FINAL TECHNICAL REPORT

May 7, 2010 to August 28, 2015

Remediation and Treatment Technology Development and Support

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Principal Investigator:

Leonel E. Lagos, PhD, PMP®

Florida International University Collaborators:

Georgio Tachiev, PhD, PE
Angelique Lawrence, MS, GISP
Siamak Malek-Mohammadi, PhD
Amy Cook, MS
Yong Cai, PhD
Guangliang Liu, PhD
Yanbin Li, PhD
Himanshu Upadhyay, PhD, MBA, PMP, MCPD, MCITP
Justin Phillips, MCP
David Roelant, PhD
Ravi Gudavalli, PhD
Mehrnoosh Mahmoudi, PhD
Shimelis Setegn, PhD
Omar Abdul Aziz, PhD
FIU Graduate Research Assistants
DOE Fellows

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FIU Applied Research Center
Florida International University

FIU STUDENTS DIRECTLY SUPPORTING DOE EM PROJECTS

DOE Fellows from the DOE-FIU Science & Technology Workforce Development Program as well as FIU Graduate Research Assistants provide direct support to DOE EM projects around the complex. The following DOE Fellows and FIU Graduate Research Assistants supported the soil and groundwater research tasks for the Oak Ridge Reservation (ORR) and Savannah River Site (SRS) under FIU Project 3:

DOE Fellows: Michelle Embon, Steve Noel
Mentor: Himanshu Upadhyay
Project Task: Geodatabase Development for Hydrological Modeling Support (ORR)

DOE Fellows: Elsa Cabrejo, Heidi Henderson, Lillian Marrero
Mentor: Georgio Tachiev
Project Task: EFPC Model Update, Calibration and Uncertainty Analysis (ORR)

DOE Fellow: Kiara Pazan
Mentor: Ravi Gudavalli
Project Task: Modeling of the Migration and Distribution of Natural Organic Matter Injected into Subsurface Systems (SRS)

DOE Fellow: Natalia Duque
Mentor: Angelique Lawrence
Project Task: Surface Water Modeling of Tims Branch (SRS)

DOE Fellow: Yoel Rotterman
Mentor: David Roelant
Project Task: Sustainability Plan for the A/M Area Groundwater Remediation System (SRS)

FIU Graduate Research Assistant: Mandar Zope (MS)
Mentor: Georgio Tachiev
Project Task: Student Support for Modeling of Groundwater Flow and Transport at the DOE Site in Moab, Utah

FIU Graduate Research Assistant: Nantaporn Noosai (PhD)
Mentor: Georgio Tachiev
Project Task: Simulation of NPDES- And TMDL-Regulated Discharges from Non-Point Sources for the EFPC and Y-12 NSC (ORR)

Addendum:

This document represents one (1) of five (5) reports that comprise the Final Technical Reports for the period of May 18, 2014 to August 28, 2015 (FIU Year 5) 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. A summary of FIU Year 1 to FIU Year 4 (May 7, 2010 to May 17, 2014) is also included.

The complete set of FIU's Technical Reports for this reporting period includes the following documents and is 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-2015-800000393-04b-237

Project 2: Rapid Deployment of Engineered Solutions for Environmental Problems
Document number: FIU-ARC-2015-800000438-04b-228

Project 3: Remediation and Treatment Technology Development and Support
Document number: FIU-ARC-2015-800000439-04b-232

Project 4: Waste and D&D Engineering and Technology Development
Document number: FIU-ARC-2015-800000440-04b-229

Project 5: DOE-FIU Science & Technology Workforce Development Initiative
Document number: FIU-ARC-2015-800000394-04b-090

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). Integrated surface and subsurface flow, transport and fate models were developed to provide analysis of contaminant patterns within each watershed. In addition, digital monitoring data available from the Oak Ridge Environmental Information System (OREIS) and related to mercury (Hg) contamination and remediation within these watersheds was used for calibration and verification of the model. Experimental studies were also carried out which provided kinetic and equilibrium data about important parameters related to Hg transport, speciation and methylation/demethylation kinetics within the watershed. The modeling work has been supported by the use of geographic information systems (GIS) technology for 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, perform statistical analyses and generate 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 can be more easily shared with other project stakeholders such as DOE personnel and site contractors.

New scope was introduced in 2013 focused on development of EM pilot studies and the use of GSR sustainability software (e.g. SITEWISE™) to evaluate the benefit of Green Sustainable Remediation (GSR) practices; to 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 environmental impact, as well as to improve system design performance and efficiency. In 2014, FIU began working in collaboration with Savannah River National Laboratory (SRNL), utilizing and building upon the capabilities developed under Project 3 in the area of soil and groundwater remediation and treatment technology to apply these approaches to similar environmental challenges at the Savannah River Site. The new tasks are synergistic with the work SRNL is performing and have involved: 1) Modeling of the migration and distribution of natural organic matter injected into subsurface systems to support environmental remediation; 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.

TECHNICAL PROGRESS FROM FIU YEAR 1 TO FIU YEAR 4

FIU-ARC has provided technical assistance and performed research on mercury remediation at the Oak Ridge site. The objective of this project was to support the remediation efforts at the Oak Ridge site by providing a better understanding of the fate and transport of inorganic and organic pollutants of concern with a focus on mercury. The project has involved numerical modeling of fate and transport of contaminants in the surface domain (rivers and overland flow) and saturated/unsaturated groundwater zones. The project also involved kinetic and equilibrium studies of the behavior of mercury under environmental conditions, which are relevant to the East Fork Poplar Creek (EFPC) watershed. Research efforts were executed in collaboration with DOE EM and DOE ORO. Student support for research at the Moab Site was also provided, which included collecting samples at the site and performing simulations with the existing groundwater transport model of the Moab site.

During 2008-2010, FIU developed integrated flow and contaminant transport models of the East Fork Poplar Creek (EFPC) and White Oak Creek (WOC) watersheds. The models were used to conduct numerical simulations of flow and transport of mercury and organics within the watersheds. In addition, experimental studies were conducted to provide more accurate information with respect to significant parameters related to mercury transport and speciation (e.g., kinetics of methylation/demethylation within the watershed). Development of GIS-based hydrological and transport models requires large amounts of data; therefore a geodatabase was developed as a strategy for supporting hydrological model data input by creating a centralized data storage system to store model parameters. The database extends the capabilities of the GIS data and allows for automating time consuming GIS processing for water resources applications. During **FY10-FY11 (FIU Years 1-2)**, the focus was on extending the sedimentation module to include the entire EFPC and Bear Creek. This research provided stochastic modeling of the system and included an analysis of the spatial and temporal patterns as a result of the stochastic variations of selected properties of the sub domain. In **FY12 (FIU Year 3)** FIU continued using the numerical model of EFPC to determine the impact of remediation alternatives on the complete hydrologic cycle, the transport overland and in surface water and rivers, sediment transport and reactions, and mercury exchange with sediments. The research was coordinated with the site and ORNL personnel. For **FY 13 (FIU Year 4)**, FIU built upon the previously developed models to analyze flow, fate and transport of site contamination and remedial activities at the Oak Ridge site which 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. In addition, the capabilities of the geodatabase developed for centralized storage and management of experimental and computed model data were extended using ArcGIS ModelBuilder and Python scripting to automate querying and geoprocessing of data for statistical analysis 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 can be more easily shared with other project stakeholders such as DOE personnel and ORR site contractors. FIU also added new scope in **FIU Year 4**, focused on EM pilot studies and the use of SITEWISE™

sustainability software 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.

EFPC MODEL UPDATE, CALIBRATION AND UNCERTAINTY ANALYSIS

The main objectives of this task were to extend the existing EFPC model by adding sedimentation and reactive transport modules, and to use the model to perform numerical simulations that are relevant for the NPDES and TMDL regulations. The simulations provide a better understanding of the flow and transport within the watershed on a regional scale. Simulations were conducted using historic observations of rainfall, evapotranspiration, and contaminant distribution within the watershed to determine transport patterns within the domain. During FY11, the focus was on extending the sedimentation module to include the entire EFPC and Bear Creek. This research has also provided stochastic modeling of the system and has included an analysis of the spatial and temporal patterns as a result of the stochastic variations of selected properties of the sub domain. In FY12 FIU continued using the numerical model of EFPC to determine the impact of remediation alternatives on the complete hydrologic cycle, the transport overland and in surface water and rivers, sediment transport and reactions, and mercury exchange with sediments. The research was coordinated with the site and ORNL personnel.

- In **FY10 (FIU Year 1)**, the EFPC model was applied to simulate groundwater flow and the fate and transport of mercury, tetrachloroethene (PCE), 1,2-dichloroethene (1,2-DCE), *cis*-1,2-dichloroethene (*cis*-1,2-DCE), and vinyl chloride (VC) in groundwater that have originated upstream of UEFPC from the Old Salvage Yard (OSY) of the Y-12 NSC. The model was calibrated using subsurface flow and concentration records extracted from the OREIS database. The simulation results were used to calculate the revised risk levels (RLR) for the chemicals of concern (COCs) and serves as a benchmark for comparison with the modeling previously performed by McLane Environmental using the SESOIL-AT123D model. Simulation results have been presented to DOE by Pro2Serve (P2S) through several PowerPoint presentations and a report was submitted to DOE including details of the simulations, input parameters and results. In addition, the report entitled, "Integrated Surface and Subsurface Mercury Transport Model of Y-12 National Security Complex, Oak Ridge, Tennessee," which provides details on development of the EFPC model, was modified and resubmitted based on comments provided by DOE reviewers. This report included: (i) Development of the hydrological model of EFPC and Y-12 NSC; (ii) Development of the sedimentation module for Y-12 NSC; and (iii) Numerical simulations of remediation activities related to changes in watershed hydrology.
- In **FY 11 (FIU Year 2),** for the subtask "*Extension of the water quality and sedimentation module",* the sedimentation module which was developed for the UEFPC (the section of EFPC upstream of Station 17) was extended to include the entire EFPC down to EFK 6.4 and Bear Creek. The sedimentation module provides the coupling between the flow and transport within the creek and the overland flow used to analyze the significance of floodplain contamination downstream EFPC. Fifty-two (52) outfalls were added to the EFPC model. Van Genuchten parameters for the unsaturated flow in the aquifer were also updated. The model was reconfigured following the incorporation of the sedimentation

module and outfalls. A series of numerical simulations have been performed using a range of Manning's number values, threshold run-off water depths, and drainage coefficients to calibrate the flow for the period of 2000 – 2008.

- MATLAB scripts were prepared for the statistical analysis of observed and computed data. Laboratory and field data on surface water level and discharge, groundwater level, and mercury contamination in soil, groundwater and surface water were obtained from OREIS database. Data was organized and incorporated into the numerical model for calibration and verification purposes.
- A progress report was drafted and submitted on 11/17/2011, outlining the incorporation of the sedimentation module, assignment of specific parameters, description of the methodology for the download, organization and analysis of field and laboratory data from OREIS database, and incorporation into the numerical model.
- For subtask *"EFPC model uncertainty and sensitivity analysis",* the probabilistic distribution of critical subsurface parameters, such as hydraulic conductivity, porosity, pore size distribution, and storage coefficients were defined specifically for the karst areas. MATLAB's statistical toolbox and scripting tools were used to develop a series of functions for a random generation of distributed hydrologic parameters based on a selected probability density function and statistical parameters. Randomly generated grids were created using the MATLAB toolbox for the uncertainty analysis. Numerical simulations were conducted for each randomly generated input grid. The output was used to generate daily timeseries for selected hydrological, fate and transport parameters, including groundwater flow velocity at selected points, potential head at selected points, rate of mercury absorption at various locations, concentrations of total mercury at the key stations (EFK 6, EFK 14, EFK 18), total mercury load at the key stations, flux exchange between subsurface and surface. The simulations were used to determine the model uncertainty in terms of stochastic variations of input parameters. Graphical plots of the variation of the output parameters were then used to present the results of the sensitivity analysis, identifying significant parameters and a range of certainty for the model.
- In **FY 12 (FIU Year 3),** a literature review was conducted related to various mercury transformation processes in the environment and also on the concept of stochastic analysis and probability distributions in an effort to further understand the analytical approach taken in analyzing model simulation results and observed data. A review of available and updated mercury data was also conducted and incorporated into the existing model. Transects with known mercury data were also developed.
- Completed student internship involving research techniques related to these tasks such as standard procedures for performing remedial work, as well as concepts such as data quality verification, GIS mapping and familiarization with instrumentation for sampling and testing for U.S. EPA compliance, was completed with DOE contractor Sullivan International Group, Inc. in Chicago, IL, and a presentation and report submitted for review. The knowledge gained from this experience is being applied to assist in execution of these tasks. A poster was created entitled "An Evaluation of Volatile Organic Compound Contamination at Two Superfund Sites", which details the procedures and findings of the 2012 summer internship of which data quality assurance and quality control (QA/QC) along with data management processes can be directly applied to the development of timeseries.

- The EFPC Model settings were evaluated and further modified to decrease simulation time and test simulations were performed.
- Presented conference paper at the 9th International Symposium on Persistent Toxic Substances held at the Miami Airport Marriott on October 26, entitled "Hydrologic and Kinetic Parameters Impacting the Total Mercury Transport within the EFPC Watershed, Oak Ridge Reservation". Announcement of the conference paper will be submitted to OSTI.
- Added groundwater monitoring wells to the model along EFPC, and determined the model's performance along a set of transects beside EFPC.
- Developed MATLAB scripts to extract observed and computed data and provide statistical analysis for model performance. MATLAB scripts were also developed for reading and extracting concentration data along EFPC.
- Executed several simulations and evaluated results for flow and depth to phreatic surface. Concluded that well timeseries need to be updated to include more observation points if possible. Calibration is needed for the groundwater wells with recorded values of depth to phreatic surface. Observation stations show a captured base flow but inconsistency in capturing peak flows. A contributing factor may be the drainage within this area. This will be explored by comparing locations relative to known outfalls or drainage structures to determine which model changes or updates would be adequate.
- Repeated a 10 year simulation (1996 – 2006) which originally failed, then implemented a series of corrective actions (i.e. resolved cross section errors and modified boundary conditions). There was a failure at 62.1% of simulation, near the end of the river network, so specific cross-sections were expanded to increase water flow in that portion of the watershed and eliminate error No. 25. These changes were successful in reducing the numerical instabilities, so water movement simulations were completed for the full 10 year period.
- Repeated water quality simulation which originally failed because boundary conditions included 6 concentration components for Ecolab. Concentration components were removed, leaving only 1, however simulation duration estimate excessively high, so currently reviewing to determine which module is slowing down the simulation (MIKE SHE or MIKE 11).
- A Master's thesis was drafted which relates to the work being conducted under this task.
- For the subtask *"Surface Water Flow and Contaminant Transport Model using XPSWMM",* preliminary research was carried out during an on-site student internship in collaboration with Eric Pierce at ORNL, to develop a replica of the storm water management system of ORNL's Outfall 211 and its contributing drainage areas using XPSWMM modeling software in order to assess flood risks. Based on availability of data, modifications to the work scope were made to incorporate:
    - Flood risk analysis of the following storm events:
        - 25 year – 24 hour
        - 100 year – 24 hour
        - 500 year – 24 hour
    - Probability of exceedance analysis of outfalls within the domain
    - Probability distribution function analysis of outfalls within the domain
- Preliminary research revealed that very limited amount of data was available for this area. TDS data was available at Outfall 211 but not within the system. Also, a few chlorine

measurements were available within the system that was used as a tracer for this model. A very rudimentary estimate of flow rates leaving the buildings via storm drains was provided by ORNL Engineering for some of the buildings.

- Copies of construction drawings of the area of interest which include buildings 4500N, 4500S, 4501, 4505, 4507, 4508 and 4556 were provided by ORNL engineering personnel. As these buildings were built at different times and stages, it was necessary to conduct an in-depth review of the construction drawings provided to determine how much of the drainage system is still located underground at this time.
- Reviewed a 'sink and drain' survey and floor plans via ORNL website in order to compare the number and locations of the storm drains leaving the buildings. Received shapefiles for the area and inserted them into XPSWMM. ArcGIS was used to convert the contours into an xyz file to view the DTM in XPSWMM.
- Developed a water balance model of the areas contributing to Outfall 211 using TSS as a tracer. Issues/Assumptions:
    - 'New' ATLAS drawings have inconsistencies.
        - Inlet to the west of MH211-3 is not shown on the drawing
        - Inlet east of 4500N Wing 1 is shown on the left of the centerline (should be on the right per field reviews)
        - Inlets east of 4500N Wing 2 are either not shown or have no symbol
        - East storm drain believed to end just east of the MH near 4500N Wing 3 (indicated by old drawings seen from Elizabeth Wright via MapInfo)
    - ArcGIS storm drain files do not contain correct elevation attribute tables.
    - Some inverts, manhole, and inlet elevations are unknown. Will make reasonable assumptions from surrounding or similar data.
    - Assumptions will be made for the building area contributing to the roof drains.
    - A single lateral for each building (possibly 2 if needed) will be shown in places where there are multiple storm laterals/roof drains because there is an overwhelming amount to begin with. There will be as a constant 2 gpm/lateral for condensate and/or cooling water discharging into the system. The 2 gpm/lateral is an estimate provided by the ORNL Engineering Department.
- Drew profiles for the 53 link – 52 node network. Input node parameters into the model: Ground elevation (spill crest elevation); Invert elevation. Input link parameters into the model: Diameter; Length; Slope; Manning's roughness coefficient. Refined the XPSWMM stormwater model by the following revisions: input user inflow for AC units; input stage-stage for Boundary Condition; input infiltration parameters (Horton's equation); revised Outfall 211 node by adding a storage area held back by a weir prior to its discharge via an orifice.
- Completed a Technical Report of the internship at ORNL outlining the research conducted for this subtask.
- A Master's thesis is being developed based on the research being carried out for this task and a first draft has been written and submitted for review. An extended thesis proposal was presented and approved by the graduate committee.
- Conducted preliminary calibration of model for steady uniform flow using constant rainfall intensity and currently checking it via mass balance equations. Provided analysis of the water balance for each catchment. Determined the response of the model for a set of

Manning's parameters to simulate the uncertainty in pipe condition, provided comparative runs for one year and determined the probability exceedances for each flow event.

- Conducted preliminary calibration of model for unsteady non-uniform flow where the rainfall intensity varies with time.
    - Data for Outfall 211 is scarce. There is no timeseries information available for Outfall 211; however, there were a few samples (flow rates measured once per day) made available for calibration of the model.
    - The sample taken on May 12, 2009 was chosen for this preliminary calibration where the precipitation for May 11, 2009 and May 12, 2009 was retrieved from the ORNL website. Precipitation near Outfall 211 is monitored by ORNL's Tower C.
    - Obtained 60 min, and 24 hour precipitation data from ORNL's website, generated several models for selected periods of time, and developed inputs for yearly simulations using 60 minute time intervals, and simulations for 1999-2012 using 24 hour time intervals.
- Conducted sensitivity analysis by running multiple simulations of monthly rainfall varying the Manning's n coefficient (0.011-0.017). Refined the model and ran yearly simulations varying Manning's n coefficient and infiltration parameters. The first analysis was for the Manning's coefficient variations (0.011-0.017, 0.035). Pipe 26 (P-26), the last pipe prior to discharging via Outfall 211 (OF-211), was analyzed for comparison. A probability exceedance (PE) curve indicated there were minute variations. Manning's coefficient of 0.014 and the evaporation default of 0.1"/day were held constant for the simulations. The second sensitivity analysis was conducted for various infiltration methods: Green Ampt, Horton, and Uniform Loss.
- A study of contaminant transport within the ORNL area was conducted using the XPSWMM model. The model was run based on the following assumptions:
    - No loss in the system (i.e. infiltration, evaporation).
    - Tracer is conservative.
    - The conservative tracer is added at nodes B-4501 and I-10.1 with constant concentration and flow of 1 mg/L and 0.1 cfs respectively.
    - 1 year rainfall with 15 minute intervals.
- These assumptions (1 & 2) were made so that the model's mass balance could be checked or calculated and easily compared to the analytical calculations. The model produced identical results to the analytical calculation results for both tracer mass loading and concentration. This indicates that the model has the capability and potential to be used to study contaminant transport.
- Currently, the model is being calibrated by comparing OF-211 data provided by ORNL. This is being conducted by simulating actual rainfall data from Tower C through the XPSWMM model and comparing the 5-minute intervals time series data provided by ORNL at OF-211 and 5-minute interval time series XPSWMM results.
- Two progress reports have been provided to DOE Headquarters, DOE ORO and ORNL personnel related to this subtask, the first providing information related to the XPSWMM model's preliminary configuration parameters (Milestone 2012-P3-M1.1 submitted 9/14/12) and the second providing preliminary simulation results (Milestone 2012-P3-M1.2 submitted 11/16/12).

- For subtask *"Surface Water Flow and Contaminant Transport Model of Y-12 NSC",* a one-dimensional surface water model of the Y-12 NSC was created using XPSWMM. This test model consists of:
    - Runoff mode (70 sub-catchments and 70 nodes).
    - Hydraulics mode (298 nodes and 311 links).
- Much of the data for this study area is currently unavailable due to security restrictions, therefore parameters used in this test model (rainfall data, location and elevation of nodes and pipes, etc.) were assumed. Infiltration was calculated using the Horton method. An imported GIS file was used to locate the outfall locations of Y-12. All the flows were linked to these outfalls. The test model was run for a 24-hr period and the flow at each outfall and pipe generated.
- A draft report of work conducted to date was prepared and serves as a working document which will be continuously updated as data becomes available and results are generated throughout the project period.
- Sub-catchments and pipes were adjusted. Divisions of sub-catchments were made with respect to land use (parking lot, building, irrigation, etc).
- Imported the Global Database (rainfall SCS type I, II, and III and applied the global storm, rainfall SCS type II, into the model. The test model was run a for 24-hr period. The "Dynamic Plan View" was used to examine the flooding nodes or the point that the water lost from the system.
- Used the design tool to calculate the pipe sizes then simulated the model again (with dynamic plan view) to make sure that all the nodes are not getting flooded. Thus, the final designate pipes can carry the flow without flooding.
- The test model (small portion of Y-12 NSC) was run with the following model conditions:
    - Rainfall data of Y-12 was replaced with SCS data (1 month).
    - The IDF data and IDF table were created and input into the model.
        - Some data was not available and had to be assumed.
        - Assumptions include 25-yr, 50-yr and 100-yr return periods.
    - The site elevation was exported from GIS in the form of contours.
    - Sub-catchments were adjusted according to land uses.
    - Node and pipe elevations were adjusted according to the GIS contours.
    - The model was run with a 1 month, 5 year return period.
        - Flow results are being analyzed.
        - Dynamic Plan View was used to examine the flooding nodes or the points at which water was lost from the system.
        - The design tool was used to calculate the pipe sizes then simulated in the model again to make sure that all the nodes were not getting flooded. Thus, the final designate pipes can carry the flow without flooding.
- The Y-12 model was expanded to cover more area of the site. The model was run with the following model conditions:
    - The steady state rainfall was input to test the accuracy of the flow hyetograph.
        - The flow hyetograph output corresponding to the steady state rainfall results were examined.
    - Model was run with 1 year (2009) rainfall data.
        - Dynamic Plan View was used to examine the flooding nodes or the point that the water was lost from the system.

  - The design tool was used to calculate the pipe sizes then simulated in the model again to ensure that all the nodes were not being flooded. Thus, the final designate pipes will be able to carry the flow without flooding.
- The study conducted in Subtask 1.3a was carried out to determine the XPSWMM model's capability and potential to be used to study contaminant transport in the ORNL area. Based on the successful results obtained, the same process is being duplicated for the Y-12 NSC.
- In **FY13 (FIU Year 4)**, FIU conducted a review of the existing Hg thermodynamic database and update for EFPC environmental conditions. 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+} investigated. A mercury thermodynamic database relevant to EFPC environmental conditions was developed and incorporated into the integrated 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.
- FIU also integrated the Hg thermodynamic database into the existing EFPC model. The integrated model derived from this task is intended to have improved capability to simulate the exchange of Hg between the creek and river, the distribution of mercury species within pore water, sorbed mercury within pores, sorbed mercury on suspended particles and "free" mercury (dissolved and chelated mercury species). Hydrological and geochemical methods and tools that can be utilized for the analysis of different remediation scenarios were explored to determine the best remediation methods. Geochemical conditions (presence of naturally occurring strong chelating agents) were varied to determine the changes of reaction kinetics and equilibrium.
- A series of simulations using the EFPC model and the thermodynamic and kinetic interactions were conducted. This task provided improved estimates for the stochastic nature of mercury fluxes within the EFPC domain. Simulations were performed to provide statistical analysis of observed data and development of timeseries, probability exceedance curves, and probability distribution models of flow, concentration and load data that integrate existing downloaded data with new data as it becomes available. Groundwater well monitoring data, concentrations in groundwater wells, outfall flow, and concentration and load data were also utilized. Simulation results were then analyzed and included in a report.

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

This task involves the use of the numerical model developed for the EFPC to simulate fate and transport of mercury, conservative tracers and VOC plumes within the EFPC watershed, to assist in analyzing the NPDES and TMDL requirements for surface water and groundwater within the EFPC watershed.

