



Worlds Ahead





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Project Description

General Objective

Support remediation efforts at ORR through better understanding of fate and transport (F & T) of inorganic/organic pollutants of concern with a focus on mercury (Hg).



Project Description

- Modeling F & T of contaminants
 - Surface (rivers & overland flow)
 - Saturated/unsaturated subsurface (groundwater)
- Green Sustainable Remediation assessment
 - Provide analysis of remediation strategies using sustainable methods to reduce environmental and social impacts of remedial cleanup and closure activities in a cost-effective way.
 - Contributing to meeting greenhouse gas (GHG) goals, reducing toxic air emissions,
 Reducing polluting wastewater discharges, Lessening the impact on ecosystems,
 Reducing waste generation, Reflecting Best Management Practices (BMPs) and good
 environmental stewardship,
 - Helping to achieve public acceptance, Reducing life-cycle costs, and Demonstrating performance in achieving environmental sustainability goals.
- Geodatabase development
 - Centralized data storage and management



Technology Needs

Regulatory requirements

- Clean Water Act States must identify waters not meeting WQ stds
- Conventional hydrologic and remediation methods limited
- State-of-the-practice tools for analysis of sustainable and green remediation alternatives needed

Project uses conventional engineering methodologies (as developed by EPA, USACE, and USGS) <u>in combination with</u> latest scientific software (1D/2D/3D F &T models integrated with reaction kinetics and thermodynamic software).

 Provides integrated solution for understanding mobility and impacts of contaminants at DOE sites, reducing costs and environmental footprint.



Technology Needs

Data storage and integration

- Accumulation of millions of spatial/temporal records related to hydrological cycle, contaminant transport, remediation technology parameters.
 - Numerical models produce gigabytes of computed spatial/temporal data for each computation node.

Geodatabase facilitates:

- Centralized storage, backup, and management of model data.
- Structured, coherent, and logical computer-supported system.
- Linkage with scalable hydrologic modeling tools/applications.
- Automation and simplification of retrieving stored GIS and timeseries data.
- Contaminant F & T analyses requiring large amounts of high-quality spatial and temporal data for reliability and validity of modeling results.



Work Scope (FIU Year 4)

Builds upon previously developed models to analyze flow, fate and transport of contamination & remedial activities at ORR.

- Task 3.1: EFPC Model Update, Calibration, Uncertainty Analysis
 - Subtask 3.1.1: Review of existing Hg thermodynamic database and update for EFPC environmental conditions.
 - Subtask 3.1.2: Integration of Hg thermodynamic database into existing EFPC model.
 - Subtask 3.1.3: Simulations using EFPC model and thermodynamic and kinetic interactions.
- Task 3.2: Simulation of NPDES & TMDL Regulated Discharges from Non-Point Sources for EFPC & Y-12 NSC
 - Subtask 3.2.1: Use of observed outfall discharges for simulations of EFPC watershed and load discharge at Station 17 using EFPC model developed with MIKE SHE/11.



Work Scope (FIU Year 4)

- Task 3.3: Sustainable Remediation and Optimization: Cost Savings,
 Footprint Reductions, and Sustainability Benchmarked at EM Sites (New)
 - Subtask 3.3.1: Benchmarking of current methodology using SITEWISETM.
 - Subtask 3.3.2: Implementation of SITEWISETM module for sustainable analysis and optimization of monitoring programs.
 - Subtask 3.3.3: Calibration and Verification of SITEWISETM monitoring program module.
- Task 3.4: Geodatabase Development for Hydrological Modeling Support
 - Subtask 3.4.1: Update of existing EFPC geodatabase.
 - Subtask 3.4.2: Development of customized Python scripts to enhance database querying capabilities.
 - Subtask 3.4.3: Use of existing geodatabase structure developed for EFPC modeling work at OR to create similar databases .





Project Wide Accomplishments (FIU Year 4)

- Draft Project Technical Plan for FY13 (FIU Year 4) submitted to DOE.
- Refereed Journal Publication:
 - 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.
- PhD Dissertation:
 - Nantaporn Noosai, PhD candidate, "Developing thermodynamic database of mercury species and integrating interactions within a flow and transport model." Dissertation completed Fall 2013.





Task 3.1: EFPC Model Update, Calibration, Uncertainty Analysis

Objective

Analysis of coupling between hydrology and Hg transport within context of decreasing risk of D&D activities.

