, and Sustainability Benchmarked at EM Sites

Background

This is a new task to be incorporated into the Project 3 work scope for FY13 (FIU Year 4). DOE's Offices of EM and Health, Safety, and Security (HSS) established a cross-programmatic team in 2012 to benchmark, train, and evaluate the cost-benefit of Green & Sustainable Remediation (GSR) practices applied to cleanup and closure projects at the field sites and Headquarters' management of those projects. EM worked with EPA and the Interstate Technology & Regulatory Council (ITRC) to certify over 130+ DOE staff and cleanup contractors in GSR principles and practice training. Federal agencies and industry are primarily using the public domain SITEWISE^{TM} software [developed and sponsored by Battelle, the Navy, and the US Army Corps of Engineers (USACE)] to improve sustainability of remedial and monitoring decisions; identify improved and more cost-effective end states; and to reduce hazardous emissions, consumption of water and energy resources, as well as footprint impact. The benefits of implementing two new ASTM standard guidance for GSR are expected to be transformative to the remediation industry, by greatly lowering costs and improving effectiveness of remediation strategies applicable to soil, groundwater, radioactive waste, and facility D&D.

The SITEWISE^{TM} software is an EXCEL-based evaluation tool designed to: 1) compare and contrast alternatives for remedial, monitoring, waste handling, and D&D design, and 2) to generate results for cost benefit and sustainable decision-making for regulatory compliance. The Navy, EPA, and USACE incorporate sustainability evaluation and decision making into their

long-standing and successful optimization programs as part of the 5-year regulatory review process. SITEWISE™ is one of many evaluation tools used in federal and industry sectors to calculate and optimize the environmental footprint of cleanup and closure alternatives. Specifically, SITEWISE™ methodology provides a baseline assessment of long-term alternative design impacts based on the sustainability factors of greenhouse gas (GHG) and critical air pollutant (i.e., sulfur and nitrogen oxides, particulate matter, etc.) emissions; energy and water usage; natural resource consumption and footprint impact; waste generation; and risk from accident death and injury.

A sustainability assessment is typically carried out using a building block approach where every alternative is first broken down into modules that mimic the implementation phases. For a remedial action, sustainability factors are calculated for the investigation, construction, operation, and long term monitoring phases to estimate the overall footprint of the remedial alternative. This building block approach reduces redundancy in the sustainability evaluation and facilitates the identification of specific activities that have the greatest environmental footprint. The objective of the methodology is to provide a decision matrix for remedy selection, design, or implementation. This approach allows for a remedy optimization stage as well. The methodology is a standard requirement for remediation and optimization led at sites by the EPA, Navy, Army, Air Force, and USACE. Data resulting from this task will be integrated into the geodatabase and will be prepared for web publishing.

Technical Approach

The proposed scope under this task for FIU Year 4 will have a 50% allocation and involves the following subtasks:

Subtask 3.3.1: Benchmarking of current methodology using SITEWISE™. The use of SITEWISE™ sustainability software will be benchmarked at one or more EM field sites with pilot-scale studies where cost benefit can be demonstrated. These pilot studies will also provide valuable insight regarding how EM cleanup and closure contracts can be modified, incentivized, and improved to attain sustainable goals and optimize existing designs. FIU will work with EM HQ and interested field sites to obtain the necessary field data to conduct pilot-scale sustainability evaluations using SITEWISE™. FIU engagement with sites and HQ to identify "pilot-scale sustainability evaluations" should include all EM's principle problem areas – High-Level Waste, Soil & Groundwater, Transuranic Waste, Deactivation & Decommissioning (others as identified) and must be FULLY coordinated with EM's Facility Engineering Program.

Subtask 3.3.2: Implementation of a SITEWISE™ module for sustainable analysis and optimization of monitoring programs. This subtask will focus on the design and development of a module in SITEWISE™ for the user to evaluate sustainable approaches, technologies, and optimization of site monitoring networks and variables. SITEWISE™ can be improved to include a monitoring design and optimization module, whereby users are guided through an expert system to select sustainable technologies and practices to reduce monitoring project costs, efforts, and footprint impact. Then, SITEWISE™ will be programmed to lead the user through data input and analytical options to generate sustainable results and lifecycle cost savings for various designs. A SITEWISE™ monitoring module will be evaluated to receive data and export results though a geographic

information system (GIS) interface to take full advantage of temporal and spatial analyses and visualizations offered by a GIS platform. For example, if a statistical or geostatiscal software, such as MAROS or GTS, is used to downsize a compliance monitoring program (i.e., remove wells, analytes, or frequencies), the monitoring module in SITEWISE^{TM} will accept these results via GIS or EXCEL to calculate the reduction in emissions, energy and water usage, waste generation, and accident risk over the program total life cycle. FIU will work with EM to create a monitoring program module with a sustainability expert system and GIS interface to improve data import, analysis, and visualization. It is likely that a monitoring program module in SITEWISE^{TM} is of equal value and interest to other federal agencies and the private sector. It could be co-developed with leveraged funding from other federal partners such as EPA, Navy, and USACE. GIS programming tools will be developed and integrated within the modules to provide capability for processing using standard spatial database and applications (such as ArcMap).