- During **FY 10 (FIU Year 1)**, a report entitled, "Mercury Interactions with Suspended Solids in the Upper East Fork Poplar Creek, Oak Ridge, TN" was prepared based on the developed model and recently extended water quality module. The report includes details of the water quality modeling in the UEFPC watershed, model calibration, uncertainty analysis, and sensitivity analysis. A graduate student thesis was completed based on the modeling work conducted. Furthermore, a scientific article entitled, "Simulation of Flow and Mercury Transport in UEFPC, Oak Ridge, TN" and a poster entitled, "Numerical Simulation of Mercury Fate and Transport in Upper East Fork Poplar Creek, Oak Ridge, TN", were presented in the poster session of the Waste Management Symposium 2011 in Phoenix, AZ. The poster was awarded best professional poster presentation by the American Nuclear Society (ANS), as well as best poster in the environmental remediation track.

- During **FY 11 (FIU Year 2)**, for the subtask entitled *"Update the database",* field and laboratory data pertaining to water quantity (surface and groundwater levels, and water flow) and water quality (i.e. temporal and spatial distribution of pollutant sources in soil, water, and sediments, bioassessment) were extracted from the OREIS database. Excel spreadsheets were developed and the data categorized based on media type (i.e., soil, surface water, sediment, and groundwater). Previously submitted reports were then updated with the newly extracted data for 2010 and 2011. The data was analyzed to identify any data gaps and additional data needs and monitoring recommendations. Spatial analysis was performed to identify spatial variations of mercury in EFPC water, in shallow and deep soil layers, and in stream bank and streambed sediments. Temporal analysis was performed to evaluate the timing of impairment and potential source loading or other conditions contributing to impairment. Specifically, the effect of rainfall and runoff flow was investigated on the concentration of mercury in the creek. The effect of rainfall/runoff and high flow conditions were investigated on the sediment transport, and thereby, mercury transport in the creek.
- For subtask *"Review and analysis of NPDES and TMDL requirements (literature review)",* a comprehensive review was conducted on NPDES and TMDL requirements for EFPC established by EPA and Tennessee Department of Environment and Conservation (TDEC). A report was developed which includes water quality criteria and TMDL target, water quality assessment and deviation from the TMDL target, water quality data analysis, and source identification.
- Water quality data analysis has been completed including temporal and spatial variations of data points, seasonal analysis of data points, and removal of data outliers and anomalies using methods suggested by the EPA.
- For subtask *"NPDES and TMDL analysis of UEFPC",* target mercury concentration for the EFPC was determined based on TDEC regulations for surface waters. The target concentration was determined to be 51 ppt for recreational use. Based on this target concentration, a "Loading Capacity" duration curve was developed.
- The flow and concentration timeseries associated with NPDES outfalls were revisited. Load and flow duration curves were developed for the outfalls and compared with simulation results. Flow duration curves were developed for two key stations along EFPC (EFK 23.4 and EFK 6.3). Flow duration intervals and zones were determined to study the effect of flow conditions on the distribution of impairments. Impairments observed in the low flow zones (dry seasons) were indicated as the influence of point sources (outfalls), while sediments (non-point sources) were determined to be effective during high flow conditions (wet seasons).

- Load duration curves were developed for key stations. A series of numerical simulations were performed to determine the percentages of the load associated with outfalls, sediments, and overland flow (load allocation analysis). Based on the numerical simulation results, waste load allocations (WLAs) were developed for continuous point source discharges using the duration curves. In the case of sediments, specific simulations were performed only with contaminant sources inside the sediments to determine the contribution of sediments to the total load observed in the creek. Load duration curves and load percentiles were developed for each source (i.e., outfalls, sediments and overland wash-off).
- A technical report entitled, "Simulation of TMDL for the Entire EFPC," which includes information on NPDES and TMDL target definition, as well as development of flow and load duration curves and load allocation analysis, was compiled and submitted in February 2012.
- For **FY12 (FIU Year 3)** the objectives of this study were met through the successful integration of the ECO Lab module to enhance the simulation of mercury transport and in the demonstration of the application of the model to the mercury TMDL analysis for the project site in the EFPC watershed.
- Modeling software MIKE SHE, MIKE 11, and ECO Lab were thus combined in a comprehensive package that simulates the flow and transport of mercury in exchange with sediment. The application of the enhanced models includes an analysis of spatial and temporal patterns stimulated by variations of selected properties of the sub domain. The impact of sedimentation on the fate of mercury was assessed through a series of simulations and using the sedimentation layer module (ECO Lab); this module addresses the dissolved mercury in the water, the adsorbed mercury concentration on suspended matter, the dissolved mercury in sediment pore water, and the adsorbed mercury in the sediment.
- In the application of the model to the EFPC watershed, previous modeling efforts, which originally included only the upper portions of EFPC, were extended to include the entire EFPC, down to station EFK 6.4 and the BC. The model is capable of simulating the entire hydrological cycle. Water quality, transport, and sediment related parameters were updated based on DOE experimental reports and journal publications to include observed data of flow, stage, and mercury concentrations in soil, surface water, groundwater and sediments at Station 17 as well as the stations previously mentioned.
- Simulations were executed for a range of input parameters to correlate stochastic hydrologic events with mercury distribution patterns and total suspended solid pattern at Station 17. The simulations were analyzed using a range of techniques, primarily comparative schematics of time-series plots, probability exceedance curves, and load duration curves. The modeling was intended to aid in the development of flow duration curves and mercury loads probability exceedances for selected stations where applicable.
- Based on the patterns exhibited throughout various observed and computed probability exceedance curves for flow and mercury, it can be concluded that the model most accurately simulates discharges and mercury loading conditions under high, moist, and mid-range flows. Although mercury loads appear to be attenuated downstream EFPC the same cannot be concluded of BC as it exhibits no significance difference in mercury loading upstream and downstream. Furthermore, results also show that the majority of the mercury in the creek is in the adsorbed form; accentuating the importance of suspended

particles and its direct connection to the total mercury concentration in the creek. Even though mercury concentrations during high flood events decreases due to dilution; post hydrological events, the mercury concentration levels are restored. Standard mercury loads probability exceedances were developed based on established limits for the site and a 90.24% reduction in loading appears to be required at Station 17.

- The model is intended to serve as a useful remediation tool since the site was characterized using relevant historical records for precipitation, groundwater levels, and river discharges obtained from OREIS and ORNL databases, which were incorporated into the model in the form of boundary or calibration conditions. The incorporation of the ECO Lab module should better characterize the mercury processes in the EFPC environment since mercury species are known to diffuse from contaminated sediment pore water to creek water in the form of diffusive transport.
- Recommendations were made to improve the study in several aspects. For instance, since the study is performed at a watershed scale it might be beneficial to consider the development and implementation of site-specific modeling applications to smaller areas at contaminated buildings and pipes. A more thorough understanding and modeling of the connections between concentrations of inorganic mercury precursors and methylmercury concentration is also needed to better predict future trends of mercury transport at the site. In the thesis research related to this task, the EPA water quality limits previously mentioned and based on water usage classification were used to establish a comparison between simulated and recorded mercury loading. An additional recommendation to improve the understanding of the EFPC system is to more specifically apply the model to understand the bioavailability and bioaccumulation in fish in order to establish a more direct connection between water quality and the DOE ROD set fish tissue concentration value of 0.3 milligrams methylmercury per kilogram of wet-weight fish tissue for the site.
- In **FY13 (FIU Year 4)** data for all 57 outfalls along the creek was obtained from OREIS. The data includes the period until 2013. The data was converted from Excel into a data format (required by the XPSWMM numerical model) which will be implemented in the surface model.
- The model updated the boundary conditions in order to extend simulations to 2012. Boundary conditions include rainfall, evapotranspiration, and timeseries of outfalls, rivers and canals. A new set of subsurface groundwater table boundary conditions were developed.
- 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”.
- Several target load-duration curves were developed for EFPC by applying the mercury target concentration of 51, 200, and 770 ppt to each ranked flow 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.
- The model was used with the newly developed ECO Lab template which incorporates methylmercury into the set of kinetic and thermodynamic equations. Several initial simulations were completed during this period and the results are in process of being reviewed.

PARAMETERIZATION OF MAJOR TRANSPORT PROCESSES OF MERCURY SPECIES

The overall objective of this task is to provide laboratory investigation of critical mercury transport, transformation, and exchange processes (i.e., methylation/demethylation, and dissolution) to be used in the numerical flow, transport and chemical reaction model. The laboratory experimental work provides insight on parameters relevant to the Oak Ridge Reservation (ORR) and which are required in the numerical model, such as dissolution rate of mercury and the proportion of mercury species available for methylation/demethylation in sediments. In addition, experimental work will aid in the analysis of the effect of significant environmental factors (pH, Eh, sunlight) on the major transport and transformation processes of Hg.

- In **FY10 (FIU Year 1**), this task originally entitled *"Laboratory Experiments for Methylation/Demethylation and Transport Parameters of Mercury"*, involved experimental work to determine the effect of various environmental factors (pH, Eh, DOC) on methylation/demethylation processes. The analyses were extended to provide information about biogeochemical processes and the sources and cycling of nutrients, sulfur, and organics in the ecosystem to examine the complex involvement of nutrients, organics, and inorganic species (including sulfur) in methylmercury production and bioaccumulation. A major focus was on ecosystem responses to variations in contaminant loading (changes in external and internal loading in time and space), and how imminent ecosystem restoration may affect existing contaminant pools. Laboratory results were published in the scientific journal, Environmental Science and Technology, in a paper entitled "Degradation of Methylmercury and Its Effects on Mercury Distribution and Cycling in the Florida Everglades". By implementing stable isotope addition experiments, MeHg photodemethylation rates in three selected ecosystems were measured: soil sediments from East Fork Poplar Creek (EFPC), surface water and sediments from Florida Everglades (FE), and seawater from Biscayne Bay (BB). The results indicate that MeHg demethylation rates varied in these three ecosystems, in the order of EFPC >BB > FE. The rate of MeHg photodemethylation in EFPC was found to be around twice of that in BB, and three times of that in FE. Experiments are being conducted to identify factors resulting in the variety of photodemethylation rates in different ecosystems. Primary pathways of MeHg demethylation and effects of sunlight spectra on MeHg photodemethylation were also investigated. It was found that MeHg is primarily degraded by sunlight, and that UV-A and UV-B radiations are the principle driver. Degradation of MeHg was not observed in the dark. Removing microorganisms had no significant effect on the degradation of MeHg. UV-B, UV-A, and visible light were calculated to account for 15, 85, and 0% of MeHg photodemethylation in surface water, respectively. In addition, further studies are being conducted to identify the processes that result in the photodegradation of MeHg in natural water. Laboratory double-spiked isotope ($^{199}Hg^{2+}$, $Me^{201}Hg$) addition experiments were carried out to investigate the methylation and demethylation of mercury in various matrices (sediment, water, floc (flocculent materials on top of soil), and periphyton). Both methylation and demethylation of Hg in natural surface water were found to be mediated by sunlight. High photodemethylation rate (9.45×10^{-3} E^{-1} m^2) and low photomethylation rate (3.90×10^{-6} E^{-1} m^2) were observed in natural water, indicating the importance of photodemethylation in decreasing the concentration of MeHg in water. Significant methylation of spiked $^{199}Hg^{2+}$ (0.007-0.074 d^{-1}, average 0.030 d^{-1}) was observed in all of the studied soil samples. Rate of Hg methylation in floc was similar to that in sediment (0.029 d^{-1}), while a slower rate was observed in periphyton (0.010 d^{-1}). Significant demethylation of MeHg was also detected in sediment, floc, and periphyton. Demethylation of MeHg was rapidest in floc (0.196 d^{-1}), followed by periphyton (0.089 d^{-1}) and sediment (0.056 d^{-1}). Finally, multiple linear regression analysis was employed to identify the major factors controlling the distribution of MeHg in water. The results indicate that methylation of Hg^{2+}, photodemethylation of MeHg, and concentration of THg in water are the major factors controlling the distribution of MeHg in water.

- During **FY11 (FIU Year 2)** Dr. Yong Cai visited ORR to present his research and to coordinate plans for the next year. A detailed Technical Task Plan (TTP) for FY 2011-2012 was then prepared for the project and submitted to DOE for review. A technical report entitled, "Parameterization of Major Transport Processes of Mercury Species," was also submitted.
- For subtask *"Photomethylation of Hg^{2+} in Natural Water",* the double isotope addition technique ($^{199}Hg^{2+}$ and $Me^{201}Hg$) was applied to measure the photomethylation of Hg^{2+} in water. A new model was developed to calculate the methylation rate constant of the spiked Hg^{2+} in water. This model corrected for the defect of previous models, in which the degradation of ambient MeHg and the newly produced MeHg was not taken into account. Methylation of Hg^{2+} was observed in natural water, with a rate of 1.14±0.02 ($\times10^{-4}$ d^{-1}). This process is mediated by sunlight. However, its rate was much slower than that of MeHg photodemethylation (kd=0.26±0.04 d^{-1}), indicating that methylation in water plays a minor role in the cycling of MeHg. In addition, the contributions of the photodemethylation of ambient and newly produced $Me^{199}Hg$ were proven not to be negligible for the variation of $Me^{199}Hg$.
- Subtask *"Estimation of the Bioavailability of Hg^{2+} and Methylmercury for Methylation and Demethylation in Natural Sediment":* The difference between the ambient and newly input Hg species in methylation/demethylation efficiency was often neglected in the previous models which may have caused a significant error. Here, we developed a method to calculate the bioavailability of Hg^{2+} and methylmercury for methylation and demethylation in natural sediment using double stable isotope ($^{199}Hg^{2+}$ and $Me^{201}Hg$) addition experiments. The percentage of bioavailable Hg^{2+} and MeHg for methylation/demethylation (x_α and x_β) was estimated to be 0.02-0.06 and 0.71-0.93, separately in studied sediments, indicating that there is a significant difference between the ambient and newly input Hg species in methylation/demethylation efficiency. The difference in methylation/demethylation efficiency of the ambient and newly input Hg

species must be taken into account when net MeHg production (or degradation) rates are estimated. If α andβ were not considered, the estimated net production (or degradation) rate of MeHg in sediment could be overestimated by a factor of 20.

- Subtask *"Effect of Thiol-Containing Compounds on Cinnabar Dissolution":* Thiol-containing compounds could significantly promote the dissolution of cinnabar. In the absence of thiol-containing compounds, Hg^{2+} concentration in water was at the level of ~1-2 μg/L. The addition of 10 μmol/L L-cysteine increased it to more than 100 μg/L. Glutathione could also increase the dissolution of cinnabar. However, its effect was much smaller compared to cysteine, suggesting that the effect of thiol varies in different thiol species. In addition, oxygen plays a significant role in the dissolution of cinnabar. The concentration of Hg^{2+} in the aqueous phase was in the order of saturated oxygen > air > anaerobic. A model based on chemical thermodynamics was developed to calculate the dissolution of cinnabar under different conditions and elucidate the relative importance of pH, O_2 and thiol-containing compounds in cinnabar dissolution. By taking into consideration the adsorption of released Hg^{2+} on cinnabar, the proposed model could well predict the dissolution of cinnabar with or without cysteine. Both model and experimental results suggest that oxidization of S (-II) may be the driving force for cinnabar dissolution in aquatic environments. Complexation of cysteine with Hg^{2+} also plays an important role in this process by inhibiting the absorption of released Hg^{2+} on the cinnabar surface.
- During **FY12 (FIU Year 3)** parameters associated with the adsorption/desorption of Hg(II) on cinnabar were measured.
- A model based on chemical thermodynamics and adsorption/desorption equilibrium is being developed to calculate the dissolution of cinnabar under different pH and Eh conditions and thiol concentrations. Parameters associated with the model were summarized or measured. The proposed model is being validated by comparing modeled results with experimental data. Effects of pH, Eh, and cysteine on cinnabar dissolution are being evaluated using this model.
- Summarized current studies on the effects of environmental factors (e.g., DOM, pH, redox condition) on the dissolution of cinnabar.
- A new technique using isotope tracers is being developed to simultaneously determine the dissolution of cinnabar and re-adsorption of released Hg^{2+} on the cinnabar surface. This technique will be used to study the effects of various environmental factors on cinnabar dissolution in the next step. A flow injection system was coupled to ICP-MS in order to analyze mercury isotopes in aqueous phase in the past month.
- Experiments were conducted to evaluate the relative importance of thiol group versus other groups in L-cysteine in cinnabar dissolution. Effects of L-serine (a chemical containing hydroxyl group) on cinnabar dissolution was examined and compared with that of L-cysteine. The concentrations of Hg (II) released from cinnabar after shaking for 24 hours were measured to be 3.2±0.9 and 116.6±1.7 µg L-1 in the presence of L-serine and L-cysteine, respectively. The molecular structures of L-serine and L-cysteine are almost identical besides the replacement of hydroxyl group in L-serine by thiol in L-cysteine. These results indicate that thiol is the functional group in L-cysteine that promotes the dissolution of cinnabar.
- ID (isotope dilution) - FI (flow injection) -ICP-MS coupled with isotope addition technique was developed and the feasibility of applying this technique in studying cinnabar dissolution was tested.

- In October 2012, $^{201}Hg^{2+}$ was spiked into the cinnabar-dissolution system and detected to monitor the adsorption of Hg^{2+} on cinnabar. Variation of $^{202}Hg^{2+}$ with time was measured to estimate the dissolution rate. Isotope dilution-flow injection ICP/MS was employed to measure concentrations of $^{201}Hg^{2+}$ and $^{202}Hg^{2+}$ in solutions. This technique is being validated and will be applied in measuring the dissolution of cinnabar and re-adsorption of released Hg^{2+} on cinnabar.
- Results of the preliminary experiment conducted in October showed that the background concentration of Hg^{2+} in the cinnabar suspension solution is too high. Efforts are being made to decrease the Hg background in cinnabar suspension solution by comparing different pretreatment procedures used for cleaning up cinnabar.
- A new technique, isotope dilutions (ID)-phenylation-purge and trap-ICP-MS, is being developed for analyzing organomercury species at trace levels. 199-labeled EtHg and 201-labeled MeHg have been synthesized in the past month.
- Experiments were conducted to study the difference of reduced glutathione (GSH) and oxidized glutathione (GSSG) in promoting cinnabar dissolution.
- A new technique using isotope addition ($^{201}Hg^{2+}$) and isotope dilution ($^{199}Hg^{2+}$) is being validated and applied in measuring the dissolution of cinnabar and re-adsorption of released Hg^{2+} on cinnabar.
- A new technique, isotope dilutions (ID)-phenylation-purge and trap-ICP-MS, is being developed for analyzing organomercury species at trace levels. This method has been applied in detecting concentrations of MeHg and EtHg standards in water phase in the past month. The detection limit and recovery of this technique will be determined in the coming month. The method will also be applied in analyzing organomercury species in sediment and fish samples.
- Experiments were conducted to study the difference of reduced glutathione (GSH) and oxidized glutathione (GSSG) in promoting cinnabar dissolution.
- Experiments are being conducted to test if eliminating oxygen during all of the pretreatment procedures can decrease the background of Hg^{2+} in HgS suspension solution.
- Submitted “Preliminary results summary of laboratory experiments” (Milestone 2012-P3-M3).

GEODATABASE DEVELOPMENT FOR HYDROLOGICAL MODELING SUPPORT

- In **FY 10 (FIU Year 1)** a geodatabase was developed to support the management of input and output data for the hydrological and transport models. A centralized data storage system was built and deployed on an advanced Windows server with the latest technology and hardware. The database provides a user interface which facilitates data access, database connectivity, web application development, numeric algorithms, and network communications. The information to be stored in the geodatabase will directly support hydrological model development and calibration and will include, for example, GIS coverages/shapefiles of the delineated watersheds, surrounding buildings and man-made structures which may serve as sources of contamination, roads, stream gauge locations, monitoring wells, bore holes, land cover and soils; raster imagery; observed/measured timeseries data such as flow rates, precipitation, evapotranspiration, mercury concentration and surface and groundwater levels; and simulation outputs including computed flow data at each node (head pressures in the saturated zone for each timestep), computed flow data in the rivers for each time step, computed concentrations in the overland, unsaturated, saturated zones and river (daily timeseries) and sedimentation information (total suspended particles, mercury concentrations, sediments). The geodatabase, which is based on the ArcHydro and ArcGIS Basemap data models, includes feature datasets and raster catalogs which contain model configuration and output data.

- In **FY11 (FIU Year 2)** FIU continued development and refinement of the geodatabase created for the EFPC model to customize it according to model input data specifications and to facilitate import/export of model data.
- A progress report entitled, "GIS & Hydrological Modeling Data Server Management," was created to provide configuration methods and parameters.
- The ORR Geodatabase was then populated with relevant model data. The import/export of spatial data into the geodatabase and execution of geoprocessing tasks as necessary for model simulations is an ongoing process.
- Data stored in the ORR Geodatabase was used for visualization, map production and analysis through the ArcGIS ArcMap interface, often utilizing the MIKE 11 GIS extension tool for timeseries file management and integration of MIKE 11 model files. Graphical plots were also generated using the observed and computed model data for reporting purposes.
- A technical report entitled, “Geodatabase Development for Hydrological Modeling Support,” was submitted to DOE in March 2012. This report has since been updated and re-submitted as a final report.
- During **FY12 (FIU Year 3)** a preliminary literature review for the use of Python scripting to automate various geoprocessing tasks and the use of ArcGIS Model Builder to generate process flow diagrams was conducted. This was to support external query and retrieval of mercury and hydrological model data from the existing ORR geodatabase. This information was used for development of a draft Project Technical Plan (PTP) for proposed FY12 work scope The following are some of the documents, presentations and technical workshops reviewed:
    - ESRI International User Conference Technical Workshops:
        - “Model Builder Advanced Techniques,” Scott Murrary, July 2010.
        - “Working with Temporal Data in ArcGIS,” David Kaiser, Hardeep Bajwa, July 2010.
    - ESRI Southeast Regional User Group (SERUG) Conference 2010 Technical Workshop:
        - “Intermediate ModelBuilder,” Kevin Armstrong.
    - Wikihow: “Creating time-series raster mosaics in ArcGIS 10 for Eye on Earth.”
    - “Model Builder Lab,” Geoinformatics, Spring 2008, Purdue University Library.
    - “Time-Series Contaminant Interpolation using ArcGIS and Spatial Analyst,” Mark K. Petersen, ESRI User Conference Proceedings 2006, Paper 1326.
- The aforementioned resources were utilized, and a preliminary model was developed and tested using ArcGIS Model Builder coupled with Python scripts which:
    - Automates the retrieval of groundwater level daily time series well data derived from OREIS by date
    - Interpolates the extracted values, and
    - Generates raster images for each day in ESRI GRID and TIFF formats.

- Conducted research to assist in development of Python scripts to enable the raster images produced to be stored in a raster catalog archived by date to facilitate visualization and animation of the temporal changes in groundwater levels for the specified study domain over a given timeframe. To date the scripts developed have enabled storage of the raster images produced in a raster catalog, however, further development is necessary for automated archival of these images by date.
- A separate model was developed using Model Builder and Python scripting to enable the export of maps from an ArcMap document within a specified data frame in PDF format. Refinement of this model is now being conducted.
- Developed model using ArcGIS ModelBuilder which iterates through selected features and exports the results in tabular format. This can be utilized to extract model input and output data contained in the geodatabase such as groundwater level, discharge and mercury concentration. Once the feature (e.g. GW well or outfall) has been selected, a field attribute such as station name is used to extract all the data for that station and export it in MS Excel or text format.
- This model is currently being extended and refined to enable greater functionality by developing new or modifying and incorporating existing Python scripts for statistical analysis of the exported data. This will be especially useful for extracting and analyzing timeseries data used in the EFPC model. Once the model is completed, a ModelBuilder workflow diagram will be generated and documented.
- A toolbox was implemented in ArcGIS which uses the scripts to analyze water stages in rivers, flow rates, groundwater levels and water quality data from wells and rivers. The toolbox was tested extracting and analyzing timeseries data used in the EFPC model. Once the model is completed, a ModelBuilder workflow diagram will be generated and documented.
- Submitted summary report providing sample Python scripts and ModelBuilder process workflow diagrams (Milestone 2012-P3-M4.1).
- For this task, **FY13 (FIU Year 4)** involved development of additional customized scripts to enhance database querying capabilities; development of a library of scripts which are coupled with other existing libraries used for mathematics, science, and engineering; and integration of the library with existing open source libraries to perform statistical analyses and which can be applied to similar databases used at other DOE sites.
- FIU also began preparation for implementing additional security protocols for access to the hydrological modeling and GIS data.
- ARC's IT team provided guidance with regards to potentially publishing the existing models on the Web.
- Update of the existing geodatabase also continued with the addition of new data obtained from model results. The geodatabase was also revised to update components such as model domains; digital orthophotos; landuse/landcover polygons; physical features including buildings, obscured areas, natural outlines, man-made outlines (polygons); transportation features such as roads, railroads, transportation structures (polylines); monthly rainfall timeseries; flow rate/discharge timeseries; and any other derived model simulation data.