Benefits

- Conventional hydrologic and remediation analytical tools (accepted by EPA, USACE, and USGS) in combination with latest scientific software (2D/3D numerical flow and transport models integrated with reaction kinetics and thermodynamic software) provides integrated solution for understanding mobility and impacts of contaminants at DOE sites.
- Provides state-of-the-practice tools for analysis of sustainable and green remediation alternatives (developed for DOD sites) needed to address long term sustainability in terms of reduced environmental and energy footprints of remedial actions.





Task 3.1: EFPC Model Update, Calibration, Uncertainty Analysis

Accomplishments

- Developed & calibrated numerical model for hydrology, sediment & Hg transport in UEFPC (1996 to present).
- Reconfigured model to incorporate sedimentation module and extended it to include 52
 additional outfalls covering entire EFPC and Bear Creek.
- Performed simulations using range of Manning's numbers, threshold run-off water depths, and drainage coefficients to calibrate flow from 2000 – 2008. MATLAB scripts were used for statistical analysis of observed and computed data.
- Provided DOE with assessment reports on effectiveness of 8 different remedial scenarios.
- Reviewed and updated existing Hg thermodynamic database specific to EFPC environmental conditions & integrated it into flow and transport models already developed for the site.
- Implemented equations in the kinetic solver (ECOLAB) which provides distribution between total-Hg and methyl-Hg species based on observed distribution coefficients (as fraction).
- Conducted preliminary tests to calibrate model using observed ratios of total-Hg and methyl-Hg concs. Initial results showed template predicts ratio between total-Hg and Me-Hg concs.





Task 3.1: EFPC Model Update, Calibration, Uncertainty Analysis

FY13 Scope

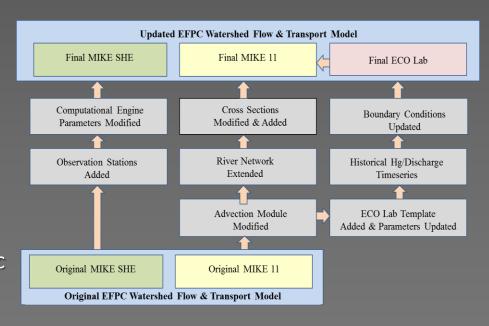
- Review of existing Hg thermodynamic database and update for EFPC environmental conditions.
- Integration of Hg thermodynamic database into existing EFPC model.
- Conduct simulations using EFPC model and thermodynamic and kinetic interactions.





Task 3.1: EFPC Model Update, Calibration, Uncertainty Analysis

- Reviewed thermodynamic database defining interactions between Hg species.
- Built-in programmable reaction solver extended to provide additional reaction equations based on literature.
- Kinetic equations and constants obtained from literature and implemented in kinetic solver of MIKE SHE/11 model (ECOLAB)
 - Provides distribution between total Hg and MeHg based on observed distribution coefficients (as fraction).





Task 3.1: EFPC Model Update, Calibration, Uncertainty Analysis

- Hg transport processes incorporated in ECOLAB as:
 - Dissolved Hg conc. in water column & sediment pore water.
 - Adsorbed Hg conc. on suspended matter and in sediment.
- For initial phase, MeHg added as dissolved species.
- Initial testing of template conducted to calibrate model using observed ratios of total Hg and MeHg concs.
 - Initial results showed template predicts ratio between total Hg and MeHg concs.
- MeHg represented using simple distribution coeff. based on observed distribution between total dissolved Hg (SHM) and MeHg concentrations (MeM):

MeM = Kmm*SHM

Based on observed data for ORR watersheds (EFPC & WOC), ratios between MeHg to total Hg ranged between Kmm = 1:500 to 1:1000.

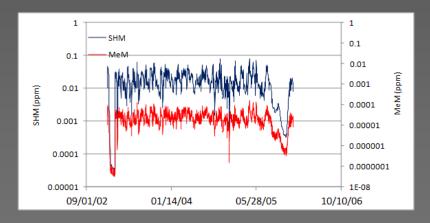


Figure showing nearly proportional distribution between dissolved mercury (SHM) and methylmercury species (MeM) based on the ECOLAB kinetic model.



Objective

Use of EFPC model for numerical analysis of contaminant flow and transport within EFPC watershed to determine impact of model parameters on TMDL.

- Ecosystem responses to variations in contaminant loading (changes in external & internal loading in time and space).
- Effect of ecosystem restoration on existing contaminant pools.

