YEAR END TECHNICAL REPORT

September 17, 2013 to May 17, 2014

Remediation and Treatment Technology Development and Support

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Addendum:

This document represents one (1) of five (5) reports that comprise the Year End Reports for the period of September 17, 2013 to May 17, 2014 prepared by the Applied Research Center at Florida International University for the U.S. Department of Energy Office of Environmental Management (DOE-EM) under Cooperative Agreement No. DE-EM0000598.

The complete set of FIU's Year End Reports for this reporting period includes the following documents and are available at the DOE Research website for the Cooperative Agreement between the U.S. Department of Energy Office of Environmental Management and the Applied Research Center at Florida International University (http://doeresearch.fiu.edu):

Project 1: Chemical Process Alternatives for Radioactive Waste
Document number: FIU-ARC-2014-800000393-04b-233

Project 2: Rapid Deployment of Engineered Solutions for Environmental Problems
Document number: FIU-ARC-2014-800000438-04b-223

Project 3: Remediation and Treatment Technology Development and Support
Document number: FIU-ARC-2014-800000439-04b-225

Project 4: Waste and D&D Engineering and Technology Development
Document number: FIU-ARC-2014-800000440-04b-220

Project 5: DOE-FIU Science & Technology Workforce Development Initiative
Document number: FIU-ARC-2014-800000394-04b-079

Each document will be submitted to OSTI separately under the respective project title and document number as shown above.

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PROJECT 3 OVERVIEW

Historically, this project has provided analysis of flow and transport for several watersheds at DOE's Oak Ridge Reservation (ORR), including East Fork Poplar Creek (EFPC), Upper EFPC (Y-12 NSC) and White Oak Creek (WOC) through the development of integrated surface and subsurface flow and transport models. The models were used to conduct numerical modeling and reviews of monitoring data available from the Oak Ridge Environmental Information System (OREIS) and related to mercury (Hg) contamination and remediation within these watersheds. The model developed for the EFPC 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 developed also includes the main components of the hydrological cycle: groundwater flow (3D saturated and unsaturated), 2D overland flow, 1D flow in rivers, precipitation, and evapotranspiration. The EFPC model was calibrated for the period of 1996-2009 using recorded stream flow and mercury concentrations measured in groundwater, surface water and soil. It was then 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.

Experimental studies were also carried out which provided kinetic and equilibrium data for important parameters related to mercury (Hg) transport, speciation and methylation/demethylation kinetics within the watershed. In addition, surface modeling work was conducted on the Oak Ridge National Laboratory (ORNL) area of the Oak Ridge Reservation using XPSWMM on the premise that this smaller system could provide the proof-of-concept and then be expanded to a larger area at Y-12. Geographic information systems (GIS) technology was employed to support the modeling work through storage and geoprocessing of spatial and temporal data required by the models. An ArcGIS geodatabase was developed for centralized storage and management of experimental and computed model data and its capabilities extended over the years using tools such as ModelBuilder combined with Python scripting to automate repetitive tasks, statistical analyses and generation of maps and reports. An investigation of downloadable free/open source GIS software along with required security protocols to facilitate online querying of the database was also conducted to determine methods by which project-derived data could be more easily shared with other project stakeholders such as DOE personnel and site contractors. New scope was introduced in FIU Year 4 that focused on the development of EM pilot studies and the use of Green Sustainable Remediation (GSR) software (e.g., SITEWISE™) to evaluate the benefit of GSR practices, to quantify the environmental footprint of remedial and other alternatives, and to develop a sustainable optimization module that allows for monitoring progress in this area at DOE EM sites. Sustainability evaluation, integrated into the existing 5-year regulatory reviews, is a common practice in industry and federal agencies to assess environmental footprint impact, as well as to improve system design performance and efficiency. Detailed task descriptions and deliverables and milestones can be found in the Project Technical Plan (Appendix 1).

TECHNICAL PROGRESS SUMMARY FOR FIU YEAR 4 (FY13)

For FIU Year 4, FIU proposed a scope which built upon the previously developed models to analyze flow, fate and transport of site contamination and remedial activities at the OR site. This work is synergistic with the work ORNL is performing and involved the integrated surface/subsurface flow and transport model developed for the EFPC and the surface model developed to study the drainage discharges from the outfalls along EFPC. A series of simulations, coordinated with the site, were 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.

FIU also added new scope in FIU Year 4 which focused on EM pilot studies and software used 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.

The following documents cover project-wide and individual task accomplishments for FIU Year 4 (FY13).

- A Project Technical Plan for FIU Year 4 (FY13) was prepared and sent to DOE on October 17, 2013. (See P3 APPENDIX I YR4 Project Technical Plan)
- A mid-year review presentation was presented to DOE HQ and DOE ORO on February 27, 2014. (See P3 APPENDIX II YR4 Research Review Feb-2014)
- Several factsheets were generated to provide short summaries of the various Project 3 tasks. (See P3 APPENDIX III YR4 Factsheets)
- This project overall has provided training for 3 DOE Fellows and 1 PhD student.

Conference Proceedings

- Research results were presented in the form of poster presentations at the Waste Management Conference 2014 in March 2014 (See P3 APPENDIX IV YR4 Conference Proceedings):
    - Display of Contaminated Locations at Oak Ridge site using ArcGIS - Michelle Embon (DOE Fellow) – Student Poster
    - Development of REST Services for Populating ESRI’s ArcGIS Spatial Modeling Applications - Steve Noel (DOE Fellow) – Student Poster
    - Environmental Remediation Optimization: Cost Savings, Footprint Reduction, and Sustainability Benchmarked on DOE Sites - Natalia Duque (DOE Fellow) – Student Poster

Refereed Journals

- A peer reviewed journal article was published based on research conducted for this project (See P3 APPENDIX V YR4 Publications):

  - Malek-Mohammadi, S., and Tachiev, G. (2013). Migration of VOC Plume in the Subsurface Domain at the Y-12 National Security Site. *Remediation*, 23(1), 139-153.

Masters Theses/PhD Dissertations

- Nantaporn Noosai, PhD candidate. Developing thermodynamic database of mercury species and integrating interactions within a flow and transport model. Dissertation completed Fall 2013. (See P3 APPENDIX VI YR4 Dissertation)

Technical Reports

- The four (4) technical report deliverables that were due May 16, 2014, for Project 3 of the FIU-DOE Cooperative Agreement, were re-forecasted for completion during the next few months. Tasks 3.1, 3.2, and 3.4 were closed in April 2014 as recommended by DOE HQ and the site contacts at Oak Ridge. Task 3.3 was put on hold by DOE HQ while re-scoping discussions were held between FIU, DOE, and SRS. Technical Reports for all the tasks related to this project have therefore been drafted and are to be submitted to DOE as follows:
  - Task 1. EFPC Model Update, Calibration and Uncertainty Analysis. The final technical report was drafted and will be submitted by July 31, 2014. The final report contains a summary of the work completed for this project during this year and includes a description of the model for EFPC, a summary of completed simulations and results. The main emphasis of the report is on the work conducted during the last year and more specifically on the development of the kinetic model and the thermodynamic database for mercury speciation.
  - Task 2. Simulation of NPDES- and TMDL- Regulated Discharges from Non-Point Sources for EFPC and Y-12 NSC. The final technical report was drafted and will be submitted by July 31, 2014. The final report contains a summary of the work completed for this project during this year with the main emphasis on an update of the hydrological and water quality data from the outfalls at the upper portion of East Fork Poplar Creek (within the Y-12 NSC).
  - Task 3. Sustainable Remediation and Optimization: Cost Savings, Footprint Reductions, and Sustainability Benchmarked at EM Sites. The task was postponed while re-scoping discussions were held with DOE-HQ. A final report will be issued for the work completed for this task by August 29, 2014. DOE-HQ in collaboration with Savannah River Site personnel has provided further direction for this task which will now focus on a sustainability plan for the A/M Area Groundwater Remediation System at SRS. This work aims to develop a set of proposed actions for the existing infrastructure of the groundwater remediation system that will reduce the environmental burden of the system while potentially reducing the duration of operation needed. The A/M Area groundwater remediation system has operated continuously for 27 years and is expected to operate continuously for the foreseeable future. Improvements in system performance, increased contaminant recovery or decreased energy consumption, will have positive enduring benefits due to the long time frame over which the benefits will accrue. This work will directly support the EM-13 Green and Sustainability Remediation (GSR) program and will be coordinated with the GSR program lead.

  - The Task 4 technical report “Remediation and Treatment Technology Development and Support for DOE Oak Ridge Office: Geodatabase Development for Hydrological Modeling Support”, was completed and will be submitted by June 30, 2014. (See P3 APPENDIX VII Task 4 Final Technical Report)

TASK 1: EFPC MODEL UPDATE, CALIBRATION AND UNCERTAINTY ANALYSIS

INTRODUCTION

The objective of this task was 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 work for FIU Year 4 involved use of the existing EFPC model to provide simulations that implement selected main thermodynamic equilibria and reactions. This included: (1) A review of the existing Hg thermodynamic database and update for EFPC environmental conditions, (2) Integration of the Hg thermodynamic database into the existing EFPC model, and (3) A series of simulations using the EFPC model and the thermodynamic and kinetic interactions. The major deliverable was 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 was integrated into the geodatabase and made available for web publishing. The following summarizes the results and conclusions derived from research conducted under this task throughout FIU Year 4. Further details will be reported in a technical report scheduled to be submitted by July 31, 2014.

RESULTS

This task provides analysis of the coupling between hydrology and mercury transport within the context of decreasing the risk of decontamination and decommissioning (D&D) activities. The work performed for FIU Year 4 supported a PhD student and included using the model to provide simulations that implement selected thermodynamic equilibria and reactions. Additionally, the methylation and demethylation reactions and the conversion between mercury and methylmercury were implemented using a reaction model which accounts for the observed ratio between mercury and methyl mercury at the Oak Ridge Site.