MODELING SUPPORT FOR NEW CERCLA DISPOSAL CELL AT ORR

FY10 (FIU Year 1): Selection of the most appropriate location for construction of the new CERCLA Disposal Cell at ORR requires data collection and analysis and an evaluation of expected technical performance. To support the DOE's current Environmental Management (EM) program in establishing the optimum site selection criteria, FIU has conducted preliminary research and prepared a comparative assessment report of four candidate sites with respect to their geologic and hydrologic transport characteristics. Three of the candidate sites (White Wing, West Bear Creek and Chestnut Ridge Paradigm) were compared to the currently proposed Environmental Management Waste Management Facility (EMWMF). A comparative risk analysis of these sites was also conducted and summarized in a spreadsheet entitled "Parametric Analysis of Relative Risk from New Candidate Sites Compared to that from EMWMF". The leachate and run-off from EMWMF contains a diverse range of chemicals (e.g. uranium, iron, copper, potassium, boron, and others) that are a potential risk for groundwater contamination. Due to the diversity of metals present in the leachate, it is important to understand the interactions between them and how this affects the equilibrium of the system. As part of the overall analysis, FIU also conducted research on various waste immobilization and debris treatment technologies using the EMWMF as a case study. The chemical composition of the principal contaminants in the EMWMF leachate and run-off were identified, and information on relevant treatment technologies specific to these contaminants was provided in a report entitled "Performance Characteristics of Waste Immobilization Technologies". Description of the immobilization technologies included both chemical and physical methodologies such as chemical precipitation, surface complexation, impermeable barriers, etc. In addition, the Code of Federal Regulations - Title 40: Protection of Environment (40 CFR Ch.1 § 268.45) establishes that hazardous debris must be treated prior to land disposal and before any immobilization technology can be applied. The best available technologies for hazardous debris treatment including extraction, destruction, and immobilization methods were therefore also provided in the report.

STUDENT SUPPORT FOR MODELING OF GROUNDWATER FLOW AND TRANSPORT AT THE DOE SITE IN MOAB, UTAH

FIU, in collaboration with DOE's Moab site project director, has utilized an existing groundwater numerical model to evaluate the tailings pore-water seepage in order to assist in effective dewatering of the tailings pile and to optimize the groundwater extraction well field as part of the DOE Uranium Mill Tailings Remedial Action (UMTRA) for the Moab site. The work was carried out with support from student interns who assisted in the collection of groundwater samples and site data and applied the existing groundwater and transport model (SEAWAT available from the public domain) to analyze the groundwater flow and transport data of the Moab site.

The objective of this model was to analyze the nitrogen and uranium cycle in the environment and provide forecasting capabilities for the fate and transport of contamination within the Moab site and to provide information which can be used to determine the efficiency of remedial actions in reducing the concentration and load of contaminants and to assist DOE in deciding the effectiveness of remedial actions. Modeling was performed with MODFLOW, SEAWAT and FEFLOW as a benchmark. The main objective was to determine the effect of discharge of a legacy ammonia plume from the brine zone after the extraction wells and injection system have been shut off. The model will be used to predict capture zones for different operating scenarios, mass removal, and time to complete remediation.

- In **FY10 (FIU Year 1)**, FIU provided a preliminary estimate of the air pollution potential when the Landshark evaporating system is used to disperse contaminated groundwater in the air at selected sites in the vicinity of the tailings, including the City of Moab and Arches National Park. Ammonia and metals were the primary contaminants addressed by the Landshark analysis and ammonia was the only contaminant addressed by the air stripper analysis. The operation of an alternative ammonia treatment using an ammonia stripping tower was also analyzed to determine the maximum concentration of emissions at the source and the ammonia mass flow rate emitted from the tower at 700 gpm treatment capacity. The average wind velocity and direction measured at the site were applied in the Gaussian air dispersion model to determine the steady state concentrations of each contaminant as a function of distance to the point source. The steady state concentrations were compared to OSHA's inhalation exposure limits for each contaminant and downwind ammonia concentrations were calculated at all major receptor points (Tailings, Offices, Matheson Wetland Preserve, the City of Moab, and Arches National Park). The ammonia concentrations were all found to be below the 8-hr OSHA exposure limits of 25 ppm (0.018 $\mu g/m^3$) and the odor threshold was 5 ppm which is within OSHA's 5-17 ppm range. In addition, the Landshark evaporator provided significant dilution (1500 times) at the point source. A graduate student worked at the site to collect field data and other information necessary for analysis of the air dispersion and to provide observed data in support of groundwater numerical modeling.
- In **FY11 (FIU Year 2)**, FIU obtained and organized the hydrological data for the analysis and modeling and completed hydrologic budget calculations to be used for developing constraints for the surface and groundwater model.
- Completed analysis of groundwater quality data adjacent to the Colorado River for calculating the flux of contamination into the river and will use results to generate water quality contour maps to assess the pattern of contaminant transport.
- Conducted simulations with the existing hydrological model (developed by a DOE consultant). Compared results obtained from carrying out simulations using the existing model with the results presented by the subcontractor of the DOE Moab Site.
- Reconfigured the existing Moab model with more current spatial and timeseries data and currently conducting numerical simulations to simulate fate and transport of contaminants including uranium and ammonia in the subsurface domain at the Moab site in Utah.
- Extracted pumping test data and regular monitoring data from literature, which will be used in the model to show the natural seasonal variations and responses to other stresses.
- DOE Fellow, Mr. Alex Henao, completed an internship during the summer of 2011 and submitted a report entitled, "Preliminary Studies of Nitrogen Concentration in Wells 0437, 0438, and 0439 at the Moab Site," in November 2011.
- Participated in a 2-day modeling webinar, "Using Groundwater Vistas," conducted by the DOE subcontractor that developed the existing groundwater model. This model is to be used for some of the planned FIU modeling work.
- Ran simulations with the Moab air dispersion model for the new location of the landsharks and created a report which included the new results.

- Finalized the Moab model and its configuration according to Advanced Simulation Capabilities for Environmental Management (ASCEM) specifications.
- Calibrated the model with water level measurements collected from several monitoring wells. Variable hydraulic conductivity values were used for the top 3 layers and uniform conductivity values for the rest.
- Pumping test data and several years of regular monitoring data which shows the natural seasonal variations and responses to other stresses was used for transient calibration of the model. The model was also used for well field optimization to predict capture zones and mass removal.
- Simulations were conducted to identify the discharge zone for the legacy plume in the brine zone and to identify areas of uncertainty.
- A technical report entitled, "Student support for modeling of groundwater flow and transport at Moab, UT site," was submitted to DOE in February 2012.
- During **FY12 (FIU Year 3)** FIU updated the Moab groundwater model with pumping test data and conducted a series of simulations for understanding the effect of seasonal variations of hydrologic parameters and the responses to other stresses.
- Updated the progress report for the Moab groundwater flow and transport model. Added a section describing the simulations using pumping and determined the changes of water and contaminant flux in the river.
- Prepared figures and tables which will be used in the annual report.
- Conducted 5 different simulations with different pumping and injection well rates to understand the effects of these variations on the existing site conditions.
- Updated the Moab groundwater model with new groundwater data and conducting simulations for longer durations (10 yrs as opposed 1 yr which was run previously).
- Developed plumes for the aqueous species of concern (nitrate and uranium) in the vicinity of the tailings pile.
- Implemented diversion ditch into the flow model (as drain cells) and will update the model once the technical details are received.
- Updated the Moab groundwater model with new groundwater data which was obtained from USGS and other publically available hydrological data.
- Developed plumes for the aqueous species of concern (nitrate and uranium) in the vicinity of the tailings pile and used the plumes to provide initial conditions for the simulations.
- Conducted 20 simulations for a 10 year period and worked on verification of model response in terms of statistical parameters. Analyzed areas with high errors and adjusted the hydraulic conductivities.
- Incorporated a diversion ditch into the flow model (as drain cells), currently testing the model response for the diversion ditch. Investigating the extraction flow rates.
- Obtained from the contractor a new configuration of the diversion ditch which will be implemented for control of groundwater flow and contaminant transport into the flow model.
- Conducted a series of simulations to ensure that the updated model provides a correct response with respect to seepage flow collected in the drainage ditch.
- Conducted 6 simulations for a 10 year period and worked on verification of model response in terms of statistical parameters. Analyzed areas with high errors and adjusted the hydraulic conductivities.

- Compiled an abstract for the waste Management Conference in Arizona 2013. The topic of the paper will be "Long-term Performance of UMTRA Tailings Disposal Cells".
- Conducted a series of simulations with the new configuration of the diversion ditch to determine the degree of control of groundwater flow and contaminant transport into the flow model and the seepage flow collected in the drainage ditch.
- The hydrologic parameters of the tailings were analyzed and a series of simulations were used to provide information which showed that prescribed-head variable upper boundary condition in eliminated the errors resulting from quantifying net infiltration and evaporation through the filter layer of the cover. Model results indicate long term a uniformly unsaturated hydraulic barrier with a low unsaturated hydraulic conductivity and a low flux under a gradient of unity and that after a few decades the tailings may transmit minimal amounts of seepage to the groundwater system.
- Analyzed the gravimetric moisture contents of more than 70 tailing samples at Moab for modeling. The volume of the sample and specific gravity of the sample was analyzed to determine the percent saturation. From the analysis it was determined that the % moisture ranges from 6.5% to 92.9%, with an average of 38.5%. The fine sand samples had the lowest values (from 6.5 to 8.4%). The data were introduced into the hydrological model and a set of simulations were performed to determine the difference with the previous simulations. This provides additional information about the uncertainty of the hydrological parameters.
- Summarized the analysis of the gravimetric moisture contents of more than 70 tailing samples at Moab for modeling. Using the data for unsaturated flow at the mine tailings. The hydrological model provided calculation about the distribution of moisture content in the soil column as a function of precipitation.
- The numerical model was modified to provide capabilities for analysis of the fluctuation of moisture content which was determined on a daily basis at different soil column heights. The purpose was to provide information about the exchange of flux between the unsaturated and saturated zones and therefore gain a better understanding of the vertical contaminant fluxes from the mine tailings to the subsurface flow, and subsequent horizontal transport to the river.
- Additional simulations were conducted to determine the transient drainage of moisture in the tailings by quantifying the vertical downward fluxes which are a result of drainage of the mine tailings.
- The model simulations were used to determine the fraction of precipitation infiltrating the tailings, the extent of infiltration, and the fraction of surface runoff during precipitation events.
- A series of probability exceedance figures were developed for each selected tailings layer to provide understanding of the behavior of the tailings during wet, median and dry conditions.
- The paper which was submitted to WM 2013 was additionally revised.
- The simulations were used to understand the dynamics of the system and changes in moisture and moisture flux. The following conclusions were derived:
    - The analysis considered the stochastic variation of all hydrological events that control flow and transport at the site. A unique modeling approach simulated the daily climatic conditions and determined the changes in moisture and moisture flux from the disposal cell for a period of ten years.

  - Modeling results indicated that increases in the saturated conductivity at the top of radon barrier do not influence flux from the tailings with time because the tailings behave similar hydraulically to the radon barrier.
  - The presence of a thin layer of low conductivity material anywhere in the cover or tailings restricts flux in the worst case to the saturated conductivity of that material. Furthermore, the precipitation is equivalent to the evapotranspiration losses from the surface layer.
  - Where materials are unsaturated at depth within the radon barrier of tailings slimes, conductivities are typically less than 10-8 centimeters per second.
  - If the low conductivity layer is deep within the disposal cell, its saturated properties are less likely to change with time.
  - The model confirmed the following trends:
    - Infiltration and evapotranspiration: The accumulated infiltration is equivalent to the accumulated evapotranspiration, resulting in no water reaching the groundwater tailings under the conditions simulated (daily precipitation and evapotranspiration). In general, for the hydrologic conditions at the site, the water from precipitation infiltrates in the shallow surface zone, where it is lost from evapotranspiration.
    - Extent of Infiltration: At a depth of 0.7 ft in the rip-rap layer (1st layer) the moisture content is very low, implying that there is a low possibility of water reaching past that layer (hydraulic conductivity is in the order of 10-10 m/s).
    - Vegetation: The vegetation affects the rate of evapotranspiration, increasing the amount of evaporation thus reducing the amount of water that infiltrates through the layer.
    - Land cover: The rip-rap rock cover variations in hydraulic conductivity ranges from 10-6 to 10-4. There is no concern that rock rip-rap is increasing percent saturations and downward moisture flux.
- The significance of this modeling approach is that the stochastic variations of a variety of hydrologic events are taken under consideration and provide a better understanding of the flow and transport within the site. Therefore, both the operation and the maintenance of the disposal cells can be minimized if they are allowed to progress to a natural condition with some vegetation and soil genesis. Because the covers and underlying tailings have a very low saturated hydraulic conductivity after transient drainage, eventually the amount of moisture leaving the tailings has a negligible effect on groundwater quality. Although some of the UMTRA sites are not in compliance with the groundwater standards, the explanation may be legacy contamination from mining, or earlier higher fluxes from the tailings or unlined processing ponds. Investigation of other legacy sources at the UMTRA sites may help explain persistent groundwater contamination.
- Submitted summary report of the Moab model's preliminary results (Milestone 2012-P3-M5.1) which described the simulations and the main aspects of the model:
  - The existing model was revised and updated with additional information related to the current remedial actions which include injection, well withdrawal, and simulating the fate and transport of contaminants, including uranium and ammonia, in the subsurface domain at the Moab site in Utah and how density dependent flow is related to brines in the groundwater system beneath the site.

Information such as ammonia surface water data collected between 2000 and 2002 were used in the analysis.
  - The existing Moab model was updated by implementing geostatistically interpolated ammonia and uranium plumes and current well operation data into the model to evaluate the effects of pumping on contaminant concentrations and determining potential surface water concentrations in riparian habitat areas for a range of operating conditions. The plumes of aqueous species of concern (nitrate, uranium) were developed with the width of the tailings that would be conservative.
  - After implementing plumes into the model as initial conditions, additional simulations were conducted to optimize mass removal and capture from the existing system. The ammonia transport was simulated by applying as initial condition, the ammonia plume (for a couple of cycles), and determining the yearly rise and fall in the river to determine if the ammonia concentrations moving up into the brine zone is due to the fluctuations of concentrations in the river.
  - The effects of the brine zone beneath the site on an overlying saline zone and the effect of discharge of a legacy ammonia plume from the brine zone after the extraction wells and injection system have been shut off and the spatial extent of the discharge zone for the ammonia legacy plume in the brine zone and its effect on natural flushing were determined.
  - A diversion ditch was added to intercept and extract water from the tailings. The ditch was implemented into the flow model (as drain cells) and by setting the head, levels will be set in each drain cell at the elevations of the drains.
  - A new configuration was implemented that includes infiltration and provides information about the reoccurrence of the concentrations within the recharge assuming the existence of a freshwater lens.
- The effect of mixing water from the river and the diversion ditch was determined along with the benefits of running a diversion ditch and well extraction at the same time.

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

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

The SITEWISE™ software is an EXCEL-based evaluation tool designed to: 1) compare and contrast alternatives for remedial, monitoring, waste handling, and D&D design, and 2) to generate results for cost benefit and sustainable decision-making for regulatory compliance. The Navy, EPA, and USACE incorporate sustainability evaluation and decision making into their long-standing and successful optimization programs as part of the 5-year regulatory review process. SITEWISE™ is one of many evaluation tools used in federal and industry sectors to calculate and optimize the environmental footprint of cleanup and closure alternatives. Specifically, SITEWISE™ methodology provides a baseline assessment of long-term alternative design impacts based on the sustainability factors of greenhouse gas (GHG) and critical air pollutant (i.e., sulfur and nitrogen oxides, particulate matter, etc.) emissions; energy and water usage; natural resource consumption and footprint impact; waste generation; and risk from accident death and injury.

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

- In **FY13 (FIU Year 4)** a literature review was conducted in relation to the cost-benefit of Green & Sustainable Remediation (GSR) practices applied to cleanup and closure projects at the field sites and Headquarters' management of those projects.
- Based on preliminary testing of SITEWISE™ (using a hypothetical site), the following information is required and needs to be provided by the site: Material production; Well materials; Treatment chemical; GAC; Construction materials; Well decommissioning materials; Bulk quantities of materials; Transportation; Personnel transportation road, air and rail; Transportation equipment; Equipment transportation road, air, rail and water; Equipment use; Agricultural equipment; Internal combustion engine; Stabilization equipment; Mixers; Other fueled equipment; Residual handling; Thermal/catalytic oxidizer; Laboratory analysis; On-site labor hours and activities.
- A review of available statistical or geostatistical software, including MAROS or GTS, was conducted. The software is used to downsize a compliance monitoring program (i.e., remove wells, analytes, or frequencies). Tests were conducted with the monitoring module in SITEWISE™ 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.
- Initial simulations were conducted and data gaps are being identified and researched.
- 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.

- The project has developed strategies for additional optimization of:
    - 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 be used to 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.
- 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 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.

EXECUTIVE SUMMARY (FIU YEAR 5)

Historically, this project entitled *“Remediation and Treatment Technology Development and Support”* 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). Integrated surface and subsurface flow, transport and fate models were developed to provide analysis of contaminant patterns within each watershed. In addition, digital monitoring data available from the Oak Ridge Environmental Information System (OREIS) and related to mercury (Hg) contamination and remediation within these watersheds was used for calibration and verification of the model. Experimental studies were also carried out which provided kinetic and equilibrium data about important parameters related to Hg transport, speciation and methylation/ demethylation kinetics within the watershed. 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 can be more easily shared with other project stakeholders such as DOE personnel and site contractors. New scope introduced in FY 13 (FIU Year 4) focused on development of EM pilot studies and the use of GSR sustainability software (e.g. SITEWISE™) to evaluate the benefit of Green Sustainable Remediation (GSR) practices; to 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 environmental impact, as well as to improve system design performance and efficiency.

For **FY14 (FIU Year 5)**, the project was renamed *“Environmental Remediation Technologies (EM-12)”*. FIU proposed a scope which utilizes and builds upon the capabilities developed under Project 3 in the area of soil and groundwater remediation and treatment technology and work with Savannah River National Laboratory (SRNL) to apply these approaches to similar environmental challenging problems at the Savannah River Site. Tasks are synergistic with the work SRNL is performing and have involved (1) Modeling of the migration and distribution of natural organic matter injected into subsurface systems to support environmental remediation; (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: MIGRATION AND DISTRIBUTION OF NATURAL ORGANIC MATTER INJECTED INTO SUBSURFACE SYSTEMS

Column experiments were conducted at the Florida International University (FIU) Applied Research Center (ARC) to estimate the sorption and desorption properties of humic acid onto Savannah River Site (SRS) sediment. Previous studies have shown that humic acid sorbed to sediments will strongly bind with sediments at a mildly acidic pH. The use of humic acid could be applied to various DOE sites for contaminant stabilization; however, column studies are required to optimize this technology and prepare it for actual field deployment and regulatory acceptance. Experiments were designed to study the behavior of humic acid, specifically Huma-K, at different pHs that would help develop a model to predict the humic acid sorption/desorption.

This report provides the background information, methodology, and results from tracer tests and humate injection tests in flow-through columns filled with soil from SRS. Tracer tests provided transport parameter values and showed that the columns have intermediate dispersion. Humate injection tests showed that pH has an effect on the sorption of HA: with an increase in the pH of the columns, humate sorption increased. Further experiments will include an injection of uranium to study the effect of HA on the mobility of uranium in porous media.

INTRODUCTION

The Savannah River Site (SRS) was one of the major U.S. Department of Energy (DOE) facilities that produced plutonium during the Cold War. The F-Area Hazardous Waste Management Facility (HWMF) consists of three unlined, earthen surface impoundments, referred to as seepage basins. From 1955 to 1988, the F-Area seepage basins had received approximately 1.8 billion gallons of low level waste solutions generated by uranium slug and irradiated fuel processing in the F-Area Separations Facility. The effluents were acidic due to the presence of nitric acid and a wide variety of radionuclides and dissolved metals (Dong et al., 2012). The waste solutions were moved approximately 3,000 feet from each processing area through underground clay pipes to the basins. Once the wastewater entered the basin, it was allowed to evaporate and seep into the underlying soil. The basins were intended to minimize contaminant migration to exposure points through the interactions with the basin soils. Although they performed as designed, due to the acidic nature of the basin influent, there was mobilization of some metals and radionuclides of uranium isotopes, ^{129}I, ^{99}Tc, and tritium migrated into the groundwater to create an acidic plume with a pH between 3 and 5.5.

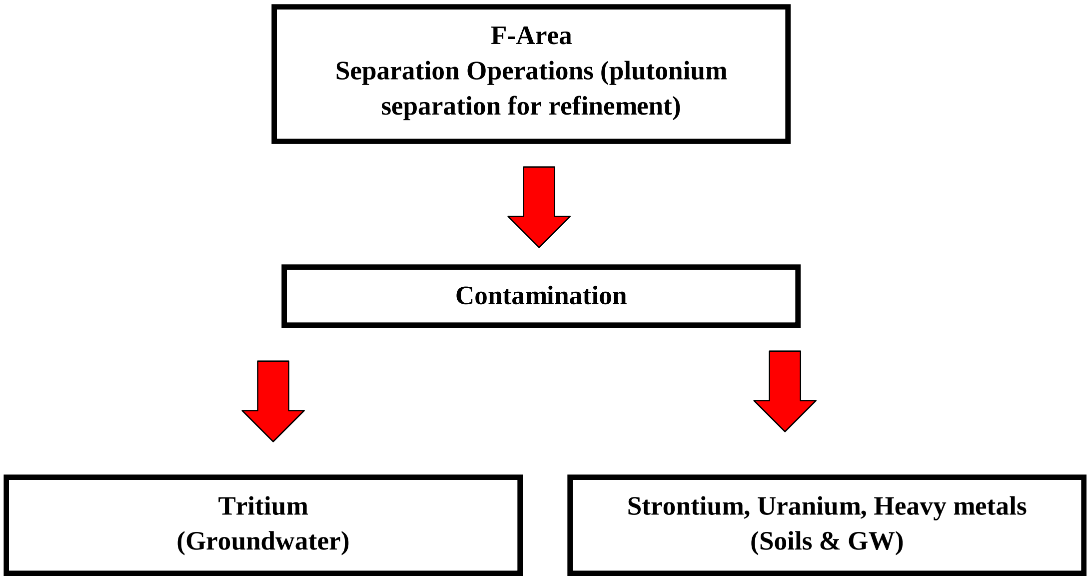

Figure 1. Source of contamination and contaminants.

Beginning in the late 1950s, the groundwater at the basins has been monitored and assessed. Remediation efforts and assessments have been applied through the years using various types and numbers of wells, seepline monitoring points and surface water locations. Although the site has gone through years of active remediation, the groundwater remains acidic, with pH as low as 3.2 around the basins and increasing to pH of 5 down gradient. In addition, U (VI) and other radionuclide concentrations remain above their maximum contaminant levels. In an effort to remove the contaminants from the groundwater, pump-and-treat and re-inject systems were implemented in 1997. Down gradient contaminated groundwater was pumped up to a water treatment facility, treated to remove metals (through osmosis, precipitation/flocculation, and ion exchange), and then re-injected upgradient within the aquifer. The pump-and-treat water treatment unit eventually became less effective, generated large amounts of radioactive waste and was expensive to maintain, prompting research for new remedial alternatives. In 2004, the pump-and treat system was replaced by a funnel and gate system in order to create a treatment zone via injection of a solution mixture composed of two components, sodium hydroxide and carbonate. The injections were done directly into the gates of the F-Area groundwater to raise pH levels. The purpose of the treatment zone was to reverse the acidic nature of the contaminated sediments, thereby producing a more negative net charge on the surface of sediment particles and enhancing adsorption of cationic contaminants. This system of remediation required a systematic re-injection of the base to raise the pH to near neutral values. However, the continuous use of high concentrations of a carbonate solution to raise pH creates a concern of possible re-mobilization of uranium that was previously adsorbed within the treatment zone since U(VI) in the presence of bicarbonate ions forms soluble aqueous uranyl-carbonate complexes.

Savannah River National Laboratory (SRNL) has been testing an unrefined, low cost humic substance known as Huma-K as an amendment that can be injected into contaminant plumes to enhance sorption of uranium, Sr-90, and I-129. A field test of humic acid technology for uranium and iodine 129 (I-129) was conducted by Millings et al. (2013) at the F-Area Field Research Site. Humic substances are ubiquitous in the environment, occurring in all soils, waters, and sediments of the ecosphere. Humic substances are complex heterogeneous mixtures of polydispersed materials formed by biochemical and chemical reactions during the decay and transformation of plant and microbial remains. Humic substances (HS) account for 50-80% of the organic carbon in the soil or sediment and are known for their excellent binding capacity for metals, while being insoluble or partially soluble. This makes HS a strong candidate for remediation efforts to reduce the mobility of uranium (VI) in the subsurface. Three main fractions of HS are identified based on their solubility in dilute acids and bases. Their size, molecular weight, elemental composition, structure, and the number and position of functional groups vary.

> ***Humic acids:*** the fraction of humic substances that is not soluble in water under acidic conditions (pH < 2) but is soluble at higher pH values. They can be extracted from soil by various reagents, which are insoluble in dilute acid. Humic acids are the major extractable component of soil humic substances. They are dark brown to black in color.
>
> ***Fulvic acids:*** the fraction of humic substances that is soluble in water under all pH conditions. They remain in solution after removal of humic acid by acidification. Fulvic acids are light yellow to yellow-brown in color.
>
> ***Humin:*** the fraction of humic substances that is not soluble in water at any pH value and in alkali. Humins are black in color.