Subtask 3.3.3: Calibration and Verification of the SITEWISE^{TM} monitoring program module. FIU will collaborate with other federal agency experts and their contractors to assure benchmark studies for calibration and verification of this module.

Task 3.4: Geodatabase Development for Hydrological Modeling Support

Background

During FY11-FY12, FIU developed a geodatabase to support the hydrological modeling work being performed at OR which serves as a centralized data management system, providing access to data generated from simulations of contaminant fate and transport to all users and facilitating storage, concurrent editing and import/export of model configuration and output data that is specific to the hydrologic and transport models being used. The capabilities of the geodatabase were then extended by creating a model using ArcGIS ModelBuilder and Python scripting to automate the process of querying the existing EFPC geodatabase, and to export data that can be used for statistical analysis and the generation of maps, graphs and reports. An investigation of downloadable freeware to facilitate online querying of the database was also conducted to determine methods by which project derived data can be more easily shared with other project stakeholders such as DOE personnel and ORR site contractors.

During FIU Year 4, the existing database will be updated with more recent ORR site and environmental data. FIU will also improve the complexity of the existing Python scripts developed during FIU Year 3 and develop additional customized scripts which will serve to enhance database querying capabilities. FIU will provide a library of scripts which can be coupled with other existing libraries used for mathematics, science, and engineering such as NumPy and SciPy, to perform statistical analyses and which can be applied to similar databases used at other DOE sites. Training will also be provided to students on how to update and query the existing geodatabase. The existing geodatabase structure developed for the EFPC modeling work at ORR will also be used to create similar databases to support modeling work being conducted at DOE's Idaho Site.

Technical Approach

The proposed scope under this task for FIU Year 4 will have a 10% allocation and involves the following subtasks:

1. **Subtask 3.4.1: Update of existing EFPC geodatabase** with more recent OR site monitoring data available from various sources including OREIS, USGS, NRCS STATSGO or SSURGO soil databases, and the U.S. EPA MRLC or NALC land cover databases. Training will also be provided to FIU graduate and/or undergraduate students on how to update and query the existing geodatabase within the ArcGIS environment.
2. **Subtask 3.4.2: Development of customized Python scripts to enhance database querying capabilities.** FIU will implement a library of scripts which can be coupled with other existing libraries used for mathematics, science, and engineering such as NumPy and SciPy, to perform statistical analyses and which can be applied to similar databases used at other DOE sites. ArcGIS ModelBuilder will be used to document ArcGIS model workflow diagrams for reporting purposes.
3. **Subtask 3.4.3: Use the existing geodatabase structure developed for the EFPC modeling work at OR to create similar databases** to support modeling work being conducted at other EM cleanup sites that may be included in Task 3.3 as pilot studies.

PROJECT MILESTONES

Milestone No.	Milestone Description	Completion Criteria	Due Date
2013-P3-M1	Task 3.3: Selection of four alternative sites for benchmarking with SITEWISE™	Memo to DOE HQ describing site analysis	1/15/2014
2013-P3-M2	All tasks: Presentation overview to DOE ORO/DOE HQ of the project progress and accomplishments (Mid-Year Review)	Presentation to DOE ORO/DOE HQ	2/18/2014
2013-P3-M3	Task 3.3: Complete analysis of the alternative sites for benchmarking with SITEWISE™ and select the first site for analysis	Memo to DOE HQ providing background information for the selected site	3/14/2014
2013-P3-M4	All tasks: Presentation overview to DOE ORO/DOE HQ of the project progress and accomplishments (Project Closeout Summary)	Presentation to DOE ORO/DOE HQ	5/12/2014
2013-P3-M5	All tasks: Submit publications to relevant journals	Submission of manuscripts	5/16/2014