Benefits

- Modeling supports development of TMDLs to estimate source loading and evaluate loading capacities that meet WQ standards.
 - EFPC identified on Final 2008 303(d) List by TDEC as impaired waterbody not supporting designated uses due to contamination by mercury, PCBs, nitrates, and phosphates.
- TMDL may be used to develop controls for reducing pollution from point and nonpoint sources to restore and maintain WQ.



Accomplishments

- Update of EFPC database with:
 - Surface and GW levels
 - Water flow
 - Spatiotemporal distribution of pollutants in soil, water, and sediments
 - Bioassessment data
- Spatial and temporal analyses conducted to:
 - Identify spatial variations of Hg in EFPC water, shallow/deep soil layers, stream bank/streambed sediments
 - Evaluate timing of impairment, potential source loading or other conditions contributing to impairment
 - Investigate effect of rainfall and runoff on Hg conc. in EFPC
- Comprehensive review of TMDL requirements for EFPC established by EPA and TDEC.
 - Target Hg conc. for EFPC determined to be 51 ppt for recreational use based on TDEC regulations for surface waters, from which "Loading Capacity" duration curve was developed.
- Report containing:
 - WQ criteria and TMDL target
 - WQ assessment and deviation from TMDL target
 - WQ data analysis and source identification
 - Development of flow and load duration curves
 - Load allocation analysis



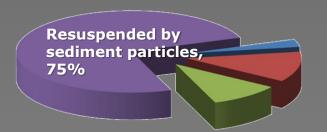


FY13 Scope

 Use observed outfall discharges for conducting simulations of entire EFPC watershed and load discharge at Station 17.



- Major mode of Hg transport is mobilization by surface water.
- Colloidal transport >85% of total Hg flux leaving UEFPC watershed.
 Possibly major cause of Hg flux under high flow conditions.
- Hg in soil & sediment sources adjacent to stream and in eroding sediment can contribute to Hg flux at Sta 17.
- Colloidally adsorbed Hg can be transported in surface water, thus
 actions that trap colloids and/or hydrologically isolate surface water
 runoff from source areas would reduce Hg flux at Sta 17.



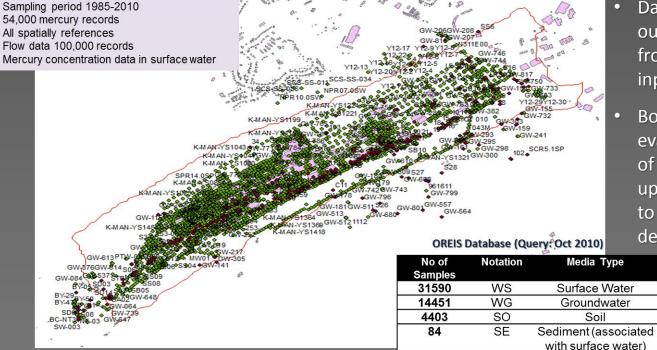
Diffused from pore water, 3%

Absorbed by water from suspended particles, 12%

Adsorbed to suspended particles from water, 10%







Mercury Concentrations in Soil in the Watershed Model Domain

- Data (up to 2013) for all 57 outfalls along EFPC obtained from OREIS and formatted for input into XPSWWM.
- Boundary conditions (rainfall, evapotranspiration, timeseries of outfalls, rivers and canals) updated to extend simulations to 2012. New GW table BCs developed.

 Target conc. for TMDLs is numeric water quality (WQ) criterion for Hg for EFPC, based on water uses/regulations by EPA, DOE, TDEC.

• Translated into TMDLs through loading capacity or as defined by EPA as "the greatest amount of loading received without violating water quality standards".





- Several target load-duration curves developed for EFPC
 - Hg target concs. of 51, 200, and 770 ppt applied to each ranked flow to generate flow duration curve.
- Hg target maximum load corresponding to each ranked daily mean flow computed by:
 - Recreation use WQ criterion (51 ppt) x Flow x Appropriate unit conversion factor
- Same calculation performed for ROD designated target conc. of 200 ppt and WQ criterion of 770 ppt established to sustain fish and aquatic life.