The dissolution mechanism of the mercury beads within the EFPC watersheds was 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+} were investigated. An extended mercury thermodynamic database relevant to EFPC environmental conditions was developed and further integrated into the coupled flow and transport models already developed for the site (PHREEQC, XPSWMM, MIKE). The task relied on thermodynamic equilibrium software and reaction kinetic software to characterize the most dominant species and processes for the environmental conditions of ORR. The model was developed using ECOLAB, which is a kinetic and reaction solver implemented as a separate module.

During this year, a set of equations were implemented in the kinetic solver which provide distribution between total mercury and methylmercury species based on observed distribution coefficients (as fraction). This is an initial approximation to ensure that the model can correctly calculate distribution of species.

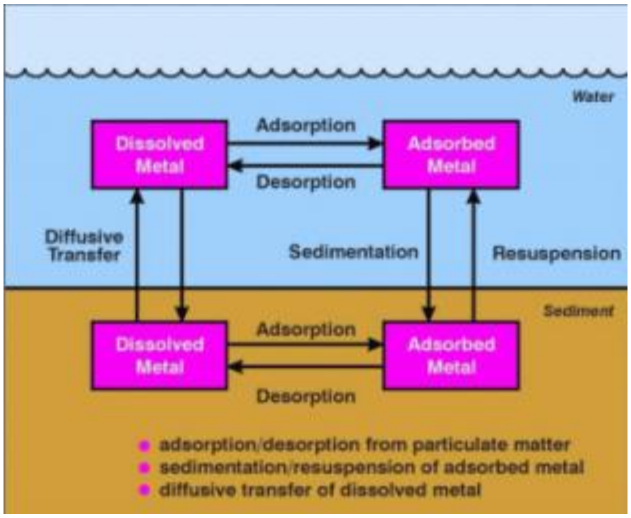

Figure 1. A summary of the processes which are currently included for total mercury and methylmercury.

The mercury transport processes which were developed and incorporated in ECOLAB are defined by specifying:

- Dissolved mercury concentration in the water (SHM).
- Adsorbed mercury concentration on suspended matter (XHM).
- Dissolved mercury concentration in the sediment pore water (SHMS).
- Adsorbed mercury concentration in the sediment (XHMS).
- Dissolved methylmercury concentration in water (MeM)

The mercury exchange between suspended solids and the water column is represented by the variable SHM. This exchange is mainly driven by the organic carbon partitioning coefficient, indicating the contaminant’s affinity towards the soil phase. Dissolved mercury is computed using the following set of coupled equations [33]:

$$\frac{dS_{HM}}{dt} = -adss + dess + difv \tag{1}$$

$$adss = k_w K_d S_{HM} TSS \tag{2}$$

$$dess = k_w X_{HM} \tag{3}$$

$$difv = \frac{f_{biot(difw)}\left(\frac{S_{HMS}}{(pors)(dzds)} - S_{HMS}\right)}{(dzwf + dzds)dz} \tag{4}$$

The equations above represent the relation between adsorption ($adss$), desorption ($dess$), and diffusive transfer ($difv$). The variables k_w, K_d, TSS, $f_{biot(difw)}$, $pors$, $dzwf$ and dz are equivalent to the desorption rate (d^{-1}), partitioning coefficient for mercury (m^3 H_2O/gDW), total suspended solids concentration (g DW/m^3 bulk), factor for diffusion due to bioturbation (dimensionless), thickness of diffusion layer in sediment (m), and thickness of the computational grid layer (m), respectively.

The methylmercury concentration is represented using a simple distribution coefficient which is based on observed distribution between total dissolved mercury and methylmercury concentrations (Figure 2):

$$\text{MeM} = \text{Kmm*SHM} \tag{5}$$

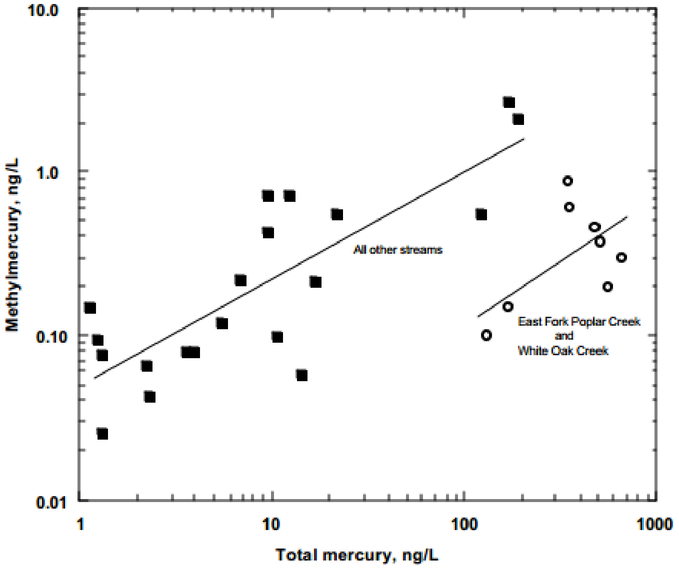

Figure 2. Relation between total mercury and methylmercury at ORR from experimental data[1].

The adsorbed mercury concentration on suspended matter within the water column results from mercury being absorbed by both the suspended solids and particles re-suspended by the river bed

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[1] Mercury and Methylmercury Relationships in Contaminated Streams in the Southeastern USA G.R Southworth, M.A. Bogle, and R.R. Turner.

layer, and eliminating the mercury desorbed from suspended solids into water column, and also those adsorbed by settling particles.

$$\frac{dX_{HM}}{dt} = adss - dess - sev + resv \tag{6}$$

$$sev = \frac{v_s X_{HM}}{dz} \tag{7}$$

$$resv = \frac{RR \frac{X_{HMS}}{X_{SED}}}{dz} \tag{8}$$

In the equations above, sev and $resv$ represent the sedimentation and re-suspension of particles. The settling velocity (m/d) of suspended solids is defined by v_s. RR is the re-suspension rate (gDW/m^2/d). X_{SED} is the sediment mass (gDW/m^2). The equations assume that the current speed is greater than the critical speed responsible for initiating movement. S_{HMS} is calculated based on the equations below:

$$\frac{dS_{HMS}}{dt} = -adss + dess - dif \tag{9}$$

$$adss = k_s K_{ds} S_{HMS} \frac{X_{SED}}{dzs \cdot por_s} \tag{10}$$

$$dess = k_s X_{HMS} \tag{11}$$

The desorption rate in sediment (d-1), metal partitioning coefficient between particulates and water (m^3 H_2O/gDW), and sediment porosity (m^3 H_2O/ m^3 bulk), are given by k_s, K_{ds}, and por_s. The variables in the above equations have been defined earlier in this section. XHMS is calculated using the following relations:

$$\frac{dX_{HMS}}{dt} = adss - dess - sev + resv \tag{12}$$

$$adss = k_s K_{ds} S_{HMS} \frac{X_{SED}}{dzs \cdot por_s} \tag{13}$$

$$sev = v_s X_{HM} \tag{14}$$

$$resv = \frac{RRX_{HMS}}{X_{SED}} \tag{15}$$

These above kinetic and thermodynamic equations were implemented within the MIKE 11 and MIKE SHE model and provide better understanding of the coupling of hydrology and mercury fate and transport with conversion to methylmercury. The equations provide the distribution between total mercury and methylmercury species based on observed distribution coefficients (as fractions).

The mercury transport processes which were developed and incorporated in ECOLAB are defined by specifying dissolved mercury concentration in the water column and the sediment pore water, the adsorbed mercury concentration on suspended matter and in the sediment. For this initial phase of development of the template, the methylmercury concentration was added in the template as dissolved species only. The template has been completed and implemented in the hydrologic and transport model. Initial testing of the template has been conducted to calibrate the model using observed ratios of total mercury and methylmercury concentrations.

Based on observed data for the ORR watersheds (EFPC and WOC), the ratios between methylmercury to total mercury ranged between Kmm = 1:500 to 1:1000. The initial results showed that the template predicts as expected the ratio between total mercury and methylmercury concentrations.

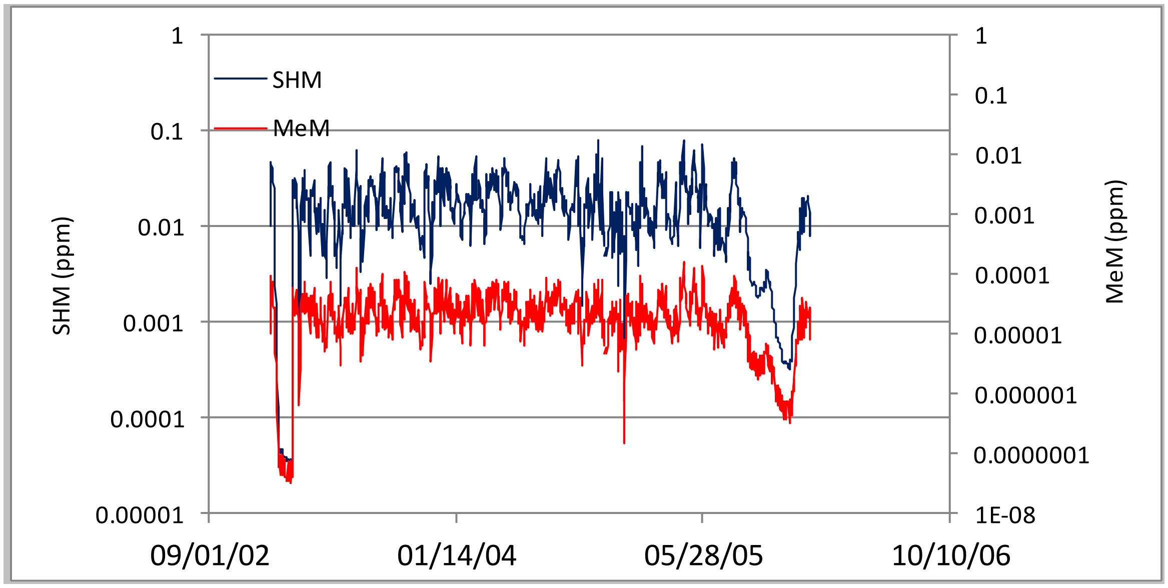

Figure 3. Nearly proportional distribution between dissolved mercury (SHM) and methylmercury species (MeM) based on the ECOLAB kinetic model

The ECOLAB kinetic provides coupling between hydrology and mercury fate and transport with conversion to methylmercury. Additional factors are required (sorption to TSS, photodegradation) to provide better understanding of the methylmercury's behavior in the environment. In the next phase of this investigation, a literature review was conducted to determine the distribution coefficient between dissolved methylmercury species and methylmercury species sorbed on organic material present in water or in sediments and this process was implemented in the ECOLAB template.