The Huma-K commercially available dry flake organic amendment was used as a source of humic acid. Huma-K is high in humic and fulvic compounds and is just one of several brands produced for large scale use as soil conditioners to boost productivity in organic agriculture and used by farmers to stimulate plant growth and facilitate nutrient uptake. Huma-K is made from leonardite, an organic rich mineral formed due to decomposition by microorganisms, by extracting the raw material with a potassium hydroxide base solution and then drying it. The high pH solubilizes the humic acid molecules and generates a dark-brown highly-concentrated solution, rich in humic acid, which can be diluted for use. Importantly, while such solutions are commonly called soluble humic acid, they are actually basic with pH greater than 7.

METHODOLOGY

Soil Characterization

Soil obtained from SRS was characterized prior to the column experiments. The soil used during the experiments was obtained from SRS's FAW-1 60'-70'. Soil was disaggregated with minimal force to avoid creating new mineral surfaces from fracturing and abrasion using a 2-mm sieve to collect sediment of a particle size ≤ 2 mm.

Bulk Density Analysis

The bulk density of a solid is defined as the ratio of the dry mass of the solid to its bulk volume (solid and void volume). The volume of the soil was measured without compaction and the mass of the solid was determined after drying a known volume in the laboratory oven (Blake et al., 1986). The bulk weight of the solid amendment mixtures was determined gravimetrically. Triplicate samples in 50-mL beakers were used and filled with soil, while the volume was noted.

The soil was dried at 105°C for one day to stabilize weight and its mass was determined after cooling it in a desiccator. Equation 1 was used to calculate the bulk density of soil:

$$Bulk\ density = \frac{Oven\ dried\ soil\ weight}{Volume\ of\ soil} \qquad \text{Eq. (1)}$$

Particle Density Analysis

The average density of the soil is the particle density. The Methods of Soil Analysis for the Pycnometer Method was used to determine the particle density of the soil. Using triplicate samples, 12.5 g of soil were air dried and weighed and introduced to an oven dried and pre-weighed 25-mL volumetric flask. Deionized water (DIW) was added to fill the flasks to the half-way point and gently boiled for a few minutes to eliminate air bubbles. After cooling, the flasks were filled to the 25 mL mark from previously boiled and cooled DIW. Temperatures were measured to ensure they were all the same and the final combined weights were determined. The particle density was determined for the soil using equation 2:

$$\boldsymbol{\rho_p = \frac{\rho_w\,(W_s - W_a)}{[(W_s - W_a) - (W_{sw} - W_w)]}} \qquad \textbf{Eq. (2)}$$

where:
ρw - Density of water in grams per cubic centimeter at observed temperature
Ws - Weight of volumetric flask plus soil
Wa - Weight of empty flask
Wsw - Weight of flask filled with soil and water slurry
Ww - Weight of flask filled with water at observed temperature

The porosity of the soil was determined using the calculated bulk and particle density, and is defined as the ratio of void volume of the soil to its total volume. Total porosity of the samples was calculated using the following formula (Danielson et. al., 1986):

$$\boldsymbol{Pt = 1 - \frac{\rho_b}{\rho_p}} \qquad \textbf{Eq. (3)}$$

The pH of the soil sample was also estimated using a 1:1 soil:water suspension ratio. In triplicate beakers, 10 g of soil and 10 mL of DIW were stirred for 15 minutes, and then settled for 15 minutes. The pH was measured using the supernatant of the soil samples.

Column Experiments

Glass columns (25 mm x 300 mm) obtained from Ace Glass Inc. were used to conduct flow-through column experiments to study the sorption/desorption of humic acid onto SRS sediment. Columns fitted with Teflon® adapters containing 350 micron screen support and a layer of glass wool (Figure 2) were filled with a known mass of oven dried soil obtained from SRS (Figure 3).

Column Tracer Test

In this experiment, a bromide tracer was injected into the column and effluent concentrations were monitored. Prior to performing the tracer tests, columns were saturated with DIW from the bottom of the column to the top in order to remove air bubbles. Once air was removed from the column, the flow was reversed to move from top to bottom and left for flow to stabilize at the desired flow rate of 2 mL/min. After flow was equilibrated, 3 ml of 1000 ppm bromide solution was injected at the top of the column. Samples of effluent were collected in pre-weighed containers at regular intervals. After each interval, the containers with samples were re-weighed and the bromide concentration was measured using a Thermo Scientific Orion Bromide Electrode (9635BNWP). Samples were collected until the bromide effluent readings reached equilibrium. Data collected allow for mean residence time to be determined, as well as the pore volume of the column. Prior to measuring the bromide concentration using a bromide electrode, the electrode was calibrated (Figure 4) using bromide standards in the range of 0.5 - 100 ppm.

Figure 2. Teflon ® adapter with layer of glass wool.

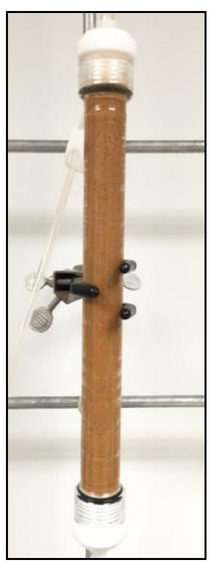

Figure 3. Column filled with SRS sediment.

The residence distribution function, E(v) as a function of volume fractions (Levenspiel, 1972) was calculated using Eq. 4:

$$E(v) = \frac{C(v)}{\int_0^{\infty} C(v)\, dv} \qquad \textbf{Eq. (4)}$$

Where:
v - Volume of effluent
C(v) - Concentration of bromide

Mean residence time (t_m), and pore volume (V_p) (Shook et al., 2005) were estimated using Eq. 5 and Eq. 6

$$t_m = \frac{\int_0^{\infty} t\, E(t)\, dt}{\int_0^{\infty} E(t)\, dt} = \int_0^{\infty} t\, E(t) dt \qquad \text{Eq. (5)}$$

$$V_p = \frac{\int_0^{\infty} v\, E(v)\, dv}{\int_0^{\infty} E(v)\, dv} = \int_0^{\infty} v\, E(v) dv \qquad \text{Eq. (6)}$$

Where:
t - Time
E(t) - residence distribution function in terms of time
v - Volume of effluent
E(v) - residence distribution function in terms of volume

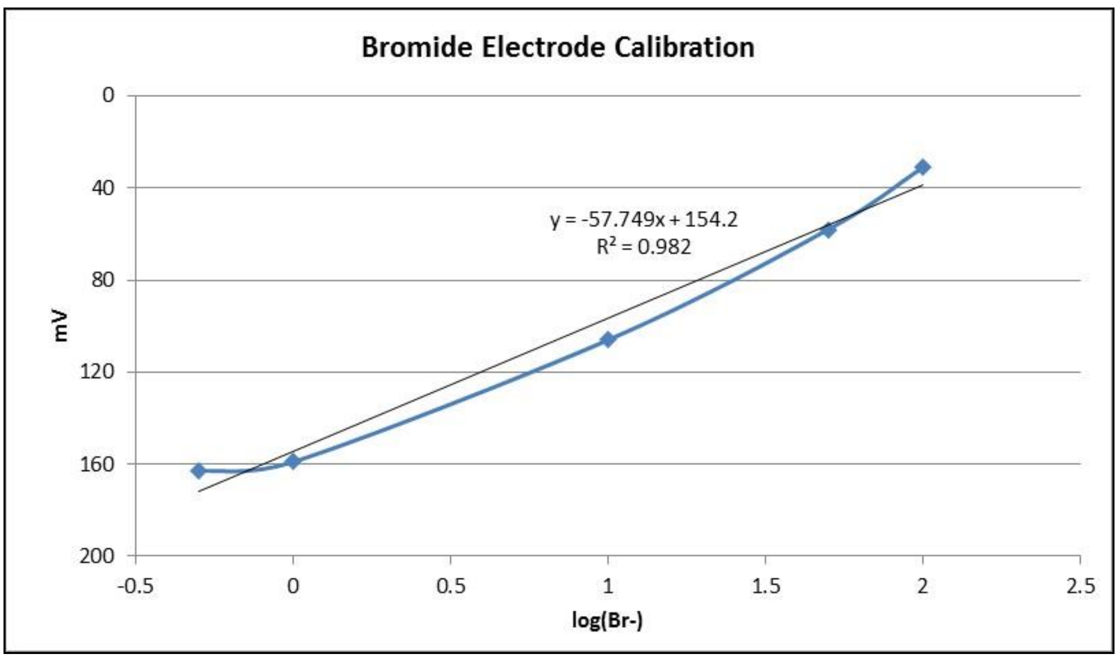

Figure 4. Calibration curve for bromide electrode.

Variance and the dimensionless Peclet number (P_e), which represents the ratio of the rate of transport by convection to the rate of transport by diffusion or dispersion, were determined by solving the 1D dispersion/advection equation (Bischoff et al., 1963; Fogler et al., 1992; Mibus et al., 2007):

$$Variance\ (\sigma^2) = \int_0^\infty (v - v_p)^2\ E(v)\,dv \qquad \text{Eq. (7)}$$

$$\frac{\sigma^2}{t_m^2} = \frac{2}{P_e^2}\left(P_e - 1 + e^{-P_e}\right) \qquad \text{Eq. (8)}$$

Where:
v - Volume of effluent
v_p - Pore volume
E(v) - Residence distribution function in terms of volume

Sorption/Desorption of Huma-K

After the tracer test, the column was preconditioned using pH adjusted artificial groundwater (AGW) prepared using a 0.01 M $NaNO_3$ solution mixed with 0.1 M or 0.1 M NaOH to reach the target pH values of 3.5 and 5. AGW was pumped from the top of the column until the pH of the effluent solution reached equilibrium. Once the pH of the effluent reached equilibrium, approximately one pore volume (PV) of 5000 ppm Huma-K solution, pH adjusted to 9 using 0.1 M HNO_3, was pumped at the same flow rate (2 ml/min) used during the tracer test. After injecting 1 PV of Huma-K solution, approximately 3 PV of AGW solution was pumped into the column and effluent samples were collected to measure the change in pH and concentration of Huma-K. Samples were analyzed using a Thermo Scientific Genesys 10S UV-Vis spectrophotometer calibrated (Figure 5) in the range of 1 to 25 ppm of Huma-K at wavelength of 254 nm, to measure the concentration of HA.

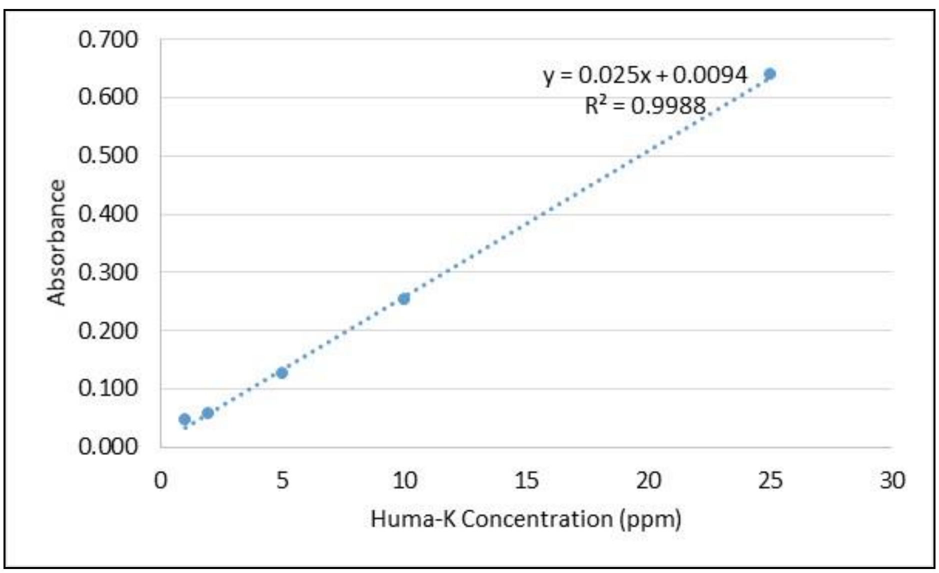

Figure 5. Humic acid calibration curve.

RESULTS AND DISCUSSION

Soil Characterization

Soil obtained from SRS's FAW-1 at a depth of 60'-70' was used in the column experiments. The soil was first characterized to measure the bulk density, particle density, porosity and soil pH. Triplicate samples were prepared and analyzed using procedures described in the methodology section and results of the average values obtained for each test are presented in Table 1.

Table 1. SRS Soil Characteristics

Bulk Density (g/cm^3)	Particle Density (g/cm^3)	Porosity	Soil pH
1.334	2.645	0.495	4.06

Humate Injection Scenarios

The information obtained from soil characterization and the data from batch experiments along with the column size were used in the model developed by SRS to estimate the flow rate and concentration of Huma-K used in the column experiments. Various concentrations and flow rates were used to identify the optimum Huma-K concentration and flow rate; the concentration used in the simulations was in the range to 5,000 - 10,000 ppm at flow rates of 1 - 4 ml/min. At high concentration (10,000 ppm), the column is completely saturated (Figure 6) even at low flow rates; a lower concentration of 5,000 ppm of Huma-K at 2 ml/min was found to be optimal for the size of the columns used in the experiments. The optimum scenario showed nice breakthrough curves with approximately 40% of Huma-K at 0.95 length of the column (Figure 7); whereas, a higher concentration of 10,000 ppm showed the column being saturated.

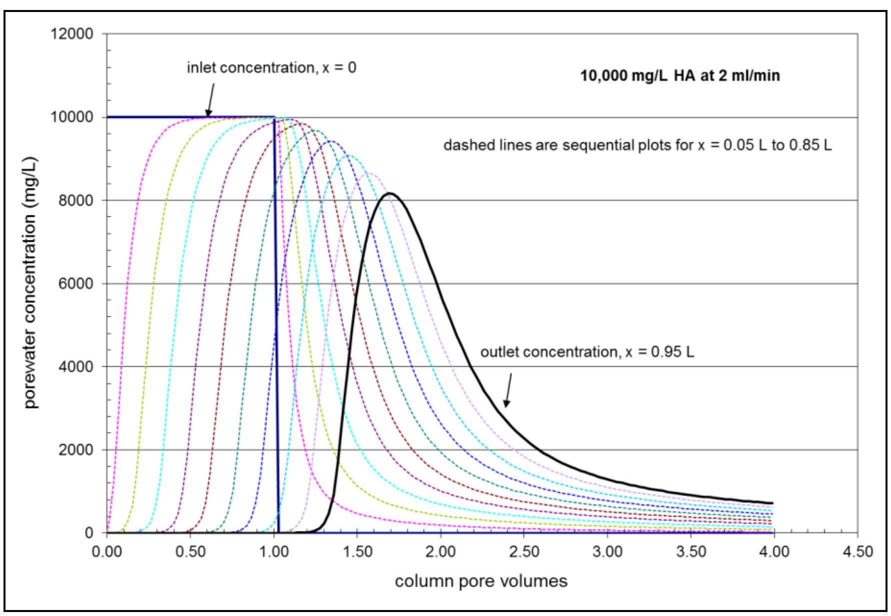

Figure 6. Huma-K injection scenario at 10,000 ppm at 2 ml/min.

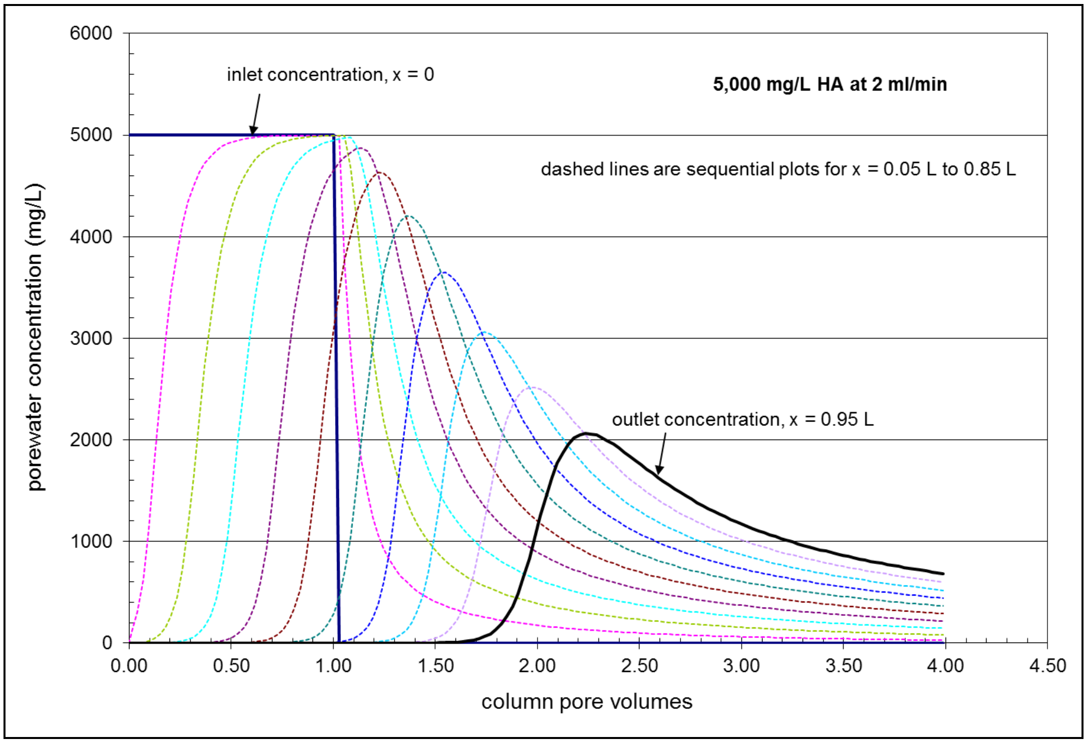

Figure 7. Huma-K injection scenario at 5,000 ppm at 2 ml/min.

Bromide Tracer Tests

Two columns were filled with oven dried SRS soil that was sieved through a 2-mm sieve; the amount of soil used in each column was 257.511 g and 266.774 g, respectively. After the columns were filled with soil, a bromide tracer test was performed by following the procedure detailed in the methodology section. The data obtained from the column experiments is presented in Figure 8, Figure 9 and Table 2. Figure 8 shows the change in concentration of bromide versus the volume of collected effluent fractions and Figure 9 shows the cumulative mass of bromide collected (bromide recovery) for both columns. Pore volume, variance and Peclet number were calculated using equations 4-8 as described in methodology sections and the data is presented in Table 2 and Table 3. The variance indicates the spread of the distribution and a greater variance value positively correlates with a greater distribution spread. Column 1 has a pore volume of 85.8 ml whereas column 2 has a pore volume of 74.12 ml; the difference could be due to the variance in soil compaction while filling the columns.

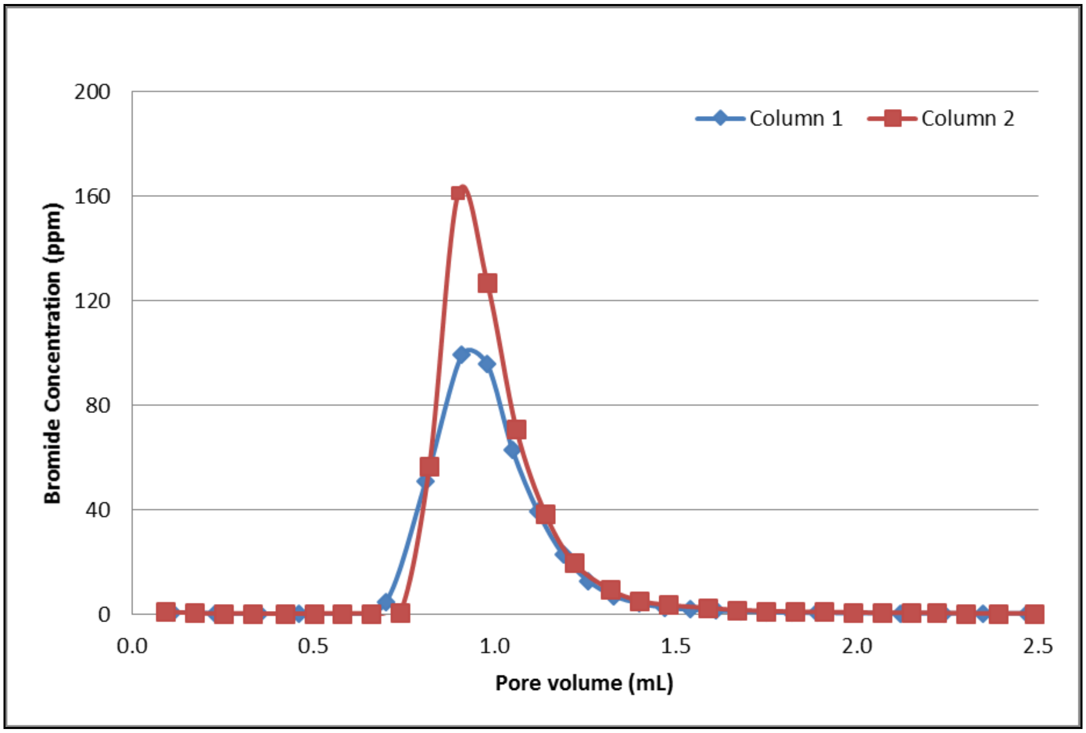

Figure 8. Concentration of measured bromide.

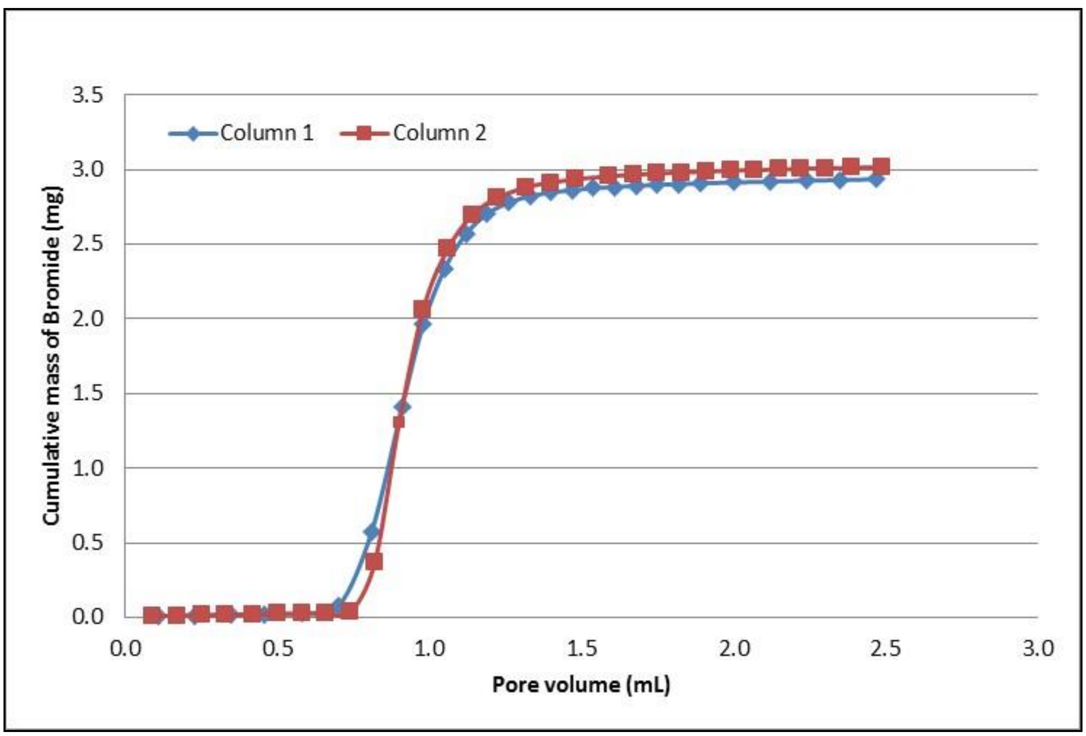

Figure 9. Cumulative mass of measured bromide.

Table 2. Tracer Test Results

Column	Soil weight (g)	Flow rate (ml/min)	Bromide added (mg)	Bromide recovered (mg)	Recovery (%)	Total fluid collected (mL)	Pore volume (ml)
1	257.511	2.0	3.0	2.94768	98.2559	236.709	85.80
2	266.774	2.0	3.0	3.01533	100.511	180.998	74.12

The dimensionless Peclet number (Pe) is defined as the ratio of the rate of transport by convection to the rate of transport by diffusion or dispersion (Eq. 9). Pe found experimentally from the tracer test was used to calculate effective dispersion (Table 3); the values of the Peclet number were used to correlate the effect of dispersion on the effluent tracer concentration. The results from Table 3 show intermediate amounts of dispersion (1/Pe) in the range of 0.024 - 0.03.

$$Pe = \frac{rate\, of\ transport\, by\, convection}{rate\, of\ transport\, by\, diffusion\ or\ dispersion} = \frac{UL}{D_a} \qquad \text{Eq. (9)}$$

Where:
L - characteristic length term (m),
D_a - effective dispersion coefficient (m^2/s), and
U - average interstitial velocity (m/s).