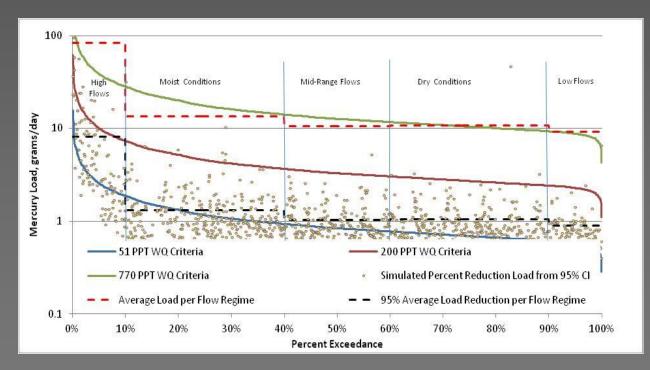


Figure 3-2 Comparison of simulated mercury loading with applied percent reduction and target TMDLs

Figure 3-2 shows:

- Standard water quality criteria compared to simulated Hg loading for which required % reduction applied.
- % reduction places
 simulated loading within
 range of 51 ppt WQ criteria
 and below 200 ppt std
 mandated by DOE ROD.





- Target load reduction criteria developed using % reduction
 - Calculated as difference between mean and WQ criteria, considering a confidence interval, and divided by mean with the incorporated confidence interval.
- Model used with newly developed ECOLAB template
 - Incorporates MeHg into kinetic & thermodynamic eqns.
- Several initial simulations completed and results being reviewed.



Objectives

NEW task focused on EM pilot studies and software to:

- Evaluate benefit of sustainable remediation practices.
- Quantify environmental footprint of remedial and other alternatives.
- Develop sustainable optimization module for monitoring program analysis on EM sites.

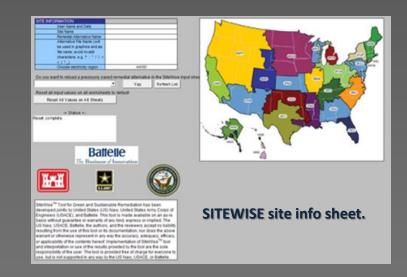
Benefits

- Building block approach will reduce redundancy in sustainability evaluation and facilitate identification of specific activities with greatest environmental footprint.
- The methodology employed will provide a decision matrix for remedy selection, design, or implementation and allows for a remedy optimization stage as well.



Accomplishments

- Review of geostatistical software including MAROS or GTS.
 - Software used to downsize a compliance monitoring program (i.e., remove wells, analytes, or frequencies).
- Tests conducted with SITEWISETM monitoring module and results used to calculate the following using MS Excel:
 - Reduction in emissions
 - Energy and water usage
 - Waste generation
 - Accident risk over the program total life cycle
- Initial simulations conducted and data gaps identified.
- Review to determine factors which may significantly impact the 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



- Development of optimization strategies for integrated surface and GW models capable of predicting contaminant F & T within site domain to achieve the following:
 - Reduction of the number of monitoring locations
 - Improvement of the chemical injection strategy
 - Reduction of the quantity of chemicals used



FY13 Scope

- Benchmarking of current methodology using $SITEWISE^{TM}$.
- Implementation of a SITEWISETM module for sustainable analysis and optimization of monitoring programs.
- Calibration and Verification of SITEWISE TM monitoring program module.



Software developed and sponsored by:

- Battelle
- US Navy
- US Army Corps of Engineers (USACE)







- Pilot-scale sustainability evaluations to include EM's principle problem areas.
 - High-Level Waste, Soil & GW, Transuranic Waste, D & D, etc.
- FULLY coordinated with EM's Facility Engineering Program.
- Analysis based on input data supplied by user that is then translated through software-specific calculations into environmental impact and footprint.



Data Inputs

Materials:

 well materials, treatment chemicals, treatment media, construction materials, well decommissioning, and bulk material quantities.

Transportation:

 Personnel and equipment transportation by road, air or rail; type of fuel used, distance traveled, number of trips taken, etc.

Equipment:

 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.



Data Inputs cont'd

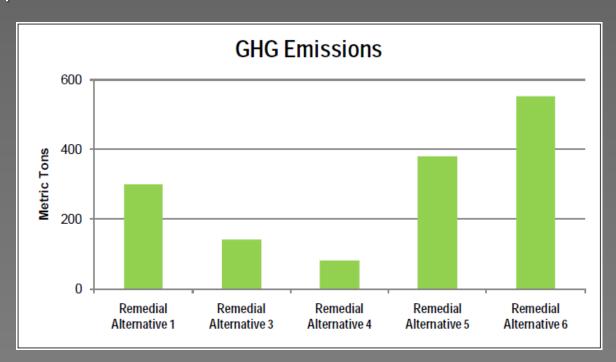
- Residual handling:
 - Residue disposal/recycling, landfill operations, thermal/catalytic oxidizers, Landfill operations, thermal/catalytic oxidizers.
- Resource consumption:
 - Water consumption, onsite land and water resource consumption.