Additionally, the literature review provided an understanding of recent experimental work on the distribution coefficients between dissolved methylmercury species and methylmercury species sorbed on organic material present in water or in sediments. This provided a means for to perform sensitivity analysis of the ECOLAB template when coupling with the MIKE SHE hydrological model. Simulations were conducted to determine the sensitivity of the kinetic parameters to the final results.

The numerical model was updated to reflect additional data obtained from the OREIS, USGS, and TDEC. Water flow is simulated in MIKE 11 via a 1-dimensional engine directly linked to the network geometry. The network developed for the EFPC model consists of reaches, nodes, grid points, and cross-sections. The river and stream network for the domain area was revised as shown below, and currently consists of 142 branches and 1288 nodes, or MIKE SHE links. Cross-sections are set to allow for overbank spilling. The left and right bank elevations and bed layer are consistent with topography files. Resistance (Manning's M) values range between 1 and 20 throughout the domain.

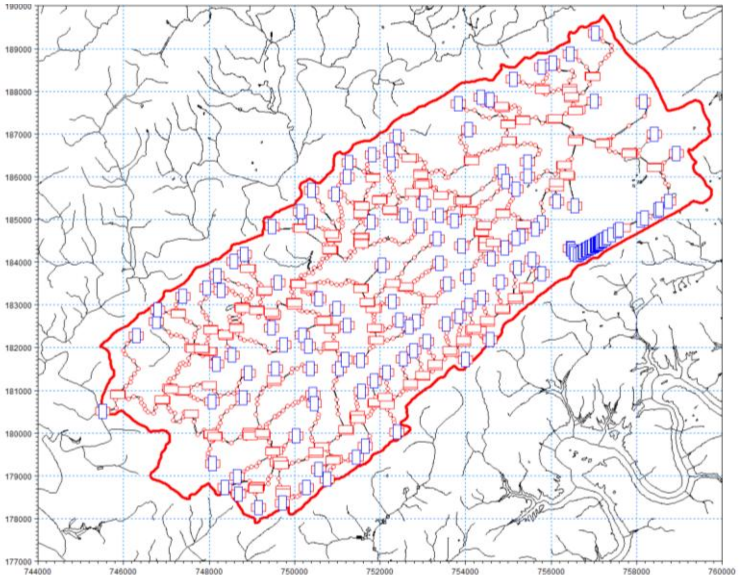

Figure 4. River network in the model indicating point nodes, boundary conditions and cross-sections.

The boundary conditions were also updated in the watershed model, and the open boundary conditions were coupled with additional boundary point sources to simulate the hydrology of the natural environment, as well as the most significant anthropological alterations to the site. Preliminary simulations were conducted to ensure the model has expected performance. The EFPC model was modified by adding outfalls (point sources) to the boundary file in both the HD and AD module. The newly developed boundary conditions file for the modules consist of the previously existing EFPC Model boundary file and the Y-12 Model. The new boundary condition file consists of a total of 176 branches of which 42 were defined as point sources.

The advection-dispersion of solutes is coupled to the simulated flows and fluxes calculated by the MIKE SHE flow model. After the modifications to the AD simulations were made (through the ECO Lab module), additional calibrations were conducted to improve the calibration of the flow model, and to calibrate the simulated concentrations and mass fluxes to the measured concentrations by adjusting only the solute transport model. The purpose of the calibration was to refine the model to better represent conditions in the most recent time period. Additional factors were taken into account:

- Uncertainty in the measurements (time, space, equipment)
- Representativeness of measurements (point/average grid values)
- Differences between the conceptual model and nature
- Uncertainty in other model parameters and data (source description etc.)
- Additional refinements that were made to account for the dual porosity parameters

Using the revised model, the mercury concentrations along East Fork Poplar Creek were summarized and compared to observed data and additional adjustments are in progress.

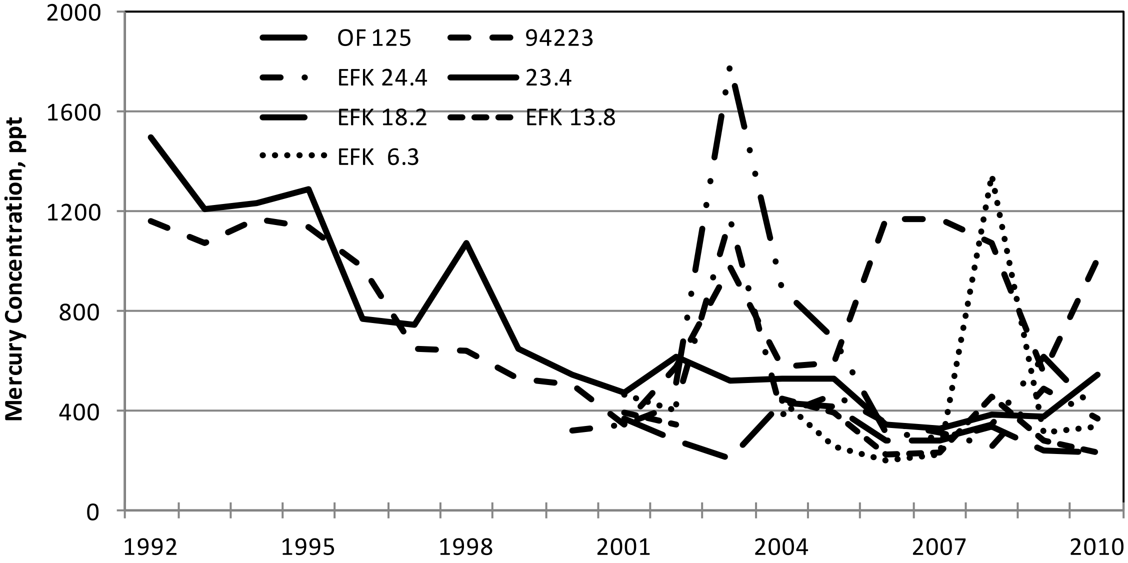

Figure 5. Monthly-based variations of average mercury concentration at selected stations along EFPC

The EFPC model was archived and all data files were versioned. The work on development of the EFPC model is placed on hold based on the low interest of the site to use the model results. The task will continue by supporting the ASCEM program and additional scope is under development for providing support for the development of ASCEM tools.

The final technical report contains additional details about the model development and the work conducted on the development of the ECOLAB template. The report was drafted and will be submitted as planned to complete the deliverable due July 31, 2014, for the "EFPC Model Update, Calibration and Uncertainty Analysis" (Task 3.1). The final report contains a summary of the work completed for this project during this year and includes a description of the model for EFPC as well as a summary of completed simulations and results. The emphasis of the report is the work conducted during the last year with a more detailed description of the development of the kinetic model and the thermodynamic database for mercury speciation.

CONCLUSIONS

The dissolution mechanism of the mercury beads within the EFPC watersheds implemented into the hydrological model and the competitive absorption on the EFPC sediment between the major cations contained in EFPC water ($Ca^{2+,}$ $Mg^{2+,}$ etc.) and Hg^{2+} was investigated. A mercury thermodynamic database relevant to EFPC environmental conditions was developed and integrated into the coupled flow and transport models already developed for the site using an enhanced PHREEQC database. The inclusion of thermodynamic equilibrium and reaction kinetic allowed characterization of the most dominant species and processes for the environmental conditions of ORR.

The integrated model was extended by implementing an ECOLAB model which was used 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 which includes dissolved and chelated mercury species (natural organic matter). The development of a mercury/methylmercury template provided details needed to improve the fate and transport model. The fate and transport model that has been developed can be used to analyze remediation scenarios and address the complexity of total mercury transport. The model also provides insight into the reactions leading to the generation or degradation of methylmercury. The reaction and kinetic model was calibrated using the observed ratio between total mercury and methylmercury.

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TASK 2: SIMULATION OF NPDES- AND TMDL-REGULATED DISCHARGES FROM NON-POINT SOURCES FOR THE EFPC AND Y-12 NSC

INTRODUCTION

During FIU Year 4 (FY13), a surface flow model for Y-12 NSC, similar to the model developed for ORNL, was developed. The purpose of the model is to determine the discharges from the stormwater drainage system and for each of the outfalls along EFPC, which will subsequently be implemented in the surface and groundwater model developed for the entire EFPC. A series of simulations were conducted to provide numerical analysis of contaminant flow and transport within the EFPC watershed and determine the impact of model parameters on NPDES and TMDL regulations. The scope involved 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 MIKE 11. During FIU Year 3 (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 simulations were conducted for available data (starting from 1991-present) to provide long term trends. Two periods were considered, prior to flow augmentation of Upper EFPC and after flow augmentation. The results were analyzed to determine the long term trends within each period, and to generate probability exceedance curves for each scenario. This data provides additional insight of the effect for the entire range of hydrologic regimes, very wet ranging to very dry conditions. The effects on diversion of clean water away from contaminated soils and storm water drains were studied as well as the possible positive impacts downstream through reducing the flood potential (by modifying the river bed), and limiting the infiltration of rainwater through areas with underlying mercury contamination.