Table 3. Transport Parameters Determined by Bromide Tracer Injections

Column	U (m/s)	Variance, σ^2	Pe	Dispersion (m^2/s)	1/Pe=D/uL	Dispersion
1	4.09×10^{-4}	107.24	33.3	3.68×10^{-6}	0.03	Intermediate
2	4.09×10^{-4}	63.34	42.35	2.90×10^{-6}	0.024	Intermediate

Sorption and Desorption Experiments

Following the bromide tracer test and preconditioning of the column, 1 PV of 5000 ppm of Huma-K with pH adjusted to 9 was pumped at a flow rate of 2 ml/min. The humic solution was stirred continuously while pumping to avoid settling. After injecting approximately 1 PV of the humic solution, 4 PV of artificial groundwater solution with pH adjusted to 3.5 and 5.0 was injected into columns 1 and 2, respectively. Effluent samples were collected at regular intervals, the pH of the samples was measured, and the humic acid concentration was measured using a UV-Vis spectrophotometer. Figure 10 shows the breakthrough curve of humic acid in the columns. It is evident from the curve that most of the humic acid injected into the column was retained in the column and no humic acid was observed in the effluent solution until after 1.5 pore volumes. After 1.5 pore volumes, the concentration of humic acid increased and reached a peak value of 6,000 ppm and 5,700 ppm for columns 1 and 2, respectively. A possible explanation is the precipitation and re-dissolution of HA as it moves through the column. When HA, pH 9, is injected in the pH 3.5 column, it may have precipitated; as more is injected, the precipitate is pushed down along with the feed solution and gravity. While HA moved down the column and the pH of the solution is increased, re-dissolution may have occurred, causing the spike in concentration for about 0.5 PV. After this, higher concentrations are no longer seen. This possibility also explains why the outlet concentration was greater than the inlet concentration. Around 2 PV, the concentration of HA started to decrease and then reached equilibrium. Because of precipitation, the amount of HA sorbed is inconclusive and the term “retained” is used over “sorbed” in this report.

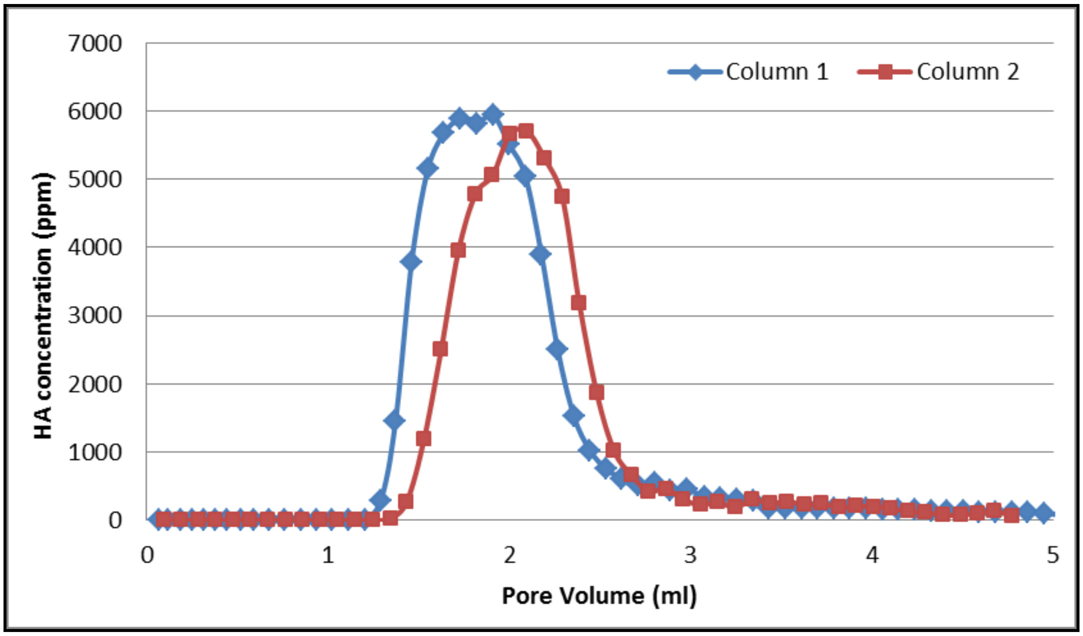

Figure 10. Concentration profile of HA in the effluent of the column.

Figure 11 shows the total mass of HA collected from the column; the amount of HA retained in the column was estimated by subtracting the amount of HA recovered from total HA injected (Table 4). Figure 12 shows the change in the amount of HA retained in the column with the pore volume of solution injected through the column.

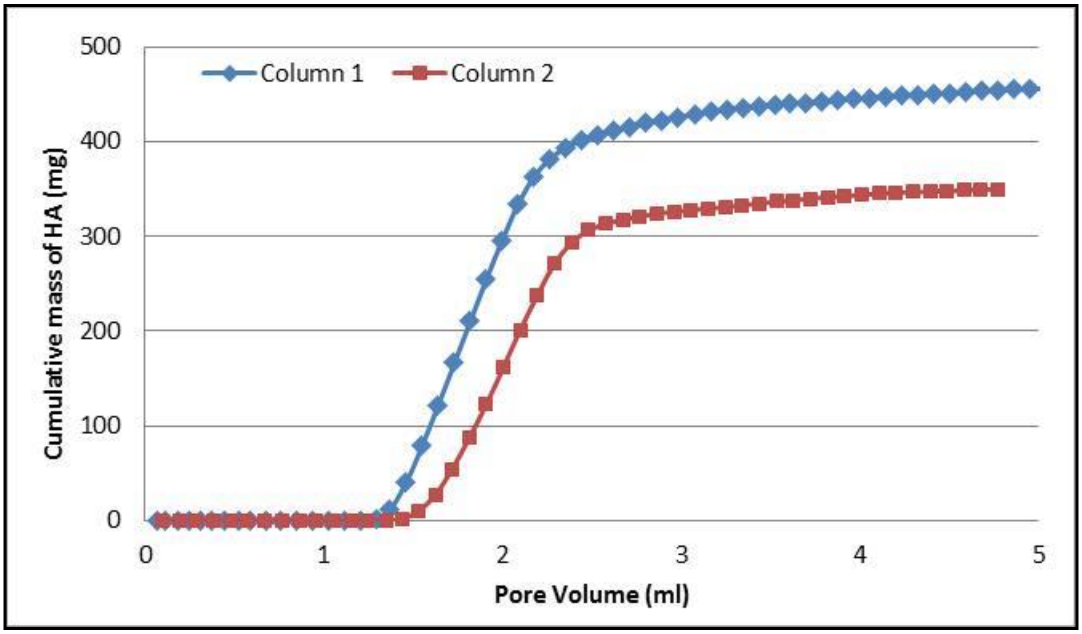

Figure 11. Cumulative mass of humic acid collected.

Table 4. Soprtion of Humic Acid

Column	Soil weight (g)	pH		Humic acid				
		Initial	Final	Volume injected (ml)	Injected (mg)	Recovered (mg)	Retained (mg)	Total Retained (mg/kg)
1	257.51	3.72	6.46	115.21	576.03	457.14	118.89	461.67
2	266.77	4.77	7.08	104.30	521.52	350.06	171.46	642.69

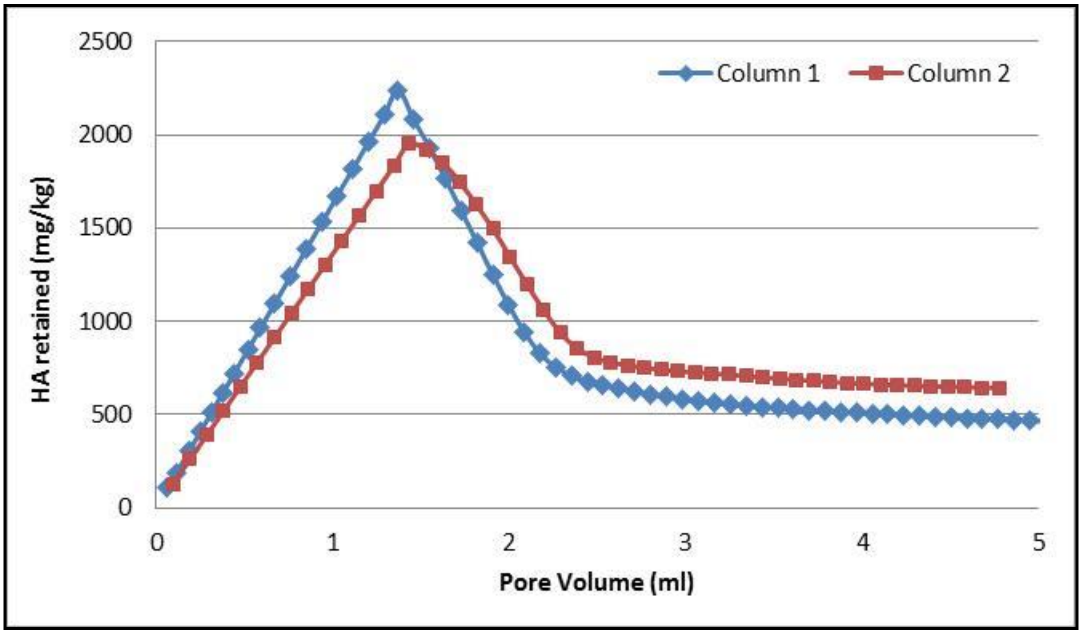

Figure 12. Retention of HA in columns.

In summary, HA may precipitate more strongly in lower pH and this explains why pH rose faster (Figure 13) in column 1 compared to column 2 where more buffering occurred, even though both eventually reached a stable 6-7 pH.

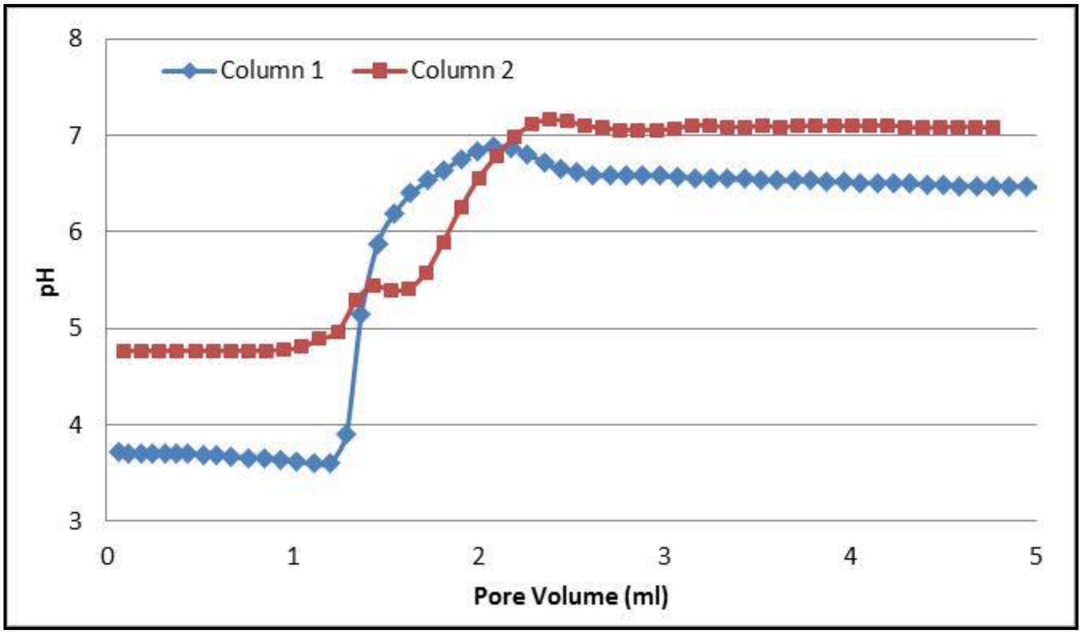

Figure 13. Change in pH of the columns.

The simple Langmuir model (Figure 6 - Figure 7), was used to observe how HA injection scenarios differed from actual column output curve. The peak concentration is 2500 ppm in the model and 6000 ppm in the experiment. The tail end concentration is 2000 ppm in the model and almost zero in the experiment. The model did not account for precipitation and re-dissolution that may have occurred, which influences the deployment approach if the results remain consistent. The model also assumes constant pH/parameters, while in the actual column, pH changes dynamically. The pH profile shows that the columns maintain 6-7 pH even after 4 PV of AGW have been injected, which can be considered in deployment for long term phases. The results demonstrate a realistic outcome and will be more useful for the development of a deployment model.

Overall, more HA was retained in column 2 preconditioned with a pH 5 AGW as compared to column 1 that was preconditioned with a pH 3.5 AGW solution. With an increase in pH from 3.5 to 5.0, the overall retention of HA increased by 180 mg per kg of soil, from 461 mg/kg in column 1 to 642 mg/kg for column 2. The results were different than what was expected, as previous studies have shown more sorption should occur at a lower pH.

Future Work

FIU will complete the humic acid sorption/desorption experiments at pH 6 and 7 to include a broad range of field conditions to be able to incorporate the results into a subsurface flow, fate and transport model of humic acid. FIU will also inject uranium into the soil columns to study the effect of sorbed humic acid on the mobility of uranium through porous media.

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TASK 2: SURFACE WATER MODELING OF TIMS BRANCH

This research is part of continued efforts to correlate the hydrology of the Savannah River Site (SRS) and Tims Branch Watershed (TBW) with the distribution of tin within the overland and river sub-domains. Tin was introduced into TBW during the application of an innovative remediation technology implemented by the U.S. Department of Energy's Office of Environmental Management, which involved the injection of stannous (tin) chloride into mercury contaminated groundwater. Understanding the fate of tin and its compounds is of primary importance due to their potential impact on the environment. Tin methylation in particular is of great environmental concern because of its toxicity to humans and animals. Although tin is primarily deposited as sediment, remobilization may occur during episodic extreme events, such as storms or heavy rainfall. In these cases, sediment can be resuspended in the water column and deposited further downstream. It is therefore important to study the fate and transport of tin during such events, in particular its potential for methylation. The main objective of this study, therefore, was to develop an overland hydrology model (MIKE SHE) capable of simulating surface flow depth and velocity throughout the TBW. The modeling application used historical precipitation, groundwater levels, geological data, and river discharges that were retrieved from government databases and input to the model. The model was developed to simulate flow discharges, flow duration, and water levels.

INTRODUCTION

The United States remains adversely affected by the nuclear arms race of the Second World War. Today, facilities like the A/M area of the Savannah River Site (SRS) in South Carolina, which contained the main SRS administrative functions and manufacturing areas, are part of a long-term clean-up strategy in the U.S. In the 1950's and 60's, SRS used millions of pounds of heavy metals, primarily mercury, and solvents such as trichloroethylene (TCE) to produce tritium and separate plutonium-239 for the nation's defense program. The A and M Areas are addressed together because of their proximity and commingled contaminants and constitute one of the largest groundwater contamination areas in the country resulting from the production of fuel and target assemblies, research and development operations, and the disposal of waste and general debris after operations were started and before the establishment of rigorous solid waste management controls. Principal contaminants include solvents in the groundwater and vadose zone; however contamination is also found in surface water and infrastructure. Mercury treatment at SRS started in 2007 by injection of stannous (tin) chloride into the contaminated groundwater. As a result, mercury was removed as a vapor and tin dioxide was precipitated in the sediment. Tin in its elemental form is not very toxic to any kind of organism, but the organic form is toxic. Organotin compounds are very persistent and not readily biodegradable; they may persist in the environment for long periods of time. They are known to be toxic to aquatic ecosystems (Amouroux et al., 2000). Therefore, understanding the fate of tin and its compounds is of primary importance due to their potential impact on the environment (Donard and Weber, 1985; Maguire et al., 1986). Tin methylation is of great environmental concern because of its toxicity to humans and animals. Although tin is primarily deposited as sediment, remobilization may occur during episodic extreme events, such as storms or heavy rainfall. In these cases, sediment can be resuspended in the water column and deposited further downstream. It is therefore important to study the fate and transport of tin during such events, in particular its potential for methylation.

Numerical modeling has proven to be a cost effective tool in studying natural processes such as hydrology and fate and transport of contaminants. Numerical modeling can provide insight into how sediment may become resuspended, transported and redistributed in a waterbody during various extreme weather scenarios. It is possible to approximately determine the path of tin through the affected watershed using advanced watershed modeling software. MIKE SHE is an integrated surface water and groundwater software that can simulate the entire land phase of the hydrologic cycle, map the vulnerability of the aquifer, and delineate the floodplain for the watershed.

The objective of this task is to develop an integrated surface water and groundwater model to predict the fate and transport of tin in Tims Branch. This report describes the preliminary development of the hydrological model of Tim Branch using the MIKE SHE model and the extensive pre-processing that was carried out to prepare the data for input into the model. The next phase of development will involve coupling of the MIKE SHE component with a 1-D river network model (MIKE 11) to estimate flow velocity and depth in Tims Branch and its outfalls. The final integrated model will include a fate and transport module (ECO Lab) which will predict the tin spatiotemporal distribution in Tims Branch under various climate scenarios.

SITE CHARACTERIZATION

Study Area

During the cold war, the U.S. Department of Energy (DOE) built various facilities around the United States to produce nuclear materials including lithium isotopes. SRS is one of the many nuclear facilities owned by DOE. SRS is in the sand-hills region of South Carolina and covers approximately 800 km^2. It encompasses parts of Aiken, Barnwell and Allendale counties and is bordered on the west by the Savannah River and the state of Georgia (Figure 14). SRS is close to several cities, including Augusta, Georgia and Columbia, South Carolina. It is located 24 km southeast of Augusta, Georgia, and 16 km south of Aiken, South Carolina. It is also within a few hours of Atlanta, Savannah, Charleston, Greenville and Charlotte (Figure 14).

SRS includes facilities such as reactors, laboratories, waste disposal sites, cooling towers, incinerators, etc. After several years of nuclear operations at the site, pollutants such as heavy metals, particularly mercury, and solvents such as trichloroethylene (TCE) have entered the environment, contaminating the soil, surface water and groundwater.

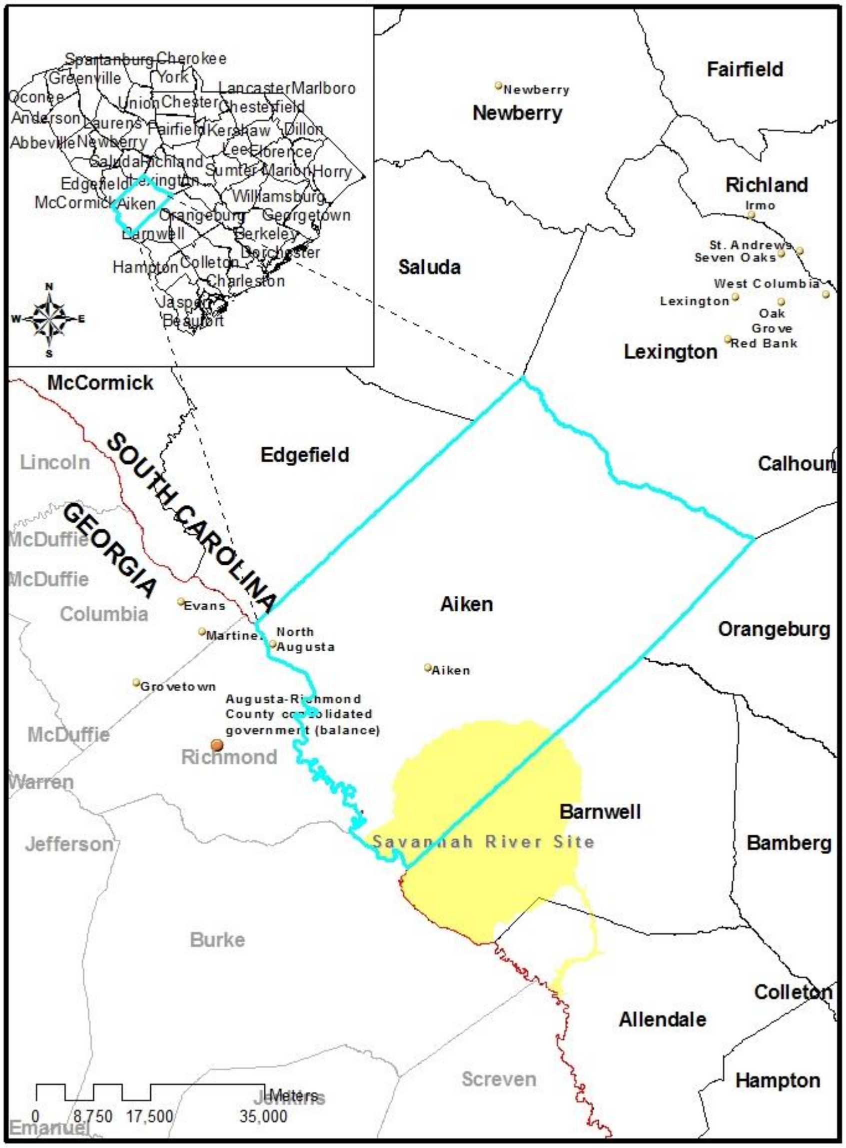

Figure 14. Location of Savannah River Site, SC.

SRS is home to the A/M area. This area is located in the northwest portion of SRS and covers approximately 0.33 km^2 (86 acres). Beginning in 1952, SRS produced nuclear materials. An important step in the production cycle was the manufacture of fuel and target assemblies in the M-Area for the nuclear reactors. The manufacturing processes in the M-Area consumed a large quantity of industrial cleaning solvents and water. Early practices included the discharge of spent solvents and water directly into the environment. The major production facilities used industrial cleaning processes and products such as trichloroethylene, tetrachloroethylene and trichloroethane, which were discarded to the M-Area Settling Basin via process sewer lines.

Tims Branch is a tributary of Upper Three Runs which is a tributary to Savannah River along the border of Georgia and South Carolina, and its watershed is contained within the larger Upper Three Runs watershed (Figure 15).

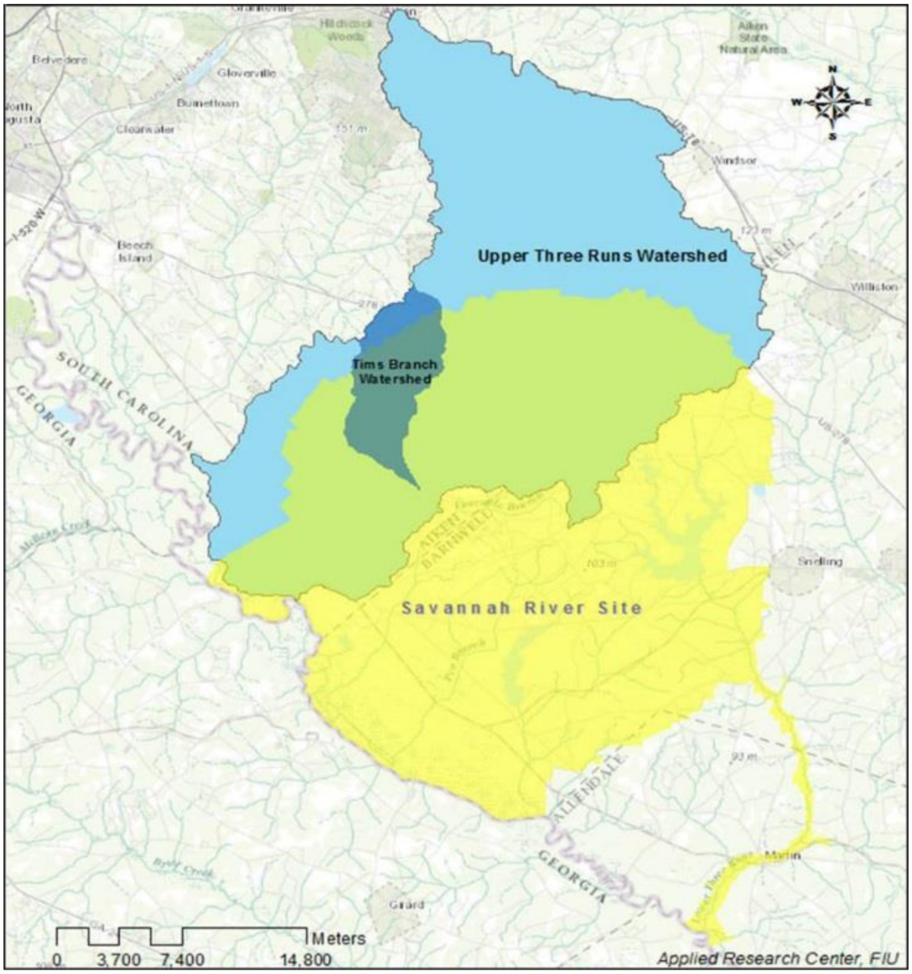

Figure 15. Tims Branch Watershed (TBW).

Tims Branch is a small braided, marshy, second-order stream within SRS that starts at the northern portion of SRS and passes through Beaver Ponds 1-5 and Steed Pond, and eventually discharges into Upper Three Runs (Figure 16). Its drainage area is nearly 16 km^2 (Batson et al., 1996). The length of this stream from outfall A-014 to Upper Three Runs is approximately 8 km. The average width of the stream varies between 2-3 m. Two major tributaries of Tims Branch are A-014 and A-011 outfalls which are approximately 230 m apart. They combine with the main stream of Tims Branch 1,400 m from the A014 outfall (Hayes, 1984). Flow in Tims Branch is strongly influenced by groundwater discharge (Mast and Turk, 1999). Because of the water table elevation and Tims Branch bed elevation, it is considered to be a losing stream (surface water discharges into the groundwater) near the A/M outfalls and a gaining stream (groundwater discharges into the stream) further south toward the confluence with Upper Three Runs (Looney et al., 2010; Varlik, 2013).