Analysis

Tool will calculate and convert 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

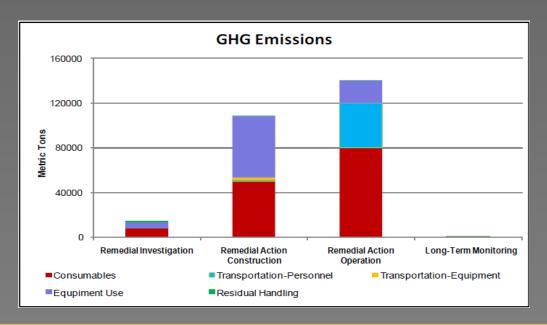




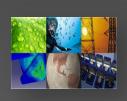


Analysis cont'd

SITEWISETM also gives detailed analysis of each remedial alternative so can identify activity with highest footprint for each metric.







Analysis cont'd

If alternative technologies for footprint reduction being used (wind, solar, renewable energy, and landfill gas microturbines), reduction subtracted from footprint produced to give net value.

Calculated environmental footprint will help support decision of appropriate remediation technology.



Analysis cont'd

Review was conducted which determined factors that may significantly impact the Green and Sustainable Remediation (GSR) metrics:

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



Analysis cont'd

SITEWISETM used with integrated surface & GW models to develop strategies for additional optimization such as:

- Reducing number of monitoring locations:
 - MAROS (Monitoring and Remediation Optimization System)
 - Geostatistical software
 - Provides strategy for formulating appropriate long-term GW monitoring programs to reduce costs.
 - Additional improvements can be provided by using numerical models to determine response of selected monitoring wells and eliminate redundant wells (i.e. wells with similar response).



Analysis cont'd

- 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.



Analysis cont'd

- Reducing 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.



Objectives

Develop geodatabase to support FIU's hydrological modeling work at ORR.

Benefits

- Centralized data management system facilitates storage, concurrent editing and import/export of data specific to hydrological models being used.
- Data Organized into 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.



Accomplishments

- Development of enterprise geodatabase to store, process and manage hydrological modeling data derived from FIU's work at ORR.
- Development of customized Python scripts to automate querying and geoprocessing of data and generation of maps and reports.
- Evaluation of free/open source GIS software and required security protocols for viewing, querying and sharing project-derived data with DOE & site contractors.





FY13 Scope

- Update existing EFPC geodatabase.
- Develop customized Python scripts to enhance database querying capabilities.
- Use existing geodatabase structure developed for EFPC modeling work at OR to create similar databases.





Existing geodatabase being updated with new data and being revised to update the following:

Spatial Data	Characteristics Represented
Admin_Features	EFPC, WOC, Y-12 & OSY Model domains (polygons)
	ORR Boundary
Admin_GRIDs	Model domains (GRIDs)
Conductivity_GRIDs	Hydraulic conductivity GRIDs
Contaminant_Conc_Features	Monitoring points (has associated timeseries attribute data)
Contaminant sources	Horizontal extent, upper level, lower level, strength
	Plume Contours
Contaminant_Conc_GRIDs	Interpolated contaminant plumes (GRIDs)
DEMs	Clinch River, EFPC & WOC Watershed DEMs
Digital_Orthophotos	ORR DOQs (.bmp)
Drainage_GRIDs	Drainage Time Constant, Drainage Codes, Detention Storage (GRIDs)
GW_Features	Groundwater level contours
GW_GRIDs	Groundwater level GRIDs
Grid codes for depth of plume	GRID code
Hydro Features	Watersheds, subwatersheds, catchments, hydroareas (lakes/ponds) (polygons)
	Floodplain polygons
	Hydrography, Hydrodrainage, hydrostructures (polylines)
Impervious_GRIDs	Paved runoff coefficient (GRID)
Landcover_Landuse_Features	Landuse/Landcover polygons
Landcover_Landuse_GRIDs	Vegetation grid codes
Manning	Manning's coefficients (GRIDs)
Monitoring_Stations	USGS SW monitoring stations, outfalls, GW monitoring wells
Network_Features	Rivers, streams, reaches, cross sections, diversion ditch, utilities (polylines)
	Nodes (points)
Physical_Features	Buildings, obscured areas, natural outlines, man-made outlines (polygons)
	Margins, man-made structures (polylines)
Soils	Geology, soils (polygons), profile definitions, van Genuchten parameters,
Topo_Features	Elevation contours
Transport_Features	Roads, railroads, transportation structures (polylines)
Water Quality Layers	Lower level, Dual porosity transfer coefficient, sorption processes, Linear kD, distribution Total mercury/Methyl mercury
Temporal Data	Characteristics Represented
Monthly_RF_TS	Monthly rainfall timeseries
Flow_Aug_TS	Flow augmentation timeseries
DHI_Timeseries	Flow rate/discharge timeseries