The following summarizes the results and conclusions derived from research conducted under this task throughout FIU Year 4. Further details will be reported in a technical report scheduled to be submitted on July 31, 2014. Dissertation research conducted by PhD student Nantaporn Noosai has been incorporated in the attached appendices (See P3 APPENDIX VI YR4 Dissertation).

RESULTS

This task utilizes the surface flow model of the East Fork Poplar Creek (EFPC) to determine the discharges from the stormwater drainage system. This task is based on measured data of flow and concentration for each of the outfalls along the Upper East Fork Poplar Creek and provides simulations of TMDL and NPDS discharges from the watershed. A new set of groundwater table boundary conditions were developed to better represent the watershed characteristics. Additionally, data for parameters including rainfall, evapotranspiration, timeseries of outfalls, rivers and canals were updated.

The target for the total maximum daily load (TMDL) analyses is the numeric water quality criterion for mercury for the EFPC waterbody. The target concentration was selected based on the detailed description of water uses and regulations established by EPA, DOE, and TDEC. These numeric water quality targets were translated into TMDLs through the loading capacity, or as defined by EPA as “the greatest amount of loading received without violating water quality standards”.

Several target load-duration curves were developed for EFPC by applying the mercury target concentration of 51 ppt, 200 ppt, and 770 ppt; each ranked flow was used to generate the flow duration curve. The mercury target maximum load corresponding to each ranked daily mean flow was computed by multiplying the recreation use water quality criterion (51 ppt) by the flow and by the appropriate unit conversion factor. The same calculation was performed for the record of decision (ROD) designated target concentration of 200 ppt and water quality criterion of 770 ppt established to sustain fish and aquatic life.

Target load reduction criteria were developed using percent reduction which was calculated as the difference between the mean and the water quality criteria, considering a confidence interval, and divided by the mean with the incorporated confidence interval.

Figure 6 shows the standard water quality criteria compared to the simulated mercury loading along with the required percent reduction which was applied. The graph shows that the percent load reduction places the simulated loading within the range of the 51 ppt water quality criteria and below the 200 ppt standard mandated by the DOE record of decision.

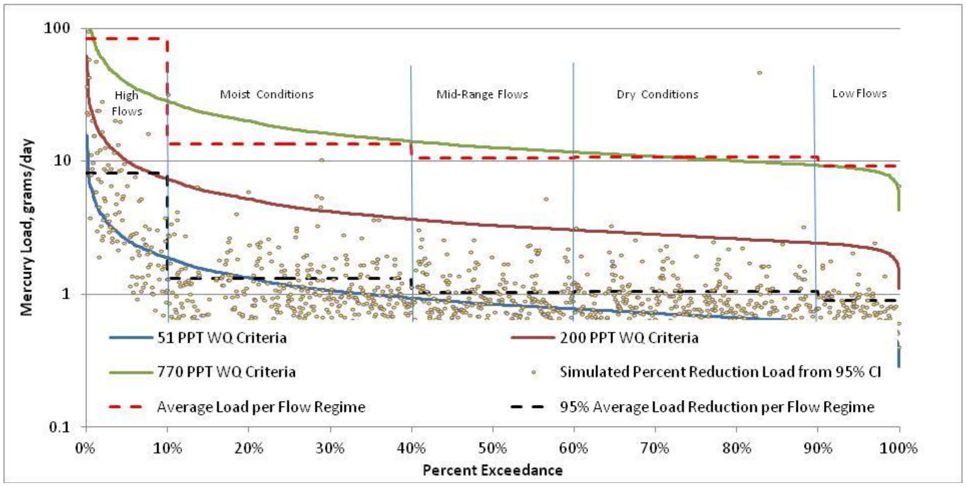

Figure 6. Comparison of simulated mercury loading with applied percent reduction and target TMDLs.

The model was used with the developed ECOLAB template which incorporates methylmercury into the set of kinetic and thermodynamic equations. A series of simulations were completed during this period to conduct calibration and validation.

The target for the total maximum daily load (TMDL) analyses is the numeric water quality criterion for mercury for the specified EFPC waterbody. The target concentration was selected based on the detailed description of water uses and regulations established by EPA, DOE, and TDEC. These numeric water quality targets were translated into TMDLs through the loading capacity or as defined by EPA as “the greatest amount of loading received without violating water quality standards”.

The simulations were conducted using the MIKE SHE model with the developed ECOLAB template which incorporates methylmercury into the set of kinetic and thermodynamic equations. The task reviewed the requirements of TMDL studies as related to ORR, including:

- Impaired watershed characterization and status, which included: i) Impairment status – Understanding the basic physical, environmental, and human elements of the watershed. ii) Data gaps and monitoring report and the existing data to identify any additional data needs and monitoring recommendations. iii) Source assessment – Identification of sources of pollutants, and magnitude of the sources. iv) Target identification – Establishment of water quality targets intended to restore or maintain beneficial uses. This step includes the calculation of the loading capacity using some analysis to link loading to water quality.
- Loading analysis: i) Linkage analyses – Select and apply approach to establish a link between pollutant loading and water quality. ii) Load calculations – Determination of natural pollutant load, and load from human activities (i.e. diffuse nonpoint sources and point discharges). ii) Loading capacity – Calculate allowable loading capacity.
- Loading allocation: i) Loading level – Select appropriate level (geographic, temporal and source) for allocations for successful implementation. ii) Allocation scenario – Evaluate allocation scenarios representing different combinations of load reductions (WLAs and LAs) and select the most appropriate and feasible allocation scenario.

The TMDL for EFPC was developed based on analysis of water quality data. Based on the most recent data, 2000 to the present, the load reductions were estimated. The percent load reduction required to decrease the mercury concentration in water from the "mean + 95% confidence interval" to the desired target level was calculated at each sampling location. The percent load reductions ranged from 85.1% to 94.0%. The highest percent load reduction was selected as the TMDL for the entire waterbody. A summary of monitoring data on mercury concentration in water from 2000 to 2013 is presented in Table 1.

Table 1. Analysis of Mercury Concentration in Creek Water (2000 - Present)

	OF125 ppb	C11 ppb	92334 ppb	EFK 23.4 ppb	EFK 24.4 ppb	EFK 18.2 ppb	EFK 13.8 ppb	EFK 6.3 ppb
Number of samples	726	138	277	3673	25	14	11	11
Minimum	0.20		0.20	0.20	0.22	0.21	0.21	0.20
Mean	0.70	0.49	0.63	0.50	0.44	0.30	0.33	0.42
Standard Deviation	1.83	0.49	0.7453	0.6550	0.3270	0.0744	0.0959	0.3181
95% CI	0.13	0.082	0.0236	0.0212	0.1281	0.0390	0.0567	0.1190
Mean + 95% CI	0.84	0.57\	0.6546	0.5172	0.5721	0.3430	0.3857	0.5400
90% CI	0.11	0.0684	0.0198	0.0178	0.1075	0.0327	0.0476	0.0999

Mean + 90% CI	0.81	0.5584	0.6508	0.5138	0.5515	0.3367	0.3766	0.5209
Target	0.051	0.051	0.051	0.051	0.051	0.051	0.051	0.051
% Reduction from 90%	93.9%	91.0%	92.3%	90.3%	90.9%	85.1%	86.7%	90.4%
% Reduction from 95%	94.0%	91.3%	92.4%	90.3%	91.3%	85.4%	87.0%	90.7%

Note. The % Reduction from 95% is calculated as follows: % Reduction = [(Mean + 95% CI) - Target] *I* (Mean + 95% CI)
The % Reduction from 90% is calculated in a similar manner.

CONCLUSIONS

The objectives of the model were to determine the discharges from the stormwater drainage system and each of the outfalls along EFPC. The discharges were implemented in the surface and groundwater model developed for the entire EFPC. A series of simulations were conducted to provide analysis of contaminant flow and transport within the EFPC watershed and to determine the impact of model parameters on NPDES and TMDL regulations. A series of simulations were executed to determine the significance of mercury reaction kinetic parameters on flow and transport within EFPC to provide analysis of the long term trends. Two periods were considered, the period prior to flow augmentation of Upper EFPC and the period after flow augmentation had been implemented. The computed data provides additional insight of the effect for the entire range of hydrologic regimes (very wet to very dry conditions). As a result of re-scoping, this task was finalized and the model was versioned.

The data computed from simulations was archived and all data files were versioned. The work on simulations with the EFPC model was placed on hold based on the low interest of the site to use the model results. The task will continue by supporting the ASCEM program and currently, additional scope is under development to provide testing and simulations using the ASCEM program.

The final technical report was drafted and will be submitted by July 31, 2014 for “Simulation of NPDES- and TMDL-Regulated Discharges from Non-Point Sources for the EFPC and Y-12 NSC” (Task 3.2). The final report contains a summary of the work completed for this project during this year with the main emphasis on an update of the hydrological and water quality data from the outfalls at the upper portion of East Fork Poplar Creek (within the Y-12 NSC).