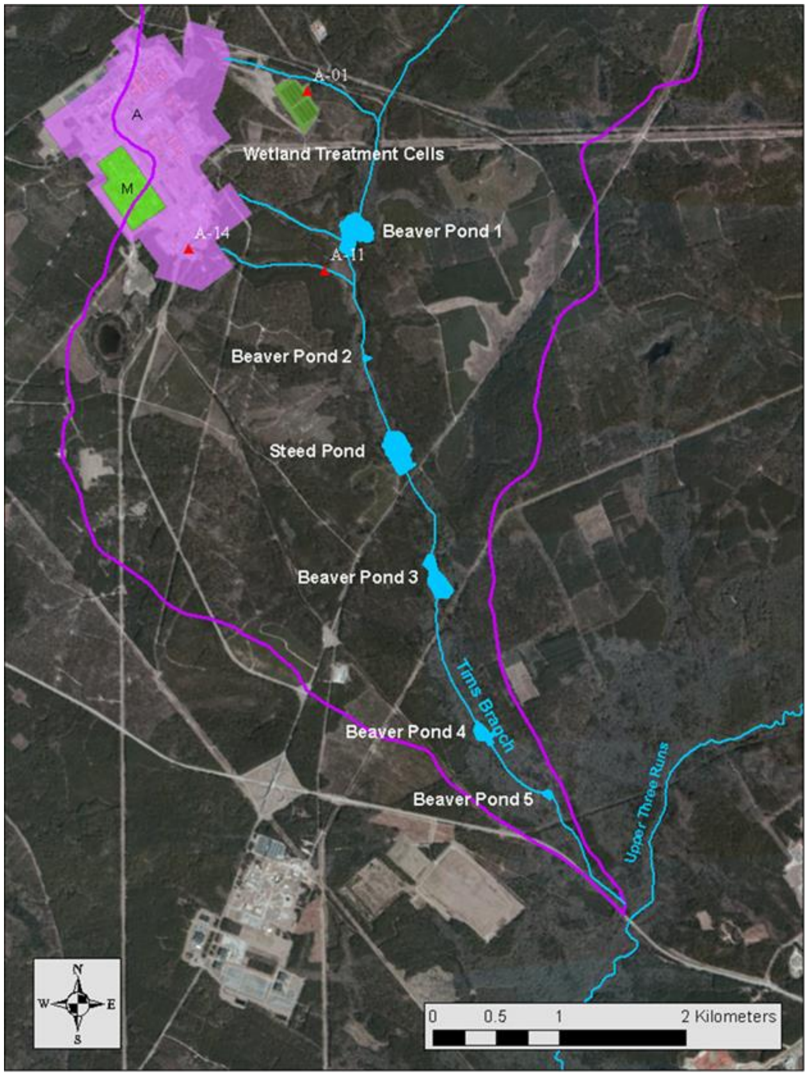

Figure 16. Tims Branch and Beaver Ponds 1-5.

Geology and Topography

SRS is a typical coastal plain watershed that includes a network of rivers and streams that are tributaries to the Savannah River which is the border between South Carolina and Georgia, and a portion of it borders the SRS (Halverson, 2008). The Savannah River is formed by the confluence of the Tugaloo and Seneca Rivers in northeast Georgia and flows southeast through the Piedmont and Coastal Plain to the Atlantic Ocean.

The general topography of SRS includes upper and lower coastal plains. Lanier (1997) described the upper Coastal Plain as consisting of rounded hills with gradual slopes, areas of highly irregular terrain, and some elevations exceeding 200 m above sea level. The highest elevation at SRS is approximately 130 m above sea level, near Tims Branch and the northwest boundary of SRS. The land surface elevation at the boundary of the upper and lower Coastal Plains, located southeast of SRS, is usually less than 60 m above sea level. Upper Coastal Plain stream slopes range from 1.0 to 4 m/km (Lanier, 1997). Figure 17 shows the Digital Elevation Model of TBW.

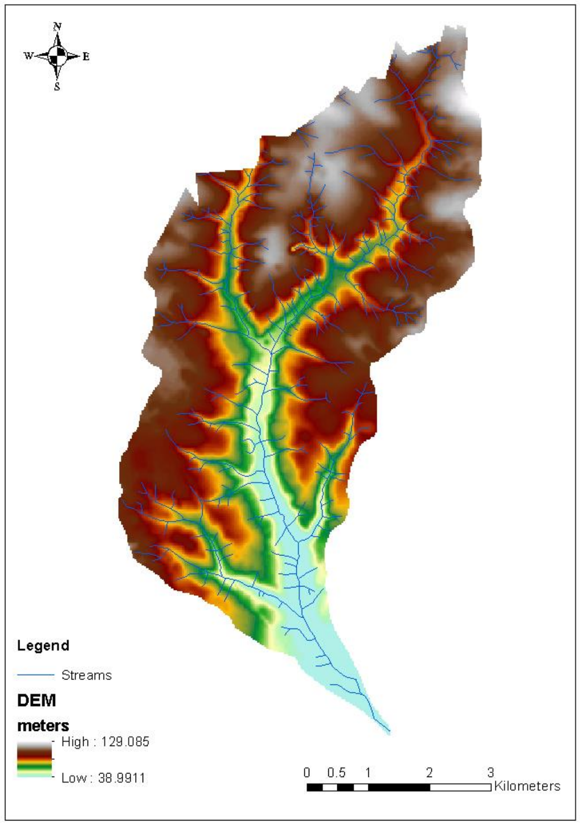

Figure 17. Digital Elevation Model (DEM) of TBW.

Figure 18 is a general geologic map of South Carolina downloaded from the South Carolina Department of Natural Resources (SCDNR) website. As illustrated in this map, the geology of the SRS area is classified primarily as Tertiary (Pliocene, Paleocene, Eocene, and Miocene) and Triassic (Triassic Basins).

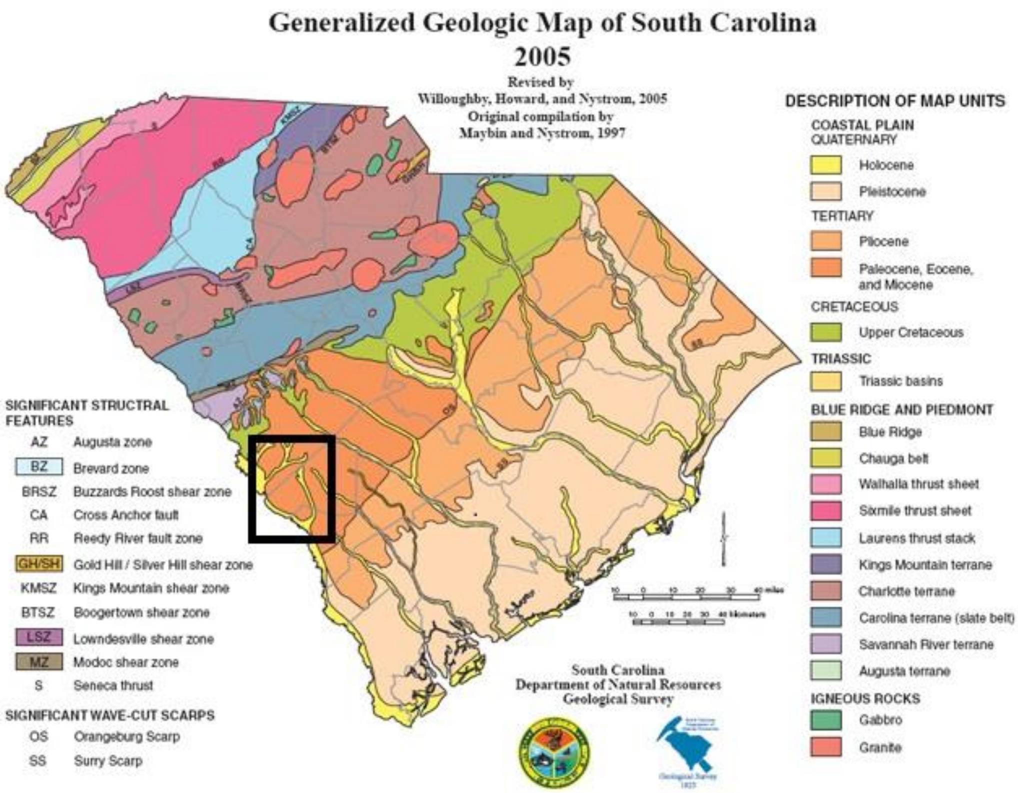

Figure 18. Map of South Carolina geology. The study area is indicated by a black rectangle. (http://www.dnr.sc.gov/geology/geology.htm).

Streams

Major tributaries from SRS to the Savannah River include Upper Three Runs, Beaver Dam Creek, Fourmile Branch, Steel Creek, and Lower Three Runs (Figure 19). Upper Three Runs Creek is a 40-kilometer (20-mile) waterway that meanders through hardwood and cypress forests on the Savannah River Site. It empties into the Savannah River. The creek is a blackwater stream because of its high concentration of naturally occurring tannic acid that gives the water its tea color. Forty-kilometers (20-miles) long, Lower Three Runs leaves the main body of SRS and runs through parts of Barnwell and Allendale Counties until it flows into the Savannah River. Government property on both sides of the stream acts as a buffer as it runs through privately-owned property. Fourmile Branch begins just upstream from Road F and flows into the Savannah River. It is about 242 km (150 miles) long and enters the Savannah River Swamp approximately 3.4 km (11,400 ft) upstream from its confluence with the Savannah River; downstream from this point, Fourmile Branch becomes braided and mixes with flow from the Savannah River.

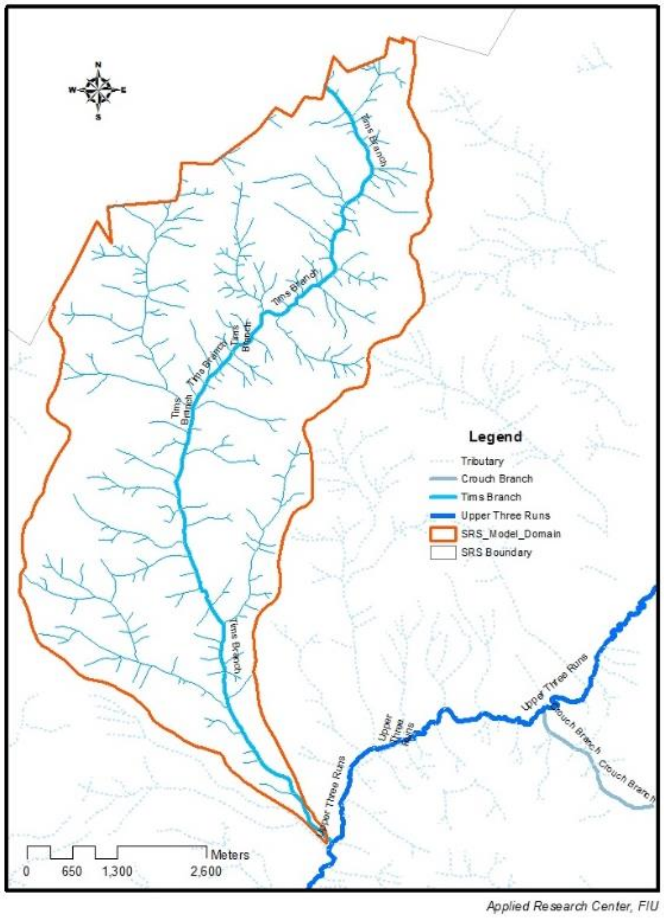

Figure 19. Tims Branch Watershed stream system.

Land Use/Land Cover

Tims Branch watershed (TBW) is home to a variety of land uses and land covers. The A/M area operates within the TBW and occupies about 14% of the total watershed area.

Figure 20 maps the developed areas of the TBW, including roads and buildings, and illustrates the percent of impervious cover. Over 6 km of the total area of TBW has an imperviousness of 14% or less. This indicates that, overall, the watershed is mostly undeveloped or agricultural land. This conclusion is compatible with the land use data, which establishes that about 80% of the watershed is forested or agricultural (**Table 5**).

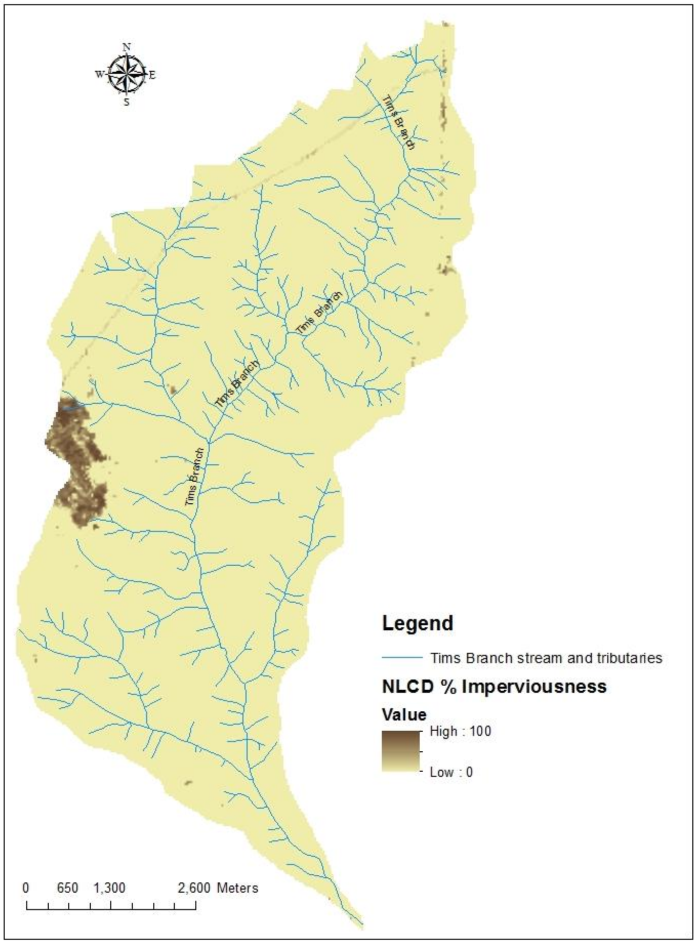

Figure 20. Impervious percentage.

Table 5. Land Use Classifications and Corresponding Manning's M Number Assigned

Land Use	Area (m^2)	%	Manning's M (1/*n*) Number
Agricultural	170,975	0.34	41
Barren Land	58,151	0.12	81
Forest	35,267,379	70.83	21
Rangeland	7,287,896	14.64	25
Urban/Built-up Land	6,816,222	13.69	90
Water	76,866	0.15	11
Wetland	115,658	0.23	23

MODELING HYDROLOGICAL PROCESSES

The hydrology of surface water is proven to be one of the key factors controlling erosion and deposition mechanisms in sediment transport processes in streams and rivers. Therefore, understanding the hydrology of Tims Branch is vital in determining the environmental conditions and the causes of enhanced sediment erosion and deposition in this stream. Developing a conceptual model and performing numerical simulations will provide an improved understanding of how an extreme rainfall or flooding episode may affect the transport of tin in Tims Branch.

A conceptual model describes the general physical framework of the relationship between physical processes that are part of an environment. The hydrologic conceptual model developed for SRS will address processes and features such as discharge points, groundwater/surface water interaction, geological formation, atmospheric characterization, infiltration, sediment erosion /deposition, etc. Very limited studies have addressed the hydrology and sediment transport mechanisms of Tims Branch and SRS. These studies are primarily based on experimental work and field data collections rather than numerical modeling approaches. Modeling hydrological processes and sediment transport mechanisms require a detailed understanding of soil and sediment characteristics, geologic formation, topography, climate, and hydraulic properties. Most of the previous hydrological modeling efforts were conducted in other areas of Savannah River and South Carolina. Conrads et al. (2006) have developed a three-dimensional model of the Savannah River estuary to simulate changes in water levels and salinity conditions in the marsh by coupling a 3D hydrodynamic river-estuary model and the marsh-succession empirical model. The coupled model, however, may not be applicable to SRS and Tims Branch because they only simulate water levels in the marsh areas. In addition, empirical modeling may not produce valid results when applied to other locations.

In a recent study, Feaster et al. (2012) investigated the relationship between hydrological, geochemical, and ecological processes on mercury concentration in fish tissue. They applied two watershed hydrology models to the Mc Tier Creek watershed in South Carolina: a topography-based hydrological model, TOPMODEL (Beven and Kirkby, 1979; Wolock, 1993), to simulate surface flow hydrology, and a grid-based mercury model, GBMM (Dai T. et al., 2005), to simulate the fate and transport of mercury. Because TOPMODEL generates stream flow based on a variable-source-area concept, the model only reflects how rainfall moves through the watershed to become stream flow, so it is not feasible to apply it for an existing stream such as Tims Branch. In a similar study, Feaster et al. (2014) investigated the potential for scaling up the previous application of TOPMODEL for the Mc Tier Creek watershed (small scale) to the Edisto River Basin (large scale) in South Carolina.

As none of the previous hydrological modeling efforts were specifically applicable to SRS and Tims Branch, it is critical to develop a site specific flow and transport model to better understand the fate and transport of tin in surface water. FIU-ARC is developing an integrated flow and transport model using the MIKE software package created by the Danish Hydraulic Institute (DHI). The integrated flow and transport model (MIKE SHE/MIKE 11/ECO Lab) analyzes the effect of hydrological events on potential tin erosion, resuspension, and transport in the Tims Branch Watershed. The model includes the main components of the hydrological cycle and sediment transport; groundwater flow (saturated and unsaturated), overland flow, precipitation, and evapotranspiration. The objective of the model is to provide a spatiotemporal distribution of tin in the sediment of Tims Branch and forecast the fate and transport of tin and its possible methylation when an extreme event happens.

CONCEPTUAL MODEL DEVELOPMENT

Considering the flow and transport pathways to Tims Branch including outfalls, groundwater flow and surface flow, and other hydrological cycle components, a data-driven site specific conceptual model has been developed for the tin transport in Tims Branch (Figure 21) which includes the location of outfalls, ponds, and other particular features in the area. Water flows into Tims Branch from two locations: A-01 and A-014.

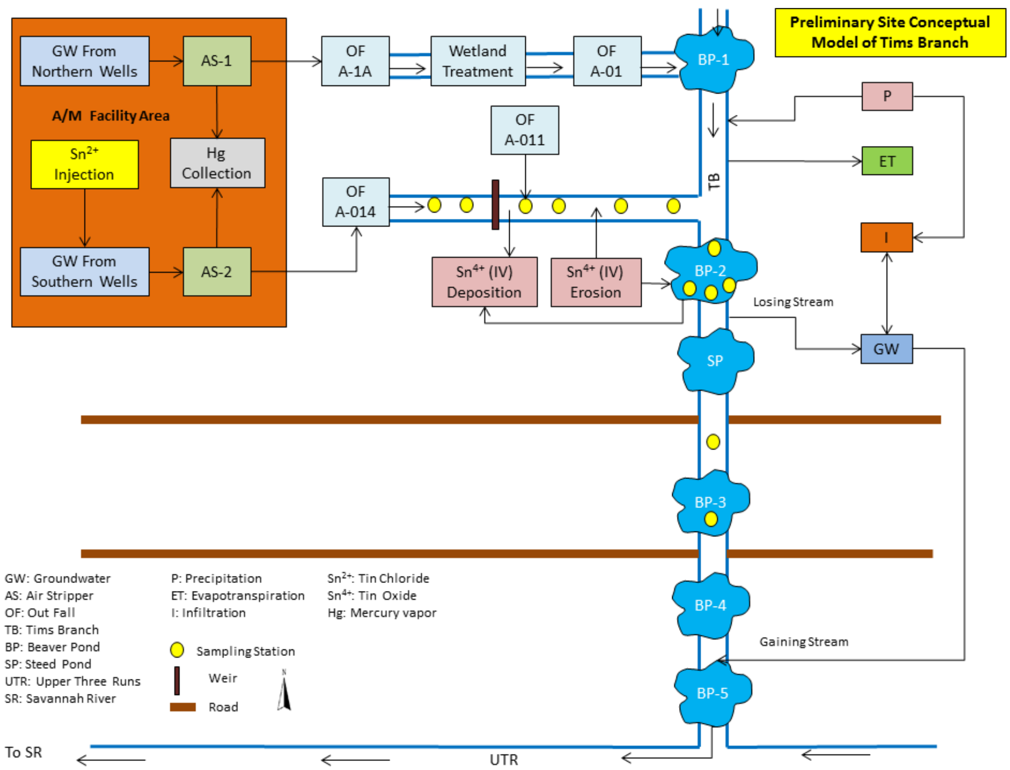

Figure 21. Tims Branch Watershed conceptual model.

A/M wastewater, including cooling water, steam condensate, groundwater treated by air strippers, storm water runoff, steam and air-conditioning condensates, laboratory drain wastewater, well flushing water, and other industrial and sanitary wastewater, are discharged into Tims Branch through several outfalls and flows toward Upper Three Runs and eventually discharges into the Savannah River (Halverson, 2008).

Since the 1950s, Tims Branch has received contaminated wastewater from the A/M area at outfalls A-1A, A-01, A-11, and A-014. The groundwater treatment process was started in 1985. The treatment process consisted of removal of chlorinated solvents using air strippers. Treated groundwater was discharged into Tims Branch. In November 2007, as part of mercury removal efforts, tin chloride ($SnCl_2$) was injected into the groundwater right before entering the air stripping system in order to convert mercury (II) to volatile mercury (0) form which could be removed through the air stripper. Dissolved mercury (II) reacts with tin chloride and produces tin dioxide (SnO_2) that precipitates as a sediment to the bottom of Tims Branch:

$$Hg^{2+} + SnCl_2 + 2H_2O \rightarrow Hg_{(g)} + SnO_{2\,(s)} + 4H^+ + 2Cl^-$$

The initial concentration of mercury in the groundwater is approximately 250 ng/L. After treatment with tin chloride, the mercury concentration has significantly reduced to approximately 10 ng/L (Looney et al., 2010). At the same time, the tin (IV) concentration, primarily as inorganic solid deposit, has increased substantially. Therefore, the sediment deposits in Tims Branch are high in tin (IV). Based on field observations and results of the present study, the best estimate of the theoretical average tin (IV) concentration in the sediment in Tims Branch from the A014 outfall downstream to the confluence of Tims Branch with Upper Three Runs Creek is approximately 28 μg/g. The depth of sediments in which tin has accumulated in significant amounts, due to the tin chloride treatment system, is between 1.5 and 3.5 inches. The estimated total tin released in Tims Branch from November 2007 to August 2011 is approximately 43 kg. Although tin (IV) appears to be less toxic than mercury, it is essential to understand tin behavior and the impacts of the treatment system (both negative and positive) in Tims Branch. The literature suggest the possibility of the generation of organotin through a methylation process (Amouroux et al., 2000; Hallas and Cooney, 1981).

There are seven potential areas in Tims Branch that tin (IV) can be deposited: weir site, Beaver Ponds (2-5), and Steed Pond (Figure 16). The weir site and Beaver Pond 2 are the only two sites that show actual accumulation of tin (IV) due to the treatment process in their sediment (Looney et al., 2010). The results from the data collection of tin (IV) concentration indicate that tin accumulation in the sediment along Tims Branch is more non-uniform with some sites showing elevated concentration while the others report less tin accumulation. This non-uniform concentration distribution may be the result of an increase in bed erosion due to a higher discharge rate (450 gpm = 0.028 m^3/s) into Tims Branch after installation of the air stripper (Looney et al., 2010; Looney et al., 2012). Although tin is primarily deposited as sediment along Tims Branch, mainly at the weir site and Beaver Pond 2, remobilization may occur during episodic extreme events such as storms or heavy rainfall. Sediment can be resuspended, enter the water body, and be deposited further downstream in Tims Branch. These suspended particles may be deposited along Tims Branch or carried by water flow further down the stream toward Upper Three Runs and eventually reach the Savannah River. If the environment along the path of particle transport is favorable, tin methylation may happen in the area where tin has been deposited.

Batson et al. (1996) investigated the remobilization of the uranium (U) rich sediment during rainfall events at SRS. Their findings show that a single storm event can effectively erode the sediment and transport it downstream towards Upper Tree Runs. They reported a 15 to 28 fold increase in U transport out of the Tims Branch system during storm events due to sediment erosion. They showed that as little as 16 mm of rainfall was needed to cause a significant increase in stream turbidity and resuspension of sediment. This process may apply to tin sediment erosion when an extreme event occurs.

Looney (2001) has identified three main uncertainties related to mercury treatment using stannous chloride: tin methylation through aerobic and anaerobic processes, tin mediated mercury methylation, and deposition and accumulation of tin in sediments. While the fraction of tin that was observed to be methylated by natural processes in many environments was relatively low and the conditions that maximize methylation (e.g., high salinity) are not present in typical freshwater streams, the potential exists for tin methylation in freshwater streams and riparian systems receiving long term discharges from outfalls being treated using stannous chloride and air stripping.