- Coordinating with ARC's IT team for publishing model data on the Web. (Project 4 – Task 5: Cyber Security Compliance and Deployment of Environmental Contamination and Remediation Models)
- Preparation for implementing secure protocols for data access is underway.
 - ArcGIS 10.2 deployed on server and currently researching requirements for deploying hydrological model results from server/PC onto secured KM-IT platform developed by FIU as part of Project 4, Task 4.
 - Users to register with KM-ITArcGIS platform for authentication and authorization to access data. This will secure the integrity of the sitespecific data considered sensitive to cyber compromise.
- ARC IT also worked on preliminary design for web interface for this feature (Figure 4-6).
- Benefits
 - Making the hydrological modeling results more easily assessable to the stakeholders.
 - Providing a secure platform from which to deploy the models.



Figure 4-6 Preliminary design for web interface for the environmental contamination and remediation model



Task 3.1: EFPC Model Update, Calibration, Uncertainty Analysis

- Subtask 3.1.1: Model update with additional reaction kinetics.
 - This subtask will focus on implementation of reaction kinetics for methylmercury species in the hydrological and transport model.
- Subtask 3.1.2: Update of EFPC data from OREIS, USGS, and other sources.
 - Timeseries; Spatial Data; Subsurface geologic conditions; Contamination data
- Subtask 3.1.3: Recalibration and validation of updated model.
 - Model adjustments to cover the new time period.
 - Conducting simulations for selected calibration and validation periods.
 - Statistical analysis of observed data and development of timeseries, probability exceedance curves, and probability distribution models of flow and concentration.
- Subtask 3.1.4: Web access to observed and computed data.



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

- Subtask 3.2.1: Simulation of the EFPC flow and transport.
 - Analysis of TMDL- and NPDES-regulated discharges using updated model.
- Subtask 3.2.2: Water quality assessment and TMDL target analysis.
 - Analysis of target loads for the TMDL analyses.
 - Calculation of daily loads for specified locations.
 - Analysis of flow exceedance from computed data along EFPC for entire watershed and selected stations with observed data.
 - Analysis of contaminant load exceedance and comparison with TMDL set criteria for selected stations along EFPC.
- Subtask 3.2.3: Investigation of additional contaminants of concern.
 - Continued work with ORR to determine opportunities where models can be utilized onsite.



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™.
 - Use of SITEWISE™ for benchmarking at EM field sites with pilot studies where cost benefit demonstrated.
- Subtask 3.3.2: Implementation of a SITEWISE[™] module for sustainable analysis and optimization of monitoring programs.
- Subtask 3.3.3: Calibration and verification of the SITEWISE™ 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.
- Subtask 3.3.4: Development of monitoring program module.
 - FIU will work with EM to create a monitoring program module using a GIS interface to improve data import, analysis, and visualization.
- Subtask 3.3.4: Benchmarking of monitoring program through incorporation of a module to:
 - Reducing the number of monitoring locations .
 - Improving the chemical injection strategy.
 - Reducing the quantity of chemicals used.
- Subtask 3.3.5: Web access to observed and computed data.



Task 3.4: Geodatabase Development for Hydrological Modeling Support

- Subtask 3.4.1: Update of existing EFPC geodatabase.
 - Recent OR site monitoring data from OREIS, USGS, NRCS STATSGO/SSURGO, U.S. EPA MRLC or NALC, etc.
- Subtask 3.4.2: Update of metadata.
- Subtask 3.4.3: Web access to observed and computed data.
 - FIU will take steps to publish project-derived hydrological model data on the web via the secured KM-IT platform.



Project Clients & Collaborators