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TASK 3: SUSTAINABLE REMEDIATION AND OPTIMIZATION: COST SAVINGS, FOOTPRINT REDUCTIONS, AND SUSTAINABILITY BENCHMARKED AT EM SITES

INTRODUCTION

This task was new and was incorporated into the Project 3 work scope for FIU Year 4 (FY13). 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 with Headquarters' oversight of those projects. EM worked with EPA and the Interstate Technology & Regulatory Council (ITRC) to train and certify over 130+ DOE staff and remediation contractors in GSR principles and practices. 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 the sustainability of remedial and monitoring decisions; identify improved and more cost-effective end states; reduce hazardous emissions, consumption of water and energy resources; and decrease the environmental footprint or impact. The benefits of implementing these 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.

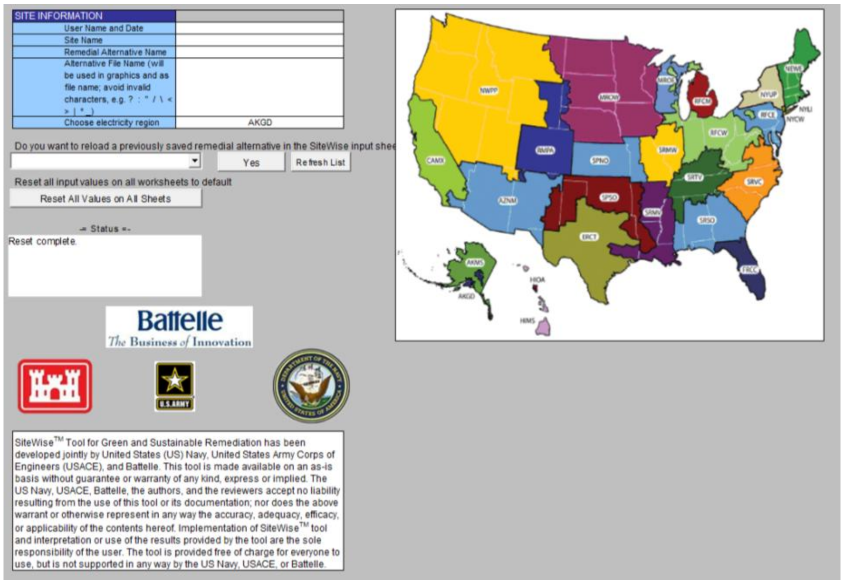
The SITEWISE^{TM} software is an Microsoft Excel-based evaluation tool designed to: 1) compare and contrast alternatives for remedial, monitoring, waste handling, and D&D design; and 2) generate results for cost benefit and sustainable decision-making for regulatory compliance. The Navy, EPA, and USACE incorporate sustainability evaluation and decision making into their long-standing and successful optimization programs as part of the 5-year regulatory review process. SITEWISE^{TM} is one of many evaluation tools used in federal and industry sectors to calculate and optimize system processes to reduce as much as possible the environmental footprint of cleanup and closure alternatives. Specifically, the SITEWISE^{TM} 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 wherein 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 environmental impact 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 potential to significantly lower the environmental impact 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 related optimization programs at EPA, Navy, Army, Air Force, and USACE sites. Data developed from this task will be integrated into the geodatabase and will be prepared for web publishing.

The scope of this task includes: (1) Benchmarking current methodology using SITEWISE^{TM}; (2) Implementation of a SITEWISE^{TM} module for sustainable analysis and optimization of monitoring programs; and (3) Calibration and verification of the SITEWISE^{TM} monitoring program module.

RESULTS

The SITEWISE^{TM} tool is designed to calculate the environmental impact footprint from user input and impact factors contained within the tool that using Microsoft Excel. SITEWISE^{TM} is designed to be used in the planning stages of a project to estimate the environmental impacts of that project using different treatment technologies. The tool can support the identification and selection of the ideal remediation technology for a given project. To this end, sustainable remediation software tools are available to treat the remediation process with a method similar to Life Cycle Assessment by considering environmental impacts from different phases of a remediation project. The tool takes into account the energy inputs and emission outputs associated with manufacturing materials and chemicals, construction processes, and continued operation and maintenance of the remediation project.



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SiteWise^{TM} Tool for Green and Sustainable Remediation has been developed jointly by United States (US) Navy, United States Army Corps of Engineers (USACE), and Battelle. This tool is made available on an as-is basis without guarantee or warranty of any kind, express or implied. The US Navy, USACE, Battelle, the authors, and the reviewers accept no liability resulting from the use of this tool or its documentation; nor does the above warrant or otherwise represent in any way the accuracy, adequacy, efficacy, or applicability of the contents hereof. Implementation of SiteWise^{TM} tool and interpretation or use of the results provided by the tool are the sole responsibility of the user. The tool is provided free of charge for everyone to use, but is not supported in any way by the US Navy, USACE, or Battelle.

Figure 7. SITEWISE^{TM} site info sheet

SITEWISE^{TM} is being used to estimate the environmental impacts associated with a particular selected remediation project. The remediation technologies used for the project will be implemented using the tool. The results will be calculated from input data supplied by the user and from software-specific calculations to translate the quantities of materials, use of equipment and vehicles, and use of energy into impacts and the environmental footprint.

A review of available statistical or geostatistical software, including MAROS or GTS, was conducted. This software is used to downsize a compliance monitoring program (i.e., remove wells, analytes, or frequencies of sampling). Tests were conducted with the monitoring module in SITEWISE^{TM} to use the results via Excel to calculate the reduction in emissions, energy and water usage, waste generation, and accident risk over the program total life cycle.

The tool requires input data of the four major remediation technology implementation phases, including:

1. Remedial investigation phase;
2. Remedial action construction phase;
3. Remedial action operation phase; and
4. Long term monitoring phase.

The required input data is primarily obtained from site technical reports and/or engineering drawings which contain construction and operation details of selected remediation technologies. Table 2 shows the input data required to calculate the impact and environmental footprint of the remediation technologies.

Table 2. Details of Required Inputs for the Four Remedial Phases

Remedial Components	Description
Baseline information	Remedial cost for all 4 phases.
Material production	Well materials, treatment chemical and materials, treatment media, construction materials, well decommissioning, bulk material quantities.
Transportation	Road transportation, air transportation, rail transportation, equipment for transportations
Equipment use	Earthwork, drilling, trenching, pump operation, diesel and gasoline pumps, blower, compressor, mixer, generators, internal combustion engines, other fueled equipment, operator labor, laboratory analysis, other onsite activities.
Residual handling	Residue disposal/recycling, landfill operations, thermal/catalytic oxidizers, Landfill operations, thermal/catalytic oxidizers.
Resource consumption	Water consumption, onsite land and water resource consumption.

Using the SITEWISE^{TM} tool, the following results are calculated.

1. From Table 2, all the data is collected and entered into SITWISE^{TM}, for all four remedial phases. The tool then calculates and converts the input data into the several categories of environmental impacts for each remedial phase, including GHG emissions, total energy used, water consumption, NOx emissions, SOx emissions, PM10 emissions, accident risk fatality, and accident risk injury.
2. The alternative technologies for the footprint reduction, including landfill gas microturbines, wind power, solar power, renewable energy, will then be selected for the reduction of footprint calculation.

3. The total footprint of the implemented remediation technologies can be calculated by the sum of the environmental footprint produced from the four remedial phases and subtracting the footprint reduction. The calculated environmental footprint will help to support the decision maker for an appropriate remediation technology use.

Initial simulations were conducted and data gaps are being identified and researched.

Based on preliminary testing of SITEWISE^{TM} (using a hypothetical site), the following information is required and needs to be provided by the site:

- Material production: SITEWISE^{TM} separates into five categories: well materials, treatment chemicals, granular activated carbon (GAC), construction materials and well decommissioning materials and calculates the GHG emissions and energy usage.

- Well materials: the environmental footprint for using PVC, steel, and high density polyethylene (HDPE; both schedule 5S and 10S, schedule 40 and schedule 80 and some SDR specifications in case of high density polyethylene) to install wells.

- Treatment chemicals: SITEWISE^{TM} includes: *in situ* chemical oxidation (ISCO) chemicals [i.e., hydrogen peroxide, biostimulant (vegetable oil), emulsified zero valent iron (EZVI), urea, fertilizer, acetic acid, sodium hypochlorite, mulch, lime, phosphate fertilizer, soda ash and iron exchange resin]. The user inputs the number of injection points, the amount of material per injection and the number of injections.

- GAC (virgin and regenerated): the mass of either virgin or regenerated GAC is required.

- Construction materials: the materials included in this category are HDPE, general concrete, gravel and cement and it requires knowledge of the total volume of the material used by entering both the area and depth required to be filled by the material in square feet and feet, respectively.

- Well decommissioning materials: includes soil, sand, general concrete, gravel, and typical cement. The amount of the material is calculated by the number, depth of wells, diameter of the well, and the material that would be used to backfill the wells.

- Bulk quantities of materials: the materials include GAC, construction, and well decommissioning materials or user defined materials which require the emission factor entries.

- Transportation: considers both personnel and material/equipment transportation to determine the environmental footprint of a remedial action. The emission factors used by the tool for calculating the environmental footprint due to transportation-related activities are provided; however, they need to be updated for the current time period.

- Transportation personnel are road, air and rail. For personnel transportation, the emission factors for air emissions are provided in mass per passenger mile based on the specific fuel used. Life cycle emission factors considered in the tool for the fuels were obtained from the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model developed by Argonne National Laboratory.

- Personnel transportation road: to calculate the environmental footprint of roads requires the user to input the distance travelled in miles, the number of travelers, the number of trips taken, the type of vehicle and type of fuel.

- Personnel transportation air: to calculate the environmental footprint of air travel requires the user to input the distance travelled in miles, the number of travelers and the number of flights taken.

- Personnel transportation rail: SITEWISE^{TM} calculates the environmental impact for three types of rail travel: intercity, commuter, and transit.