PRE-PROCESSING OF MODEL DATA

Development of hydrological models requires data that may include thousands of groundwater monitoring wells, boreholes, stream reaches with gauges, weather stations, land cover, vegetation, soil type, topography, geology, water quality and satellite imagery. The MIKE SHE model uses an extensive amount of geographic information systems (GIS) data inputs for many of its configuration parameters. In order to support hydrological model development for the Tims Branch Watershed, GIS tools were used to (1) develop an ArcGIS geodatabase to store and manage GIS and timeseries data; (2) pre- and post-process model-specific data; (3) automate repetitive geoprocessing tasks; and (4) produce maps for visualization and reporting purposes. The application of GIS technology enables integration of data derived from multiple sources, which often have different spatial references, are at different scales, and are from different time periods, into a single manageable system.

Development of the SRS Geodatabase using ArcGIS

Development of the geodatabase structure involved the following steps:

1. Import of the XML file generated from an existing geodatabase formerly developed for the Oak Ridge Reservation (ORR) to create a preconfigured database structure for the new SRS geodatabase.
2. Modification of the new SRS geodatabase configuration based on model requirements.
3. Import of GIS and timeseries data.
4. Documentation of the geodatabase design using ArcGIS Diagrammer.

Import of ORR Geodatabase XML File

The SRS geodatabase was built upon the database framework originally developed for hydrological modeling work conducted by FIU-ARC at the Oak Ridge Reservation. The ORR Geodatabase was created based on the ArcHydro and ArcGIS Base Map data models with modifications made for MIKE SHE/11 model-specific input parameters. The Arc Hydro data model is designed to support water resources applications within the ArcGIS environment and possesses a structure that enables linkage with scalable hydrologic modeling tools and applications to model hydrologic systems (Maidment, D. R., 2002).

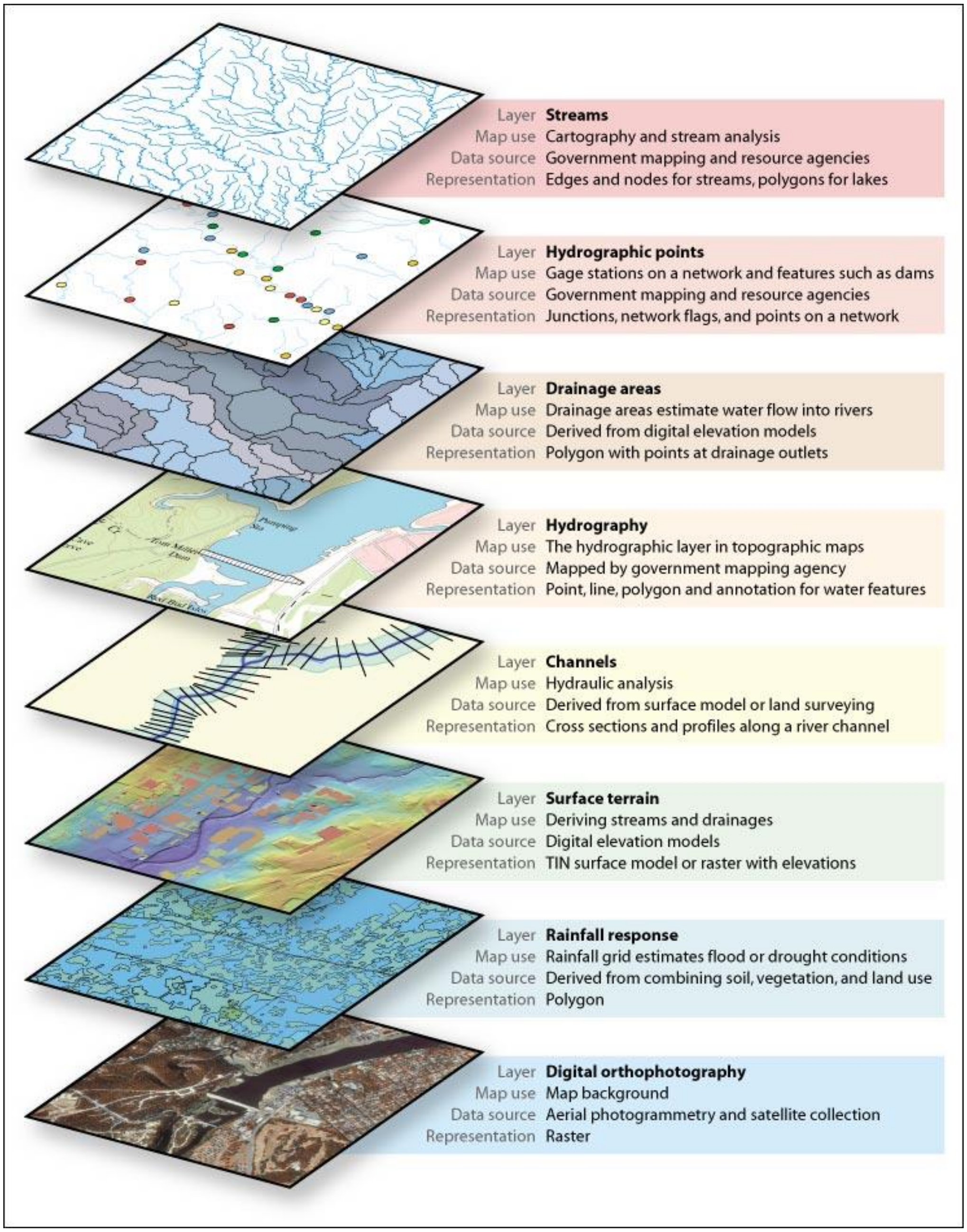

Figure 22. The ArcHydro data model (Maidment, D. R., 2002).

An ArcGIS geodatabase is an XML-based GIS data exchange system which facilitates the export and import of preconfigured data as XML files which contain both the data definition and the data itself. The SRS geodatabase was therefore created by exporting the ORR geodatabase schema using ArcGIS tools as an XML file, and then importing the XML file into an empty file geodatabase to create the new preconfigured SRS geodatabase. Since the ORR database was primarily developed based on the ArcHydro data model, the new preconfigured SRS geodatabase possesses a spatial relational database management (RDMS) schema and relationship structure specific to hydrologic systems where spatial relationships between hydrological parameters and geographical features can be defined. The SRS geodatabase has a standardized data structure which helps in the organization of hydrologic features (e.g. channel cross sections, stream geometric networks and nodes, monitoring points, watersheds and sub-watersheds, and other hydrographic and drainage files) and their relationships to each other, providing a common framework that can be utilized by various hydrologic models. The geodatabase structure also facilitates concurrent multi-user access, editing capability and management of spatial data within the ArcGIS framework and is comprised of a series of tables which contain feature, raster and attribute data, as well as metadata.

The SRS geodatabase structure also adheres to the appropriate security and quality assurance protocols necessary to maintain data integrity. This process exerts control on the type of access all users have to the geodatabase and its datasets, and enables specification of user data management privileges. Connection to the geodatabase requires Windows-authenticated credentials, and specific roles and permissions can be set if necessary. Besides the FIU-ARC firewalls and the built-in software and hardware security protocols, the geodatabase resides on computers which must adhere to FIU's University Technology Services (UTS) Security and IT Policies which are outlined in detail at http://it.fiu.edu/security/index.shtml.

Modification of the SRS Geodatabase Configuration

Once the preconfigured SRS geodatabase was generated, modifications were made with respect to the spatial domain as well as the feature dataset and raster catalog names and properties to configure the SRS geodatabase specific to the study area. GIS data in the ORR geodatabase was stored with the following spatial reference properties: North American Datum (NAD) 83, State Plane Projection (Zone 5301), Units Meters. This was converted in the SRS geodatabase to: North American Datum (NAD) 83, UTM (Zone 17N), Units Meters.

Import of GIS and Timeseries Data

Modeling of hydrologic systems requires large amounts of historical data for development and calibration and includes, for example, GIS coverages/shapefiles of the delineated watersheds, surrounding buildings and man-made structures which may serve as sources of contamination, roads, stream gauge locations, monitoring wells, bore holes, land cover and soils; raster imagery; and observed/measured timeseries data such as flow rates, precipitation, evapotranspiration, contaminant concentration and surface and groundwater levels. Figure 23 below shows the SRS geodatabase system workflow design which depicts the various geospatial and timeseries data types stored in the geodatabase and the implementation of GIS tools for data geoprocessing to convert the files to compatible formats that can be used in the hydrological model.

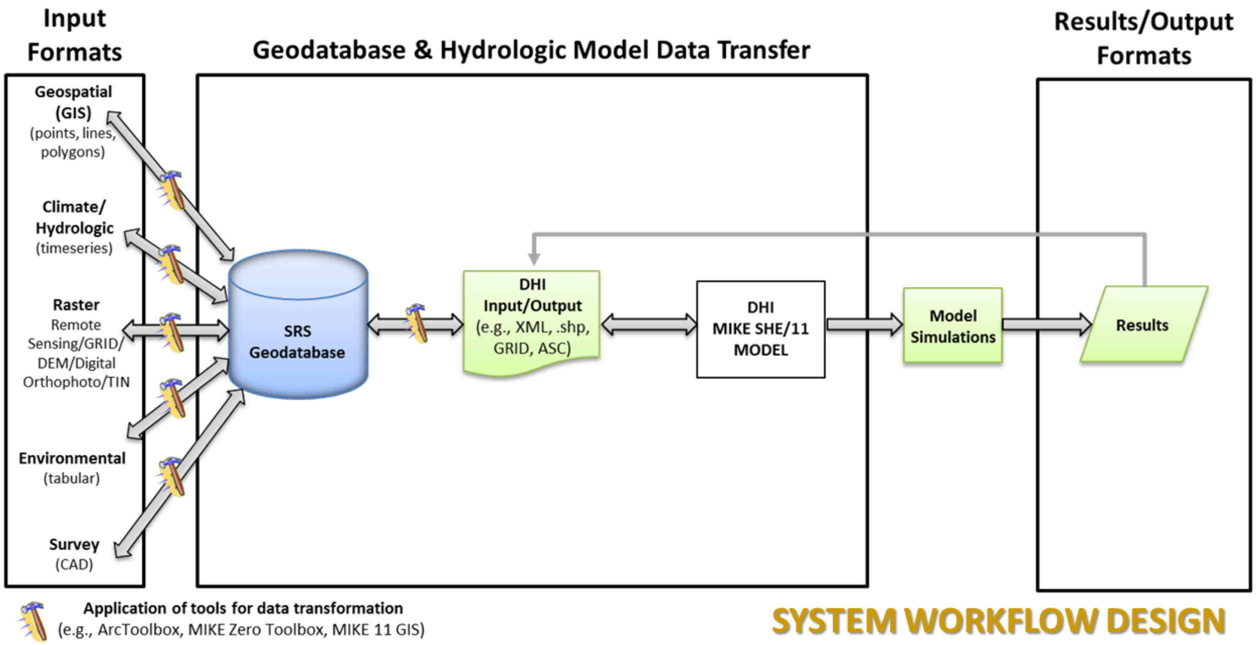

Figure 23. SRS geodatabase system workflow design.

The MIKE SHE/MIKE 11 model uses GIS data inputs for many of its configuration parameters which contain spatial features within the model domain, such as points representing monitoring stations, lines representing rivers/stream networks, or polygons which outline areas such as watershed and catchments (Figure 24).

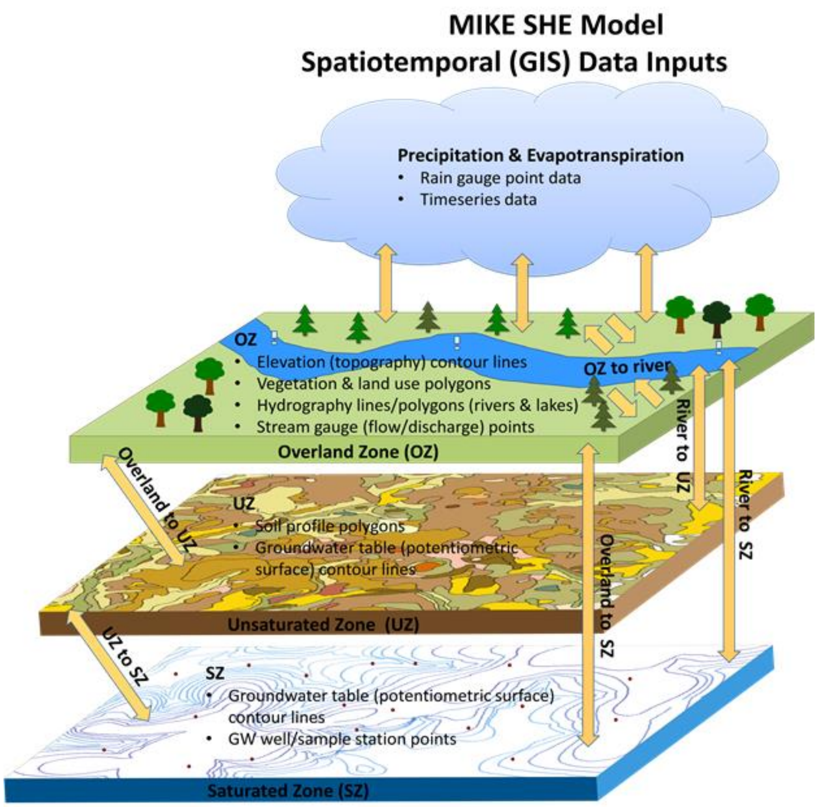

Figure 24. MIKE-SHE model spatiotemporal (GIS) data inputs.

The significance of using GIS data is not just the spatial representation of hydrologic features, but their association with timeseries data attributes such as flow rates and directions, contaminant concentrations, water levels, precipitation, etc. Availability of data in this format shortens the time for data preparation and ultimately model development. Table 6 below shows some of the significant spatial and temporal data inputs used for model development. In Table 6, spatial data names with "FC" at the end represent geodatabase feature classes, while those with "GRID" at the end represent raster/gridded data.

Table 6. Model Configuration Files Stored in the SRS Geodatabase

Spatial Data	Characteristics Represented
Admin_FC	Administrative boundaries (e.g. state, SRS, facility area)
Biota_FC	Threatened & endangered species survey areas
Buildings_FC	SRS buildings
Conductivity_GRIDs	Hydraulic conductivity in grid format
Contaminants_FC	Contaminant plume contours and waste areas
Contaminants_GRIDs	Interpolated contaminant plumes
DEMs	Tims Branch watershed digital elevation model
Digital_Orthophotos	ORR DOQs (.sid files)
Drainage_GRIDs	Drainage time constant, drainage codes, detention storage
Geology_FC	Geological layers (e.g., surface geology, boreholes, fault lines)
GW_FC	Water table lines, piezometer points
GW_GRIDs	Interpolated groundwater level data
HydrographyNet_FC	River network, junctions, flow lines, etc.
Hydrology_FC	Ponds, lakes, streams, flood zones, wetlands, drains, etc.
Impervious_GRIDs	Paved runoff coefficient (GRID)
LandUse_FC	Land Use/Land Cover classification polygons
LandUse_GRIDs	Land Use/Land Cover classification in grid format
Mannings_GRIDs	Manning's roughness coefficients in grid format
Monitoring_Stations_FC	USGS SW monitoring stations, outfalls, GW monitoring wells
Soils_FC	Soil classification polygons
Topography_FC	Elevation contours
Topography_GRIDs	Interpolated elevation contours
Transportation_FC	Roads, railroads, transportation structures, etc.
Vegetation_FC	Vegetation classification polygons
Vegetation GRIDs	Vegetation classification in grid format
Watershed_FC	Watershed boundaries
Temporal Data	**Characteristics Represented**
SRS_rainfall_data_1964_2014	Daily rainfall timeseries
SRS_temp_C_data_1964_2013	Daily temperature (°C) timeseries
SRS_temp_F_data_1964_2013	Daily temperature (F) timeseries
Outfalls_Flowrates	Flow rate timeseries
DHI_Timeseries	Flow rate/discharge timeseries

The majority of GIS data for the hydrological modeling work being conducted by FIU-ARC at SRS was provided by the Savannah River Nuclear Solutions (SRNS) Geotechnical Engineering Department at SRS in the form of an ArcGIS 10 map package. The supporting metadata for many of these files were provided in the form of XML files. ArcMap 10.2 was used to view the GIS data provided, which was stored in several small geodatabases. The ArcToolbox import utility was then used to consolidate the GIS data into the single SRS geodatabase created. The XML metadata files were then were then appended to their associated GIS feature classes using the metadata editor within ArcCatalog.

The accuracy and predictive forecasting ability of 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 SRS site monitoring data sources used in this project include USGS, NRCS STATSGO or SSURGO soil databases, and the U.S. EPA MRLC or NALC land cover databases. Timeseries data (daily rainfall, stream flow and temperature) as well as several reports and journal publications from which several hydrological model parameters were derived, were also provided by Savannah River National Laboratory (SRNL). FIU-ARC researchers also conducted an extensive literature review in order to characterize the study area and retrieve additional data required for model development and calibration. The data derived from these multiple sources was also imported into the SRS geodatabase.

Documentation of the SRS Geodatabase Design Using ArcGIS Diagrammer

Documenting the geodatabase design can assist in representation of the map layers, metadata and other elements specific to the data model used to create the geodatabase. ArcGIS Diagrammer for ArcGIS 10.2 is a downloadable diagramming utility used to create, edit or analyze geodatabase schema. It generates diagrams and reports in the form of editable graphics within an interface similar to Microsoft Visual Studio and serves as a visual editor which accepts XML workspace documents that are created from ESRI’s ArcMap or ArcCatalog.

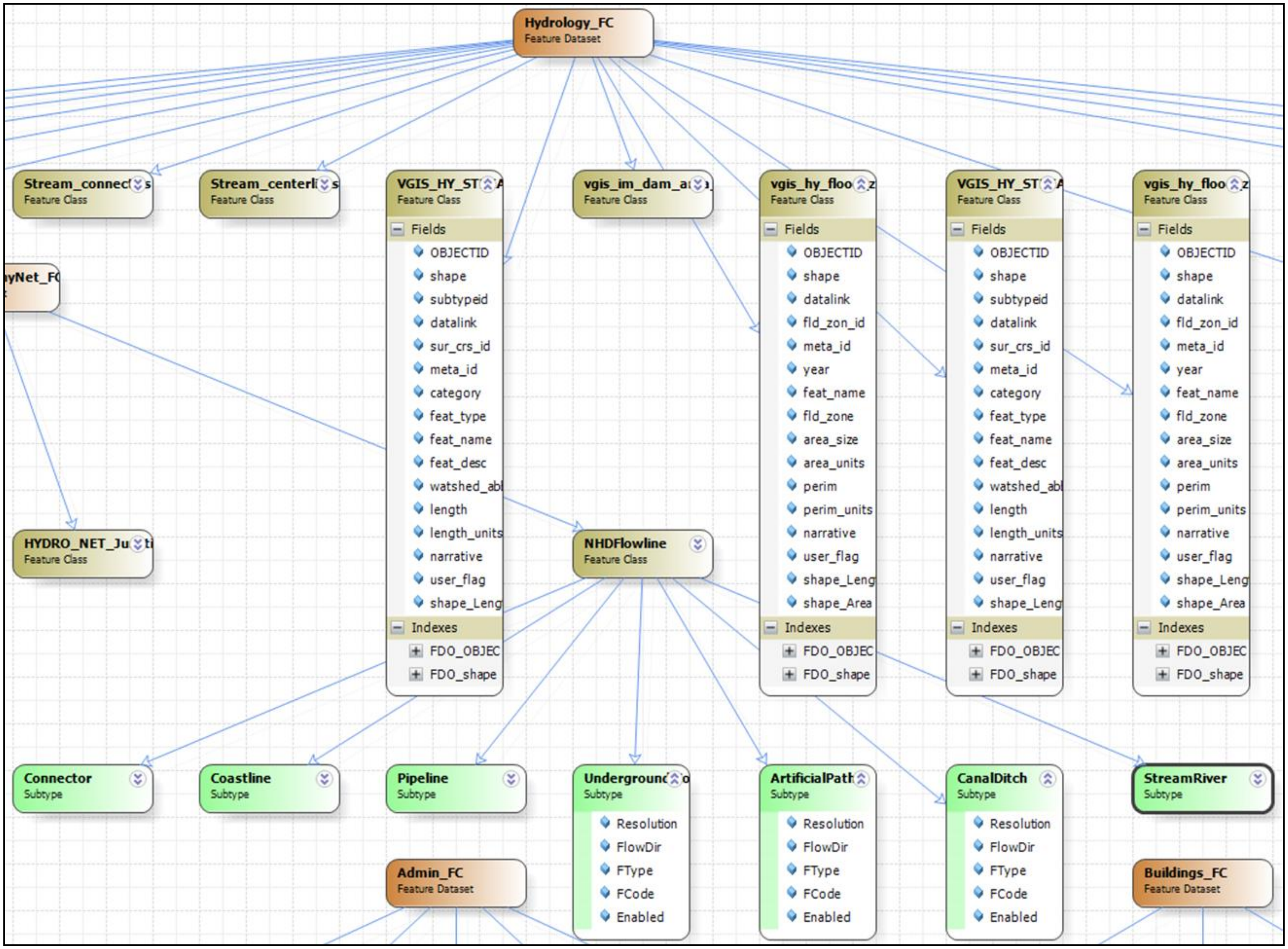

Figure 25. Partial view of the SRS geodatabase schema generated using ArcGIS Diagrammer.

Once the GIS data and associated metadata were imported into the SRS geodatabase, an XML file was exported using the ArcCatalog GUI. This XML file was then imported into ArcGIS Diagrammer to create the SRS geodatabase schema diagram (Figure 25) and data reports (see APPENDIX A. ArcGIS DIAGRAMMER DATA REPORT) which depict the SRS geodatabase structure and details of the features, rasters and tables that have been used or generated during hydrological model development, as well as any existing relationships and spatial references.

The data definition is what provides the basic information for creating a schema diagram described above as well as information related to the feature classes. Subtypes, domains, and relationship classes can also be specified. The data part provides the data values to be inserted into each feature class or table. Some of these key elements are described below:

- **Datasets** – ArcGIS Diagrammer displays the dataset properties to the right of the schema diagram, as seen in Figure 26. Specifications such as feature type (i.e., feature class, raster, relationship class, etc.); shape (i.e., point, line or polygon); spatial coordinate properties (i.e., map projection, horizontal and vertical coordinate systems, spheroid, datum, XY units, and z and m properties); and field names and field types among others can be observed. If subtypes exist, their properties can be viewed here as well.

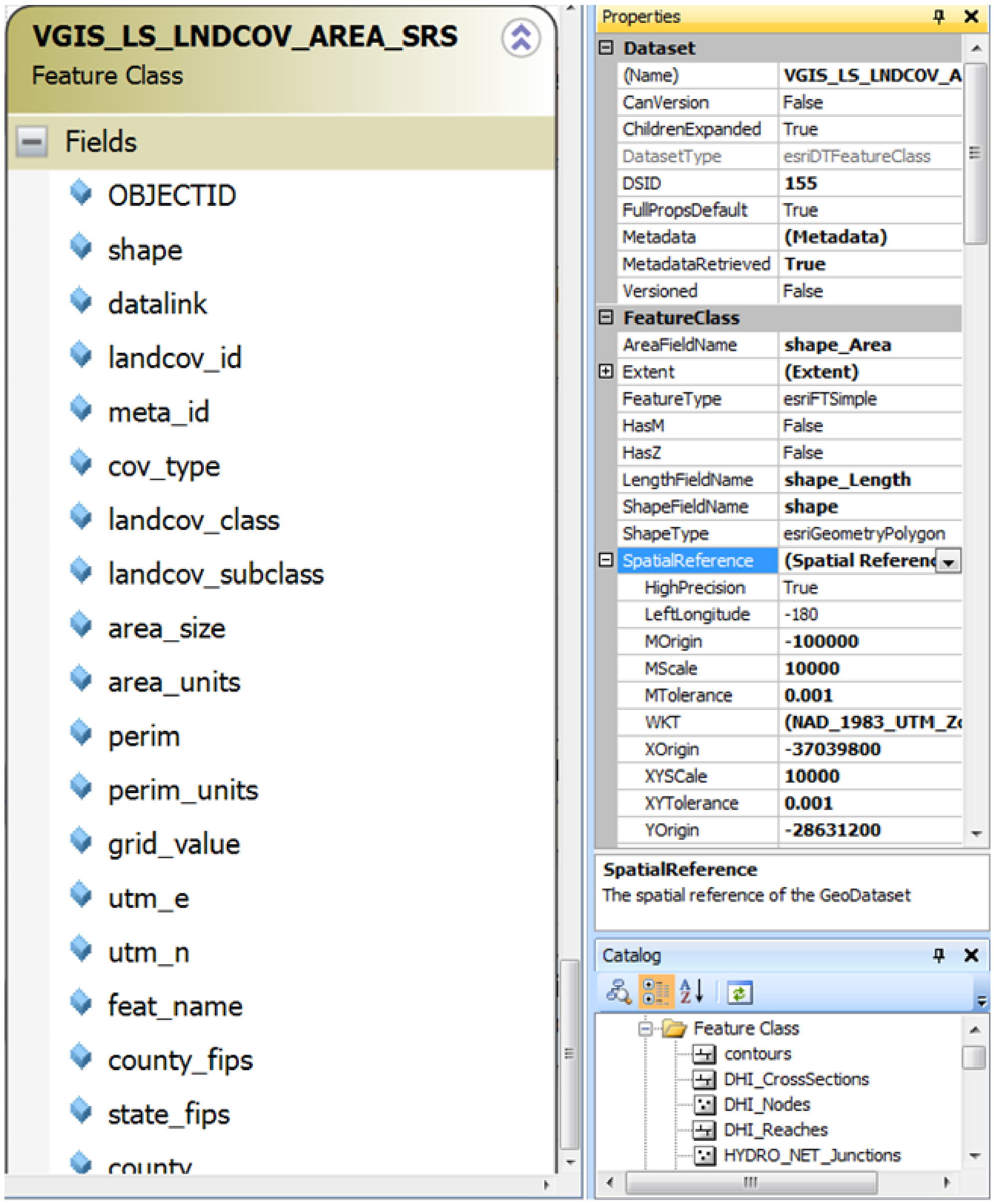

Figure 26. Properties of the SRS land cover dataset viewed using ArcGIS Diagrammer.