DELIVERABLES

Client Deliverables	Responsibility	Acceptance Criteria	Due Date
Draft Project Technical Plan	Project Manager	Acknowledgement of receipt via E-mail two weeks after submission	10/17/13
Quarterly Progress Reports	Principal Investigator/Project Manager	Acknowledgement of receipt via E-mail two weeks after submission	Quarterly
Memo for theselection of four alternative sites for benchmarking with SITEWISE™ (Task 3.3, associated with milestone 2013-P3-1)	Project Manager	Acknowledgement of receipt via E-mail two weeks after submission	1/15/2014
Presentation and midyear report of project progress and accomplishments for all tasks	Project Manager	Acknowledgement of receipt via E-mail two weeks after submission	2/18/2014
Complete analysis of the alternative sites for benchmarking with SITEWISE™ and select the first site for analysis (Task 3.3, associated with milestone 2013-P3-M3)	Project Manager	Acknowledgement of receipt via E-mail two weeks after submission	3/14/2014
Technical report on geodatabase structure, customizations and scripting capabilties	Project Manager	Acknowledgement of receipt via E-mail two weeks after submission	4/18/2014
Technical Report for "EFPC Model Update, Calibration and Uncertainty Analysis" (Task 3.1)	Project Manager	Acknowledgement of receipt via E-mail two weeks after submission	5/16/2014
Technical Report for "Simulation of NPDES- and TMDL-Regulated Discharges from Non-Point Sources for the EFPC and Y-12 NSC" (Task 3.2)	Project Manager	Acknowledgement of receipt via E-mail two weeks after submission	5/16/2014

Technical Report for "Sustainable Remediation and Optimization: Cost Savings, Footprint Reductions, and Sustainability Benchmarked at EM Sites" (Task 3.3)	Project Manager	Acknowledgement of receipt via E-mail two weeks after submission	5/16/2014
Technical Report for "Geodatabase Development for Hydrological Modeling Support" (Task 3.4)	Project Manager	Acknowledgement of receipt via E-mail two weeks after submission	5/16/2014
Draft Year End Report	Project Manager	Acknowledgement of receipt via E-mail two weeks after submission	06/30/2014

COMMUNICATION PLAN, ISSUES, REGULATORY POLICES AND HEALTH AND SAFETY

Communication Plan

The communication with the clients and relevant experts at DOE EM/ORO/Moab Site is a critical component of the project. The mode of communication will be e-mails, telephone/conference calls and meetings at the site. Though site-specific contact persons have been identified, constant communication will be maintained with client stakeholders at DOE HQ and the DOE sites to ensure all parties involved are aware of the project progress.

Information Item	Client Stakeholder	Schedule	Communication Method	Responsible Stakeholder
Status Update Teleconferences	DOE EM, ORO, Moab	Monthly	Phone	Project Manager
EM-HQ Status Update Phone Call	DOE EM	Bi-Monthly	Phone	Principal Investigator
Quarterly Report	DOE EM	End of Q1, Q2, Q3, Q4	E-mail	Project Manager
Draft Year End Report	DOE EM, ORO, Moab	30 working days after completion of performance period	E-mail	Project Manager
Papers and presentations	DOE EM, ORO, Moab	As developed for conferences (e.g., WM13)	E-mail	Project Manager
Milestone completion E-mail	DOE EM, ORO, Moab	At completion of milestone	E-mail	Task Manager

The following individuals will serve as points of contacts:

Site DOE Contacts

- Elizabeth Phillips, DOE-ORO, (865) 241-6172
- Don Metzler, DOE Moab, (970) 257-2115

DOE EM (HQ) Contacts

- Kurt Gerdes, (301) 903-7289
- G. (Skip) Chamberlain, (301) 903-7248
- Justin Marble, (301) 903-7210
- Mark Williamson, (301) 903-8427

Oak Ridge Field Office/Moab Site Technical Contacts

- Richard Ketelle, (RSI), (865) 574-5762
- Eric Pierce (ORNL), (865) 574-9968
- Liyuan Liang (ORNL), (865) 241-3933
- David Watson (ORNL), (865) 241-4749

Anticipated Issues

Subtask 3.2.1: Re-creation of the existing Y-12 NSC stormwater management system layout via a numerical surface water one dimensional XPSWMM model will require information from the site with respect drainage system, this task will be postponed until May 2014 to ensure that required data are available. This task has no dependencies of other tasks and if data are not available, the efforts and resources planned for this task will be reassigned to tasks 3.3.1, 3.3.2 and 3.3.3 and additional scope will be developed.

No other issues are anticipated.

Regulatory Policies and Health and Safety

This project involves primarily computer-based modeling and information technology development, therefore standard health and safety issues normally associated with field activities and laboratory experiments do not directly apply. All pertinent FIU on-site task activities, however, will be performed in accordance with FIU-ARC's Project-Specific Health and Safety Plan (PSHASP).

Much of the environmental and GIS data used for hydrological model development has been derived from the secured Oak Ridge Environmental Information System (OREIS) database. As such, cyber security measures will be established to ensure that data integrity is maintained. In addition to the FIU-ARC firewalls and the built-in software and hardware security protocols, all computers used in this project must adhere to FIU's University Technology Services (UTS) Security and IT Policies which are outlined in detail at *http://it.fiu.edu/security/index.shtml* and *http://security.fiu.edu/Pages/policies.aspx*. Security measures such as password protection will also be implemented in addition to an effective security strategy for sharing the database via the internet with other project stakeholders such as DOE or DOE site contractors.