- Transportation equipment: includes transportation by road, air, rail and water. For each mode of transportation, the environmental footprint is calculated based on the mass of material or equipment transported.

- Equipment transportation road: for transporting equipment by road, SITEWISE^{TM} considers transportation using an on-road truck. A default fuel economy of 7.2 mpg is used for the on-road truck.

- Equipment transportation air, rail and water.

- Equipment use: includes using pumps (electrical and run by fuel), earthwork equipment, blowers, compressors, generators, agricultural equipment, mixers, and stabilization equipment. The emission factors used by the tool for calculating the environmental footprint due to equipment.

- General electrical equipment and generators are included. The electrical equipment in the model includes blowers, compressors, mixers, and others. Three inputs are required to calculate the impact of air emissions by using generators during remediation. The fuel type (gasoline, diesel, biodiesel 20 or e-diesel) and the horsepower range are required.

- Agricultural equipment: requires the fuel used by the equipment (diesel, biodiesel 20 or e-diesel) and the soil condition (firm untilled soil, previously tilled soil and soft or sandy soil) and the soil type (clay, loam or sand).

- Internal combustion engine (ICE): to provide analysis for equipment that is not currently a part of current model due to the fact that ICE (or a modified version of ICE) are part of the working mechanism of several pieces of equipment that are used. The required input includes operating hours and fuel consumption rate for the ICE and the type of fuel.

- Stabilization equipment: determines the environmental impact of a roller or paver (and the corresponding fuel type). Requires the area to be stabilized (ft^2) and the time that it will take as inputs required to determine the environmental impact of stabilization equipment.

- Mixers: the total amount of fuel and time required for use of the mixer are required.

- Other fueled equipment: equipment with a different type of fuel can be analyzed to determine the emissions.

- Residual handling: the residual handling section calculates the air emissions footprint from transporting residual waste (similar to transporting material by on-road truck), incinerating waste, and using a thermal oxidizer to oxidize contaminant waste.

- Thermal/catalytic oxidizer: The environmental footprints of several different types of thermal oxidizers are determined based on the type of thermal oxidizer (simple, recuperative, regenerative, flameless, recuperative flameless, fixed bed catalytic and recuperative catalytic oxidizer).

- Laboratory analysis: the cost of laboratory analysis, the corresponding footprint associated with the laboratory analysis and the emission factors for this analysis are determined based on a U.S. EPA study.

- On-site labor hours and activities: on-site labor hours and activities require labor hours for several categories of activities. Emission factors are based on data from the Department of Labor.

A review was conducted to determine the factors which may significantly impact the Green and Sustainable Remediation (GSR) metrics, including:

- Excessive number of monitoring locations;
- Inefficient chemical injection strategy;
- Excess quantity of chemicals used;
- Inefficient power usage by over-sized equipment;
- Installing less energy efficient equipment ;
- Unnecessary continuously running equipment; and
- Unnecessary unit operations.

Project 3 has developed integrated surface and groundwater models which are capable of predicting the contamination fate and transport within the site domain. The project has developed strategies for additional optimization by:

- Reducing the number of monitoring locations - One of the strategies for reducing the costs of long-term monitoring is to use optimization algorithms which reduce the number of the monitoring wells. For example, MAROS (Monitoring and Remediation Optimization System) is a software program which was developed to provide a strategy for formulating appropriate long-term groundwater monitoring programs to reduce the costs. Additional improvements can be provided by using the numerical models to determine the response of selected monitoring wells and to eliminate redundant monitoring wells (wells with similar response).

- Improving the chemical injection strategy - Injecting chemicals in the subsurface environment can be improved by simulating injection. Simulation of injections can provide an understanding of the mixing patterns in the subsurface environment and can determine the best strategy (rate, duration and location of injection). The existing surface and groundwater models provide analysis of the plume which will be created by injecting specific chemicals. In addition, the model can be used to determine the fate and transport of the chemicals which are used for remediation.

- Reducing the quantity of chemicals used - Reducing the quantities of chemicals is critical for cost and environmental footprint reduction. In order to reduce the quantities, a set of simulations can be developed which use the surface and groundwater models to determine the required mass of chemical to maintain the required concentration within a given extent of the contaminant plume.

Additionally, geostatistical methods for reducing the number of the wells were reviewed. The Monitoring and Remediation Optimization System (MAROS) provides an optimal monitoring network solution. The software uses statistical plume analyses (parametric and nonparametric trend analysis) and allows users to enter External Plume Information (empirical or modeling results) to determine the most optimal sampling frequency, location and density. Particular attention was given to the ability to interface MAROS with modeling results obtained using current models surface and groundwater models developed by the project.

A discussion with the ORR site was conducted on the possibility of providing an analysis of the waste treatment plant which will treat approximately 3000 gpd of mercury contaminated water. Relevant information was prepared and sent to the site for additional coordination.

The literature was investigated for various aspects of mercury treatment including potential zero-mercury discharge technologies. Particular attention was given to strategies that limit the quantity of mercury which would enter the waste treatment plant.

Preliminary analyses were conducted to test the software by performing a case study of the Outfall 200 Mercury Treatment Plant at ORR. Two alternatives were analyzed using SITEWISE^{TM}. Both remediation technologies used granular activated carbon (GAC) as a treatment medium for mercury contaminated water. Alternative A used virgin GAC while alternative B used regenerated GAC as another footprint reduction practice. The tool calculates and converts input data into several categories of environmental impacts for each remedial phase:

- GHG emissions
- Total energy used
- Water consumption
- NO_x emissions
- SO_x emissions
- PM10 emissions
- Accident risk fatality
- Accident risk injury

SITEWISE^{TM} also gives detailed analysis of each remedial alternative, so it can identify activity with the highest footprint for each metric. If alternative technologies for footprint reduction are being used (wind, solar, renewable energy, and landfill gas microturbines), the reduction is subtracted from the footprint produced to give a net value. The calculated environmental footprint will help support the decision of the most appropriate remediation technology.

A review was conducted which determined factors that may significantly impact the Green and Sustainable Remediation (GSR) metrics, including:

- Excessive number of monitoring locations
- Inefficient chemical injection strategy
- Excess quantity of chemicals used Inefficient power usage by over-sized equipment
- Installing less energy efficient equipment
- Unnecessary continuously running equipment
- Unnecessary unit operations
- Improving the chemical injection strategy:
    - Simulating injection of chemicals into subsurface can assist in understanding subsurface mixing patterns and determination of the best strategy (rate, duration and location of injection).
    - Existing surface and GW models provide analysis of plume created by injecting specific chemicals.
    - Models can be used to determine fate and transport of chemicals used for remediation.
- Reducing the quantity of chemicals used:
    - Critical for cost and environmental footprint reduction.
    - To reduce quantities, simulations can be developed which use surface and GW models to determine required mass of chemical to maintain required conc. within a given extent of the contaminant plume.

Benefits include:

- Centralized data management system facilitates storage, concurrent editing and import/export of data specific to hydrological models being used.
- Data organized into a structured, coherent, logical computer- supported system.
- Facilitates automation and simplified retrieval of stored GIS and timeseries data.
- Versioning tools enable security management and quality assurance while editing.
- Database structure enables linkage with scalable hydrologic modeling applications.
- XML-based GIS data exchange system facilitates import/export of preconfigured data as XML files which can contain both the data definition and the data itself.

SITEWISE^{TM} is capable of comparing two or more remediation technologies to evaluate the cost-benefit of GSR practices. It calculates the remedy footprint generation and helps identify areas and methods for potential footprint reduction. In this case study, it was found that no one alternative was the best; however, it was possible to identify aspects of both which can be combined in order to provide the most appropriate remediation technology.

Conference calls were held with DOE-HQ which provided further direction for this task. Additional studies will provide an analysis of the available tools for green and sustainable remediation and will compare SITEWISE^{TM} with other systems used for environmental and financial footprint reduction.

SITEWISE^{TM} Version 3 (2013) was obtained and the latest user manual was reviewed. Version 3 has been modified to address observations made by a benchmark team as part of the Naval

Facilities Engineering and Expeditionary Warfare Center project, “Quantifying Life-Cycle Environmental Footprints of Soil and Groundwater Remedies.” These revisions provided updates on: i) improving the applicability and accuracy of footprint results; and ii) improving the usability or formatting of the tool. The task reviewed alternatives to SITEWISE^{TM} tools used for green and sustainable remediation (including Life-Cycle Analysis, Sustainable Remediation Tool, guidance documents from ITRC, Greener Cleanup Matrix, SuRF-UK, U.S. SURF framework document, Green Remediation Evaluation Matrix, Carbon Footprint Tools). Below are snapshots of small sections of the GSR and SITEWISE^{TM} flowcharts currently under development.

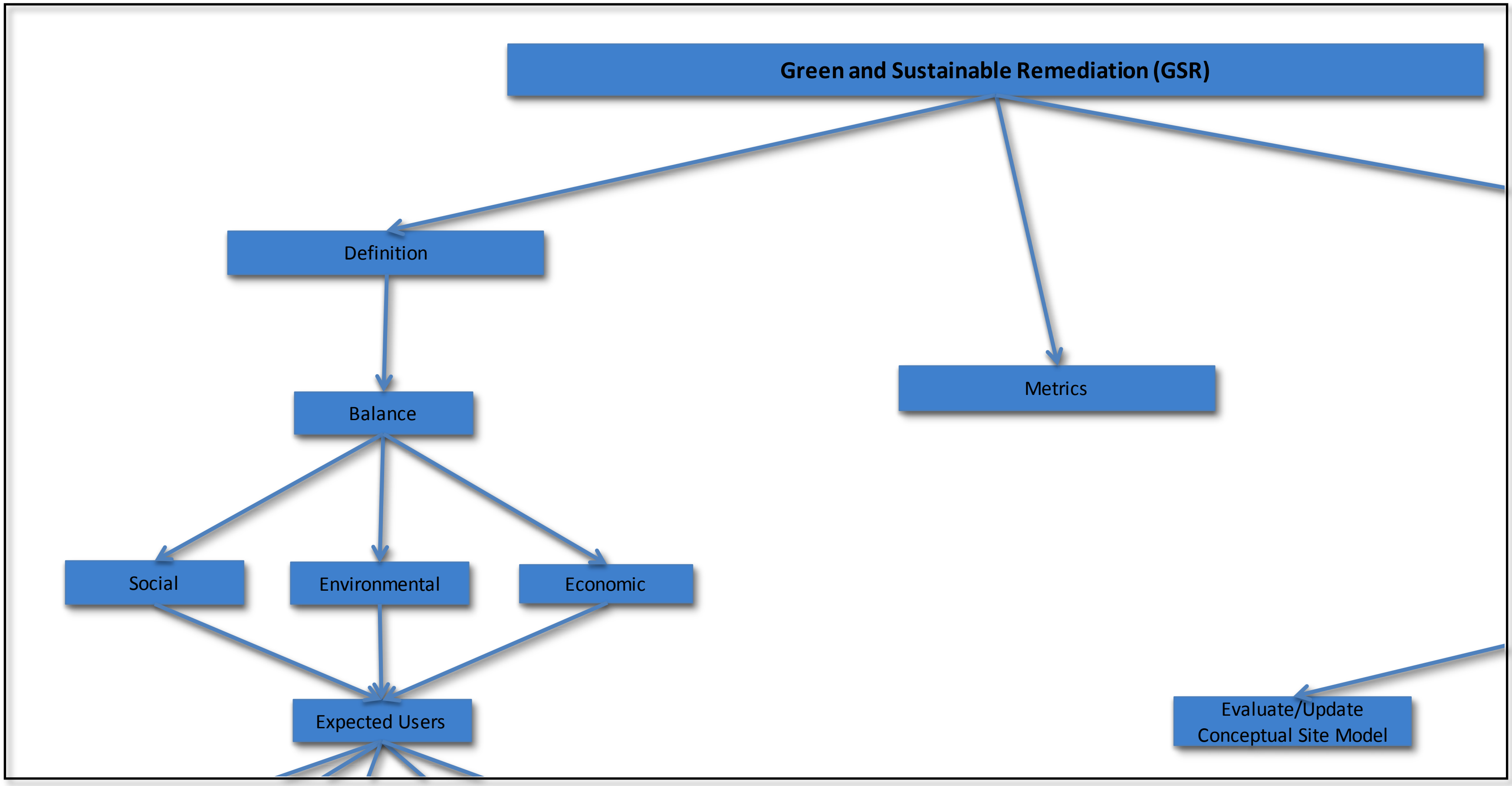

Figure 8. GSR Flowchart

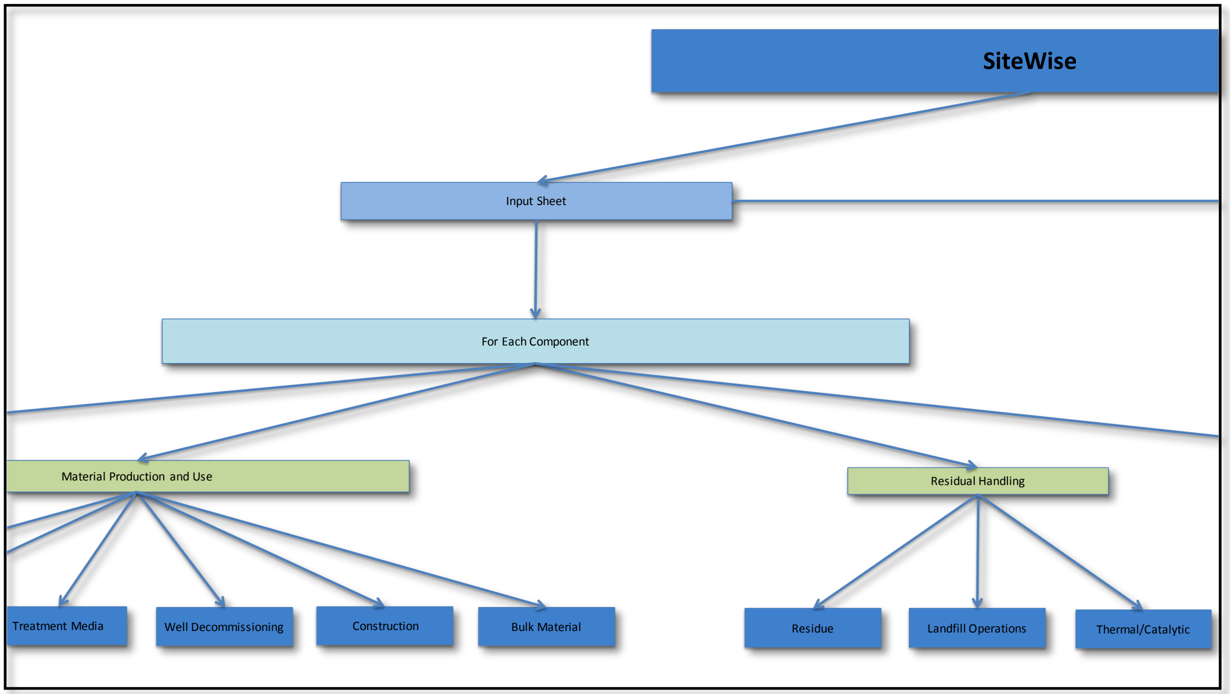

Figure 9. SITEWISE^{TM} Flowchart

Re-scoping discussions with DOE-HQ provided further direction for this task which will now focus on a sustainability plan for the A/M Area Groundwater Remediation System at SRS during FIU Year 5. This task going forward will develop a set of proposed actions for the existing infrastructure of the groundwater remediation system that will reduce the environmental burden of the system while potentially reducing the duration of operation needed. The A/M Area groundwater remediation system has operated continuously for 27 years and is expected to operate continuously for the foreseeable future. Improvements in system performance, increased contaminant recovery or decreased energy consumption, will have positive enduring benefits due to the long time frame over which the benefits will accrue. This work will directly support the EM-13 Green and Sustainability Remediation (GSR) program and will be coordinated with the GSR program lead.

CONCLUSIONS

A detailed study was done on the many available environmental sustainability tools available, especially Green Sustainable Remediation (GSR) and SITEWISE^{TM}. Data requirements were analyzed for the tools and cross referenced to the availability of this type of data at DOE sites. Often data on the usage of fuel, power, other energy, water and other resources are collected on units larger than a particular technology or system (e.g., buildings, complex of buildings and facilities, etc.) and not available for subsystems. That said, there are methods of estimating the data required from the aggregate data. Results from implementation of GSR and SITEWISE^{TM} at federal sites were also studied with attention toward the implementation process and the data collection used in these implementations. FIU worked with DOE EM to identify a DOE EM site or failing that, another federal remediation site, for FIU to apply SITEWISE^{TM}, including Oak Ridge and Hanford. DOE Savannah River and SRNL has shown interest in FIU supporting the development of a GSR program there, especially one that begins by analyzing the A/M Area groundwater remediation system,

For this reason, this task was re-scoped for FIU Year 5 and will now focus on the development of a set of proposed actions for the existing infrastructure of the groundwater remediation system that will reduce the environmental burden of the A/M Area groundwater remediation system at the Savannah River Site. Successful implementation of GSR for the groundwater remediation system would provide the impetus for further implementations at SRS.

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TASK 4: GEODATABASE DEVELOPMENT FOR HYDROLOGICAL MODELING SUPPORT

INTRODUCTION

FIU-ARC has been providing technical assistance and performing research on mercury remediation at the Oak Ridge Reservation (ORR), TN, to support their remediation efforts through hydrological modeling in order to provide a better understanding of the fate and transport of inorganic and organic pollutants of concern with a focus on mercury (Hg). FIU developed a geodatabase to support the hydrological modeling work performed by FIU, which involves the use of three integrated watershed models for the Y-12 National Security Complex, White Oak Creek (WOC), and East Fork Poplar Creek (EFPC) to simulate the fate and transport of contaminants. More than a hundred simulations were completed for the purpose of calibrating the models, deriving model uncertainties, and for providing the analysis of remediation scenarios, resulting in gigabytes of simulation data. Therefore, there was a need for an advanced spatial data structure that would be used to address the management, processing, and analysis of spatial and temporal numerical modeling data derived from multiple sources, and to produce hydrogeological maps for visualization.

The existing geodatabase structure developed for the hydrological modeling work at ORR was structured to be replicable for application at other DOE sites and 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 work for FIU Year 3 (FY12) extended the geodatabase capabilities and created models using ArcGIS ModelBuilder and Python scripting that automate the process of querying the existing EFPC geodatabase and the generation of maps. Investigation of easily downloadable free/open source geographic information systems (GIS) software for viewing and querying the hydrological modeling data and for generating maps, graphs and reports, was then conducted to determine a simple way of sharing project derived data with other project stakeholders such as U.S. Department of Energy (DOE) personnel and ORR site contractors.

Work carried out during FIU Year 4 has included an update of the existing geodatabase with more recent ORR site monitoring data; development of additional customized Python scripts to further enhance the database capabilities to perform statistical analyses by implementing a library of scripts which can be coupled with other existing libraries used for mathematics, science, and engineering such as NumPy and SciPy; training of FIU undergraduate students (DOE fellows) on how to update, query and perform geoprocessing tasks within the ArcGIS environment; and research to determine the best way to share project data via the Internet over a secured platform. The following summarizes the research conducted under this task throughout the FIU Year 4 period of performance. Further details are reported in the attached technical report under “P3 APPENDIX VII Task 4 Final Technical Report”.

RESULTS

The accuracy and predictive forecasting ability of the hydrological models largely depend on the availability of timeseries data (daily/monthly/annual) as well as the period of time this data covers. The various ORR site monitoring data sources used in this project such as OREIS, USGS, NRCS STATSGO or SSURGO soil databases, and the U.S. EPA MRLC or NALC land cover databases, are being constantly updated and as such, it is necessary to periodically download and update the ORR geodatabase with more recent data. FIU's Year 4 work scope has therefore involved an update of the existing geodatabase with recent ORR site monitoring data. The GIS data derived from OREIS has been replaced with the 2006 flyover vector and raster data. Updated timeseries data from OREIS for parameters such as flow/discharge, chemical contaminant concentrations, conductivity, surface water depth, depth to groundwater, have also been downloaded and used in the models and resulting project-derived simulation data added to the geodatabase.

Additional customized Python scripts were developed to calculate model performance statistics for a subset of existing flow and contaminant monitoring stations. This was achieved by implementing a library of scripts coupled with existing libraries used for mathematics, science, and engineering such as NumPy and SciPy.

There has also been progress on research related to the publishing of hydrological modeling results via the Internet. The ArcGIS for Server architecture being implemented includes three software technologies including: (1) ArcMap for creating, editing, and viewing the geospatial data and maps; (2) ArcGIS Server, which provides the platform for storing and sharing GIS resources with the user community; and (3) the Web Adaptor, which adds an intermediate layer of protection between the end user viewing published maps and ArcGIS Server where the information is actually stored.

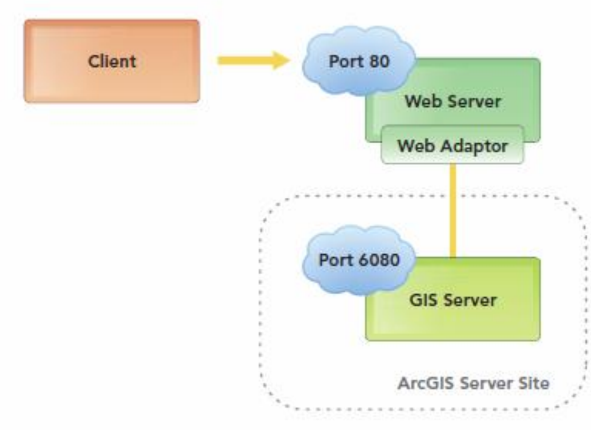

Figure 10. ArcGIS for server architecture.

In order to display project data on the web, a map containing GIS-based hydrological data was created using ArcMap and then published using ArcGIS Server. Once published on the server, the map and associated data files become accessible as a GIS service or web service through port 80. However, to add an extra layer of protection and control to the web service, ArcGIS Web Adaptor was installed on an ARC-FIU GIS server, which ensures restricted access to the GIS service exclusively through the Web Adaptor.

With the Web Adaptor installed, a website was created that communicates with the web adaptor and consumes the GIS web service information displaying it in an interactive map that users can view. The website uses ESRI’s JavaScript API to create a map object from the web service created and using the map information, generates different map layers which are added to the map object to show all the different features in the map document.

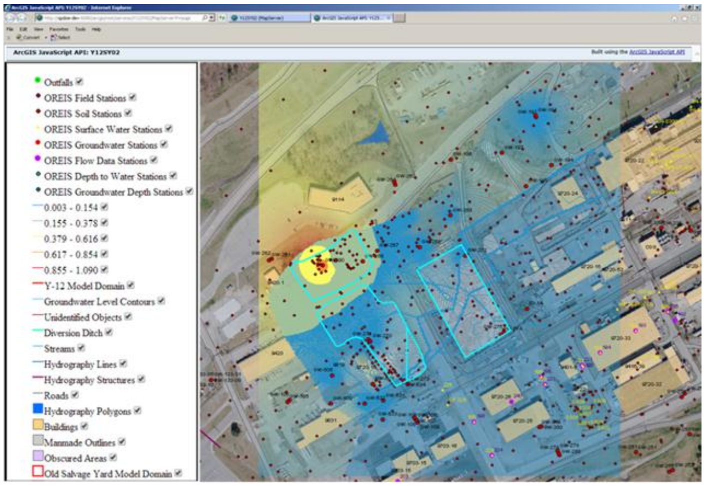

Figure 11. Prelminary website development.

A map Legend was also created to inform the user what the different geometries on the map represent. This functionality also uses JavaScript to retrieve the different map layer information from the web service and manipulates the web page to visually display this information to the user. Another feature added to the website is the ability to toggle different map layers on and off using checkboxes in the legend. Large maps can be crowded with many different layers and points of data; therefore, the layer toggle feature allows the user to view meaningful layers of information and omit irrelevant data crowding the map. Zooming and panning are also features implemented on the map, allowing users to move and pan to any location within the map object.

Further development of the website then incorporated a layer selection feature. This feature allows the user to select a layer from the Legend which will also highlight and select the respective layer on the map. The Layer Selection feature also works in conjunction with the popup feature. Once a user has selected a Layer, it will then be possible to click on a particular feature on the map from that layer and a popup will appear displaying the feature’s attribute information, geometry and an interactive chart showing timeseries data.

CONCLUSIONS

This report details the final work provided for this task. The task was closed in April 2014 based on recommendations by DOE HQ and the site contacts at Oak Ridge. The task has provided support to the hydrological modeling work being performed by FIU-ARC at the Oak Ridge Reservation (ORR) through development of a GIS-based database (geodatabase) which provides an advanced spatial data structure for management, processing, and analysis of spatial and temporal numerical modeling data derived from multiple sources. ArcGIS ModelBuilder coupled with Python scripting was used to extend the geodatabase capabilities to more easily query data and automate many of the repetitive geoprocessing tasks required for pre- and post-processing of hydrological modeling data. Finally, a web-based GIS map which depicts hydrological modeling results was created to so that project derived data can be more easily shared project stakeholders including DOE personnel and ORR site contractors.

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FUTURE WORK

This Year End Report provides details of the final work conducted for the Oak Ridge Reservation under this project. Tasks 1, 2 & 4 were closed in April 2014 based on recommendations by DOE EM HQ and ORR. The entire project has been re-scoped and the site contacts have changed to Savannah River National Laboratory (SRNL).

For FIU Year 5, FIU is working with SRNL contacts and is proposing a scope which utilizes and builds upon the capabilities developed under Project 3 in the area of soil and groundwater remediation and treatment technology. Tasks will be synergistic with the work SRNL is performing and will involve: (1) Modeling of the migration and distribution of natural organic matter injected into subsurface systems; (2) Fate and transport modeling of Hg, Sn and sediments in surface water of Tims Branch; and (3) Analysis of baseline, optimization studies and development of a system improvement plan for the A/M Area groundwater remediation system.

Task 1: Modeling of the migration and distribution of natural organic matter (NOM) injected into subsurface systems

This work aims to assemble, integrate and develop a practical and implementable approach to quantify and model potential natural organic matter (NOM, such as humic and fulvic acids, humate, etc.) deployment scenarios for the range of conditions at DOE sites. SRNL has performed initial laboratory experiments and have generated an initial set of simplified models. They currently plan to extend these studies (additional batch and column testing) with the support of FIU students (DOE Fellows and other interns).

Task 2: Surface Water Modeling of Tims Branch

The task will perform modeling of water, sediment, mercury and tin in Tims Branch at the Savannah River Site (SRS). This site has been impacted by 60 years of anthropogenic events associated with discharges from process and laboratory facilities. Tims Branch provides a unique opportunity to study complex systems science in a full-scale ecosystem that has experienced controlled step changes in boundary conditions. The task effort includes developing and testing a full ecosystem model for a relatively well defined system in which all of the local mercury inputs were effectively eliminated via two remediation actions (2000 and 2007). Further, discharge of inorganic tin (as small micro-particles and nanoparticles) was initiated in 2007 as a step function with high quality records on the quantity and timing of the release. The principal objectives are to apply geographical information systems and stream/ecosystem modeling tools to the Tims Branch system to examine the response of the system to historical discharges and environmental management remediation actions.

Task 3: Sustainability Plan for the A/M Area Groundwater Remediation System

This work will be performed in support of EM-13 (Office of D&D and Facilities Engineering) under the direction of Mr. Albes Gaonas. FIU will develop a set of proposed actions for the existing infrastructure of the groundwater remediation system that will reduce the environmental burden of the A/M Area groundwater remediation system. Reducing the duration of operation for the treatment system could be a recommendation of these studies. The A/M Area groundwater remediation system has operated continuously for 27 years and is expected to operate continuously for the foreseeable future. Improvements in system performance, increased contaminant recovery, or decreased energy consumption, will have positive enduring benefits due to the long time frame over which the benefits will accrue. This work will directly support the EM-12/EM-13 Green and Sustainability Remediation (GSR) program and will be coordinated with the GSR program lead.

APPENDICES

The following documents are available at the DOE Research website for the Cooperative Agreement between the U.S. Department of Energy Office of Environmental Management and the Applied Research Center at Florida International University: http://doeresearch.fiu.edu

1. P3 APPENDIX I YR4 Project Technical Plan
2. P3 APPENDIX II YR4 Research Review Feb-2014
3. P3 APPENDIX III YR4 Factsheets
4. P3 APPENDIX IV YR4 Conference Proceedings
5. P3 APPENDIX V YR4 Publications
6. P3 APPENDIX VI YR4 Dissertation
7. P3 APPENDIX VII Task 4 Final Technical Report