- **Relationship Classes** – Relationships between various features are defined in the same manner as in all RDBMS applications. Common attributes in each table are linked to each other through a common field and the rows in one table can be associated with rows in another table as a one-to-one, one-to-many, or many-to-many relationship.
- **Domains** – Domains can be represented in the database schema for each feature to specify valid value lists or ranges for each attribute column, which serves as a means by which data integrity can be enforced.

Spatial relationships and rules such as topologies and networks can also be documented in the geodatabase XML schema diagram in addition to map layer specifications (i.e., how the map features and labels are symbolized and rendered).

Development of Process Flow Models using ArcGIS ModelBuilder

Simple tasks such as retrieving data from the SRS geodatabase; pre-processing the data; exporting for use in hydrological model development; subsequent import and post-processing of model data; data analysis; and production of graphs, maps and reports are repetitive but necessary. The objective of this task, therefore, was to develop a reusable GIS tool which can iterate over the set of spatial MIKE SHE input data parameters, perform geoprocessing actions, calculate statistical parameters and generate maps and reports. The use of ArcGIS ModelBuilder assists in automating these tasks which saves time and can facilitate batch processing of this data. Customization of the geoprocessing tools is also possible using Python scripts if there are hydrological model-specific requirements.

ArcGIS ModelBuilder which has built-in ArcGIS tools was used to automate repetitive model-specific geoprocessing tasks, for example, clipping all of the GIS feature classes to the study domain being used in the MIKE SHE model and then projecting them to UTM coordinates. ArcGIS ModelBuilder generates model workflow diagrams (Figure 27 and Figure 28) to document and visually represent the tools and scripts (if any) that have been incorporated in the data model.

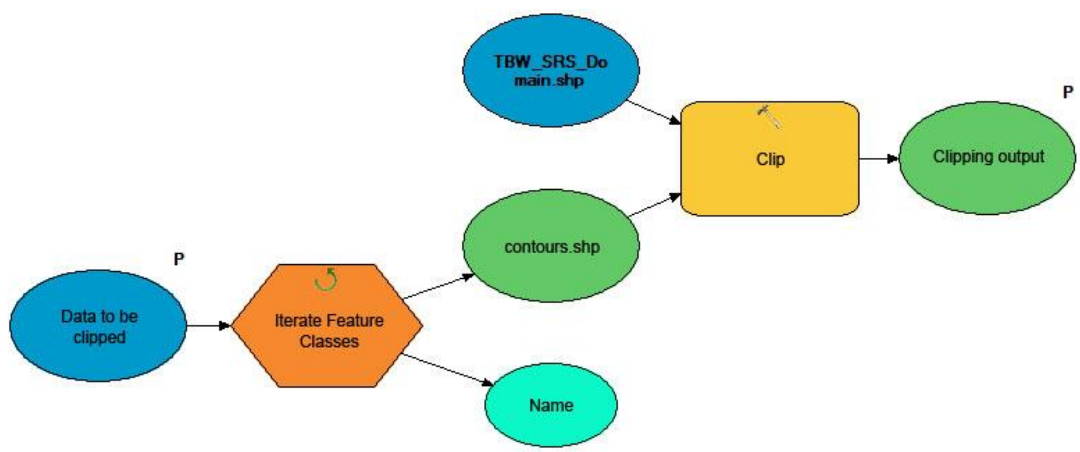

Figure 27. ArcGIS ModelBuilder workflow diagram for clipping GIS data to the study domain.

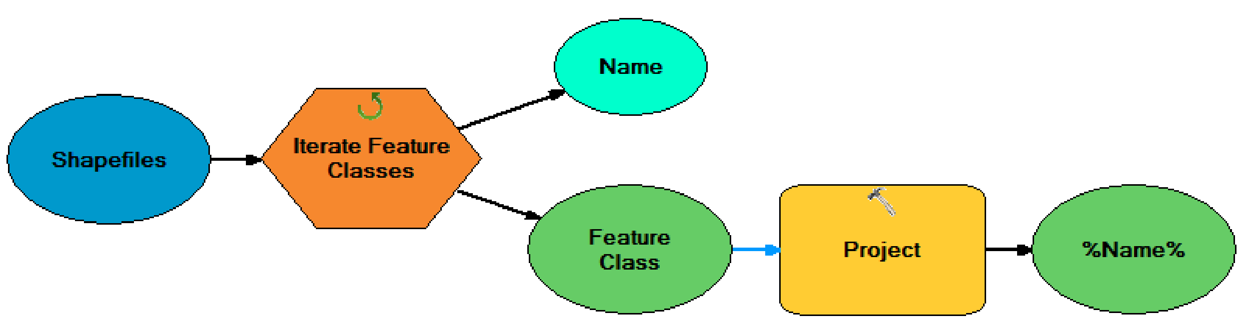

Figure 28. ArcGIS ModelBuilder workflow diagram for projecting GIS data to UTM coordinates.

FIU's work at Oak Ridge Reservation involved the development of customized Python scripts which required additional programming of built-in automated geoprocessing tools to call or retrieve data from the ORR geodatabase. A toolbox which combined built-in ArcGIS geoprocessing tools coupled with customized Python scripts was developed and calibrated for use with the East Fork Poplar Creek (EFPC) model. This toolbox, however, is a scalable and reusable application that can be implemented for other DOE sites and will therefore be utilized for the hydrological modeling work now being conducted at Savannah River Site. The tools and scripts developed automate the query and retrieval of timeseries data, including contaminant flow and transport parameters (e.g. contaminant concentration, surface water and groundwater flow, discharge, groundwater levels, etc.), from the specified geodatabase. The ArcGIS data model iterates through selected features and exports the results in tabular format. The toolbox also allows the ArcGIS program to iterate over several GIS files for pre- or post-processing of data to be used in or that are derived from hydrological modeling. The models developed have capabilities to:

- Add GIS files to ArcMap and create layer files.
- Select features within a specified area (e.g. the study domain) and clip/extract selected features and create a new layer file of selected subset.
- Export clipped feature in format to be used by MIKE SHE/11 model.
- Export attributes of clipped feature in MS Excel or text format for statistical analysis and generation of graphs and reports.
- Export map extent in various formats (e.g. JPEG, TIFF or PDF) for development of reports.
- Interpolate timeseries data collected at various monitoring points, generate gridded surfaces, and create and export mapped results.

New process flow models using ArcGIS ModelBuilder will be developed to support the hydrological modeling effort at SRS; however this will be complemented by the use of those previously developed by FIU-ARC researchers for the work carried out at ORR.

Development of Model-Specific Input Files

During hydrological model development, input file modification was often necessary either for use of the data at smaller scales or to modify appended timeseries or attribute data to generate compatible MIKE SHE/11 files. As previously mentioned, ArcGIS ModelBuilder was used to automate the clipping of the GIS data to the model domain, however, in some cases, further editing of the attribute data was also necessary. The MIKE SHE model uses GIS data inputs for many of its configuration parameters and as such, GIS data in shapefile (.shp) format can be directly input into the model. There are instances however, where although MIKE SHE accepts the GIS shapefile, the attribute field with the relevant data required is not read by the model due to an incompatible field type. For example, a non-integer numeric field may be "single", however, the field type accepted by the model is "double". As a result, modification of the attribute table is necessary to create a new field with "double" as the field type into which the required numeric data can be copied.

Timeseries

Precipitation is one of the critical variables in the integrated hydrological model, which determines the surface water flows in the watershed and the dynamics of the groundwater table. For use in MIKE SHE, the Precipitation Rate can be specified as a rate (e.g., mm/hr) or as an amount (e.g., mm). Rainfall timeseries data was provided by SRNL for approximately 50 years (01/01/1964 - 9/29/2014) in inches/day in an MS Excel spreadsheet. This data was copied into a MIKE SHE timeseries (.dfs0) file and input into the MIKE SHE model as precipitation. The model automatically converts the units to mm/day in the graph generated and will only use the data within the specified Simulation Period.

Tims Branch has received discharge from various outfalls in the A/M area. Major outfalls include A-001, A-003, A-1A, A-01, A-011, and A-014. Timeseries data of discharge from these outfalls was provided by SRNL. Other historical timeseries of discharge was acquired from the US Geological Survey (USGS) monitoring stations at Steed Pond (USGS 02197306), upstream (USGS 021973026 & USGS 021973028), and downstream (USGS 02197309) of Tims Branch. The USGS discharge data was recorded on a daily basis while the discharge data collected by SRS was collected weekly or monthly. The USGS data will be used for calibration and validation of the model. Figure 29 provides graphs of USGS discharge timeseries data in m^3/s for several outfalls in the Tims Branch watershed study domain at SRS.

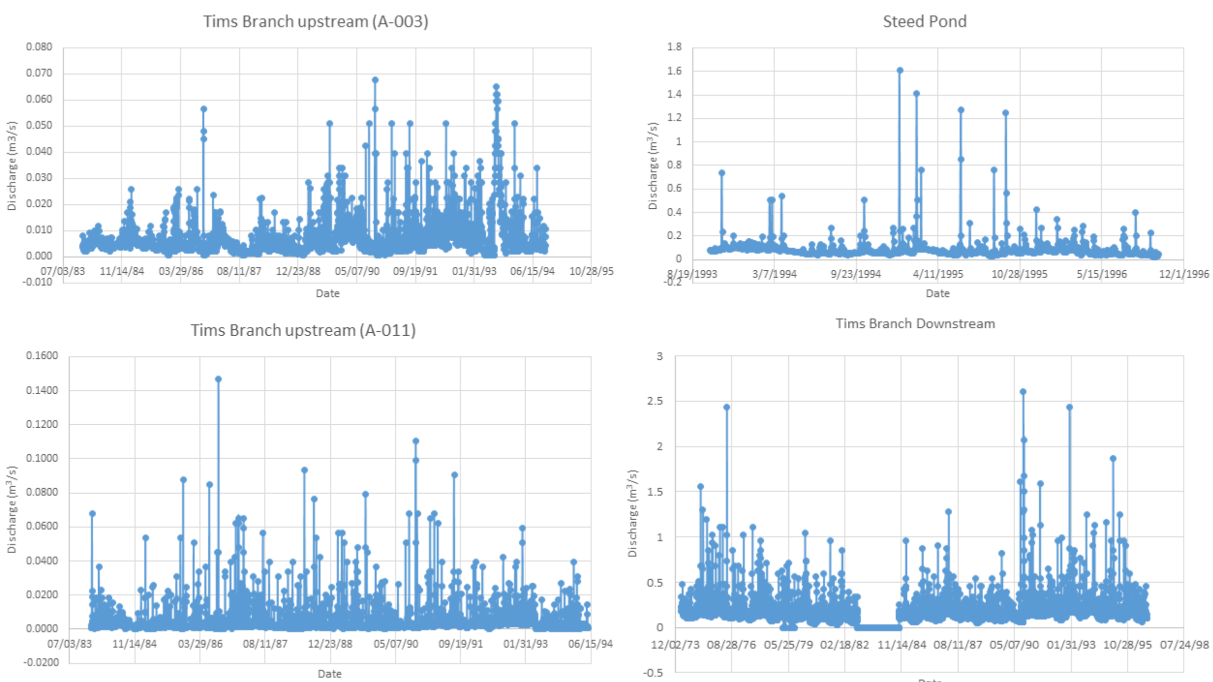

Figure 29. USGS discharge data (m^3/s) for various outfalls within the SRS study domain.

Topography

The model input for topography was generated by converting a 10 foot (~3m) resolution digital elevation model (DEM) to a point shapefile which contained XY coordinate data with associated elevation values. The model interpolates this point data via a triangular interpolation method into a gridded surface (Figure 30). This was then exported as a .dfs2 file, which is a native MIKE SHE grid file format. The .dfs2 file was then used to replace the point shapefile in the model. The USGS DEM format used was generated from 7.5 minute DLG hypsography data and was downloaded from the South Carolina Department of Natural Resources (SCDNR) GIS Data Clearinghouse.

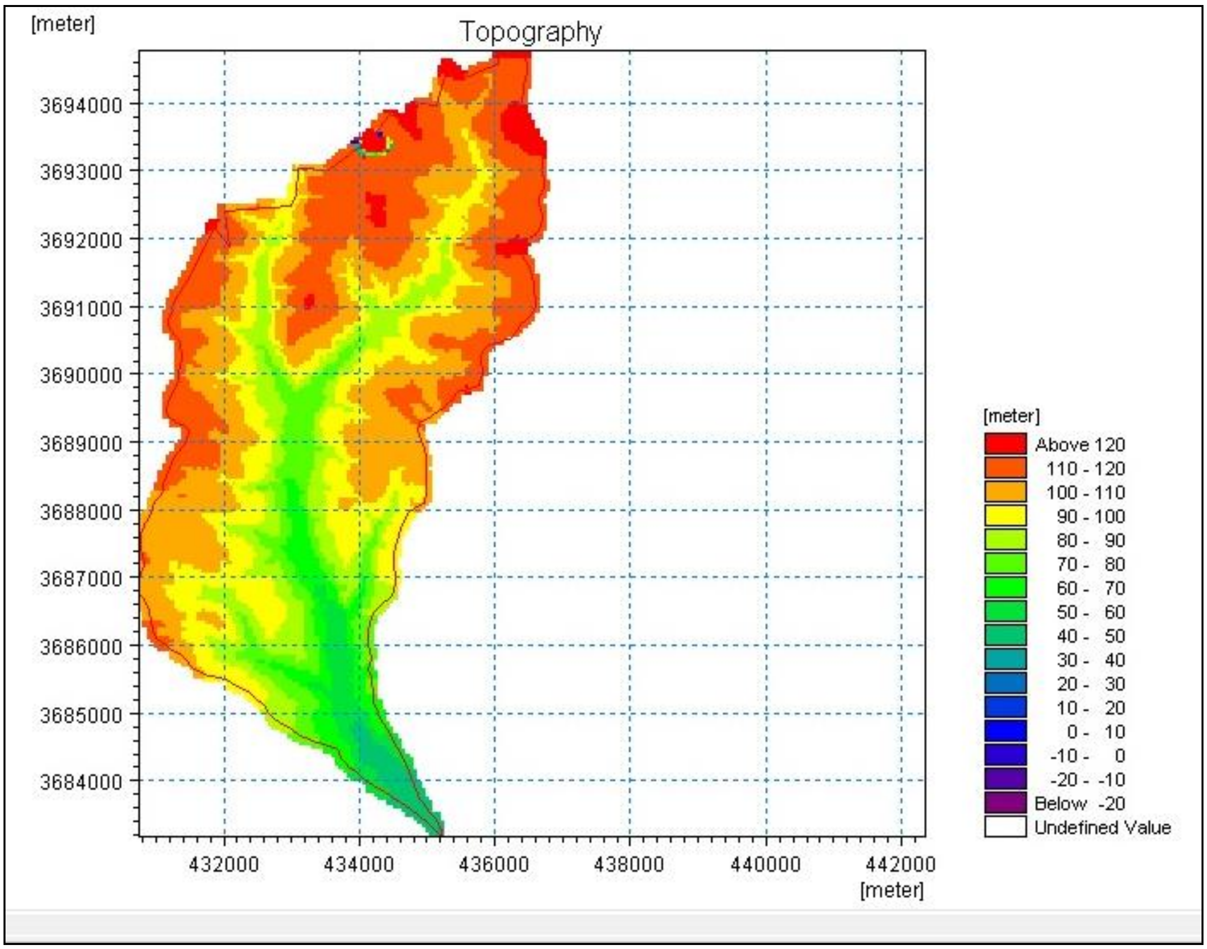

Figure 30. MIKE SHE grid file representing the topography within the Tims Branch Watershed model domain that was derived from a digital elevation model (DEM).

Land Use

Land cover data for the northwestern portion of Savannah River Site was provided in the form of a GIS feature class, which was clipped to the project's study domain, exported from ArcMap as a shapefile and then imported into the MIKE SHE model. Figure 31 displays snapshots of the polygons (highlighted in red in each figure) as viewed in MIKE SHE representing various land use classifications.

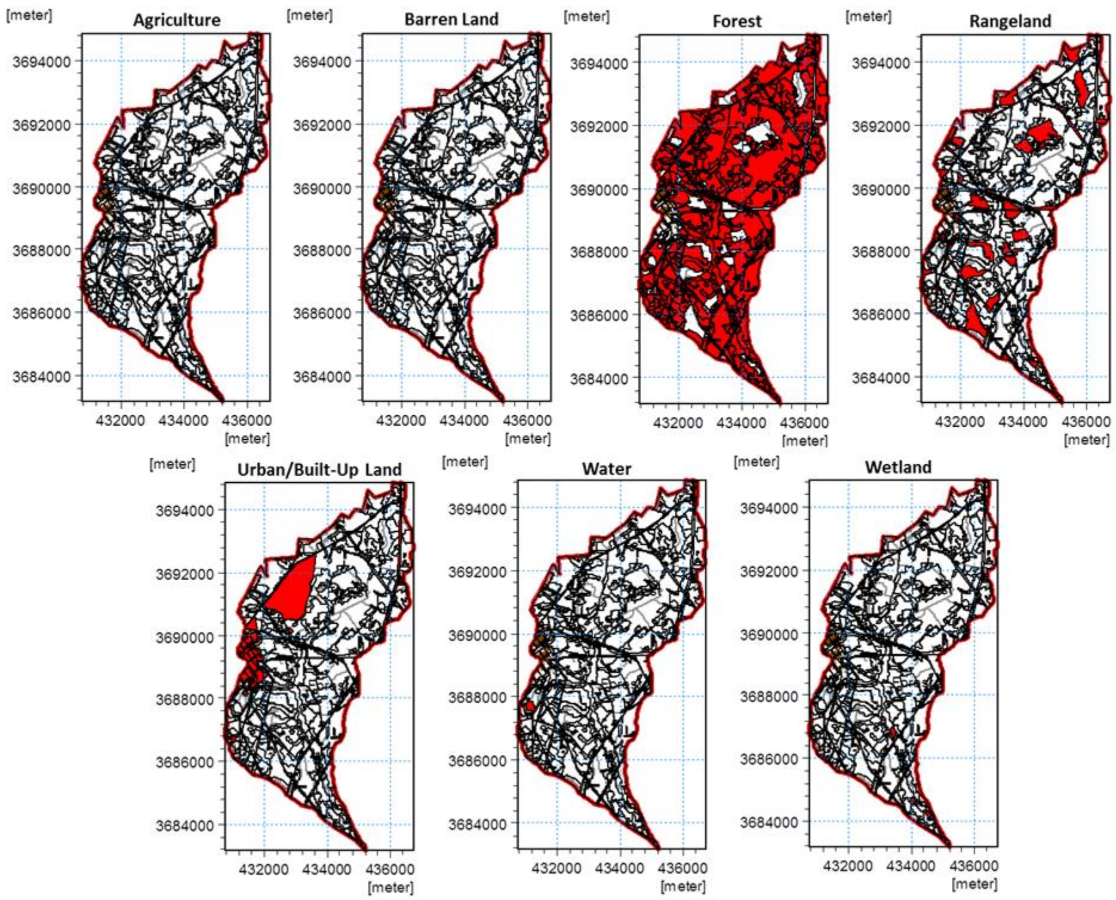

Figure 31. Land use maps.

Manning's Roughness Coefficient

Computation of flow in an open channel requires evaluation of the channel's resistance to flow, which is typically represented by a roughness parameter, such as Manning's *n*. (Phillips et al, 2007). **Table 5** shows the values of Manning's *n* that were assigned to each land use classification in the land cover shapefile previously described. Manning's *n* values were obtained from standard civil engineering Manning's tables available online as well as *n* values derived from the technical report by Tachiev et al, 2014, "Remediation and Treatment Technology Development and Support for DOE Oak Ridge Office: EFPC Model Update, Calibration and Uncertainty Analysis". The land cover shapefile attribute table was then modified to include a new field of Manning's M (i.e., 1/*n*) numbers. This added field was then used as the basis for generating a new polygon shapefile to represent the Manning's Roughness Coefficients within the SRS/Tims Branch study area. As the MIKE SHE model only accepts point/line shapefiles for spatially distributed Manning's M, ArcGIS tools were used to convert the polygon shapefile to a point shapefile which was then input into the model. The model then interpolated the values to generate a gridded surface which was saved as a MIKE (.dfs2) grid file. This grid file was then used to replace the shapefile in the model configuration (Figure 32).

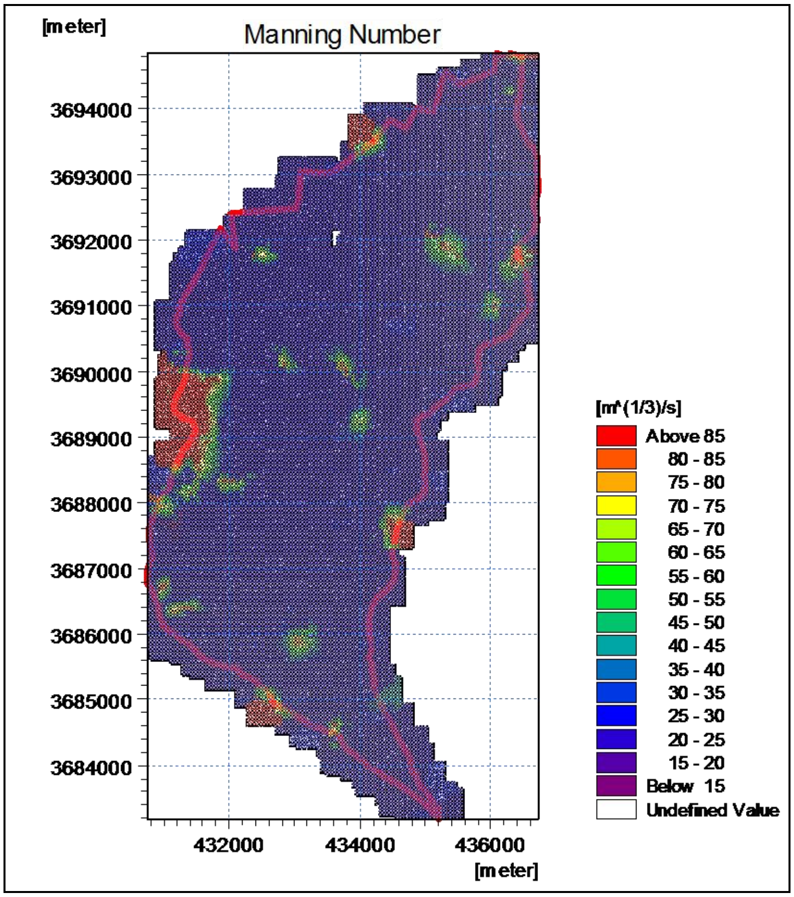

Figure 32. Manning's M (1/*n*) grid file as viewed in MIKE SHE.

Paved Runoff Coefficient

Paved runoff coefficient values were derived from the [1]Clean Water Team Guidance Compendium for Watershed Monitoring and Assessment State Water Resources Control Board 5.1.3 FS-(RC) 2011, which specifies the runoff coefficient (C) as a dimensionless coefficient relating the amount of runoff to the amount of precipitation, with larger values for areas with low infiltration and high runoff (pavement, steep gradient), and lower values for permeable, well

[1]Source: Clean Water Team Guidance Compendium for Watershed Monitoring and Assessment State Water Resources Control Board 5.1.3 FS-(RC) 2011 is a factsheet prepared by the California Environmental Protection Agency State Water Resources Control Board that can be accessed online at the following URL: http://www.waterboards.ca.gov/water_issues/programs/swamp/docs/cwt/guidance/513.pdf.

vegetated areas (forest, flat land). This data is required by the MIKE SHE model and can be a significant parameter indicating flooding areas during storm events as water moves fast overland on its way to a river channel or a valley floor. Paved runoff coefficient values were assigned to the land use classifications outlined in **Table 5** above. A value of 0.7 was given to the Urban/Built-up Land and a value of zero assigned to all other land use types. In the same manner as described above for development of the Manning's Coefficient GIS shapefile, the land cover shapefile attribute table was modified to include a new field of runoff coefficients. This added field was then used as the basis for generating a new polygon shapefile to represent the Paved Runoff Coefficients within the SRS/Tims Branch study area. As the MIKE SHE model only accepts point/line shapefiles for spatially distributed Paved Runoff Coefficients, ArcGIS tools were used to convert the polygon shapefile to a point shapefile which was then input into the model. The model then interpolated the values to generate a gridded surface which was saved as a MIKE (.dfs2) grid file. This grid file was then used to replace the shapefile in the model configuration (Figure 33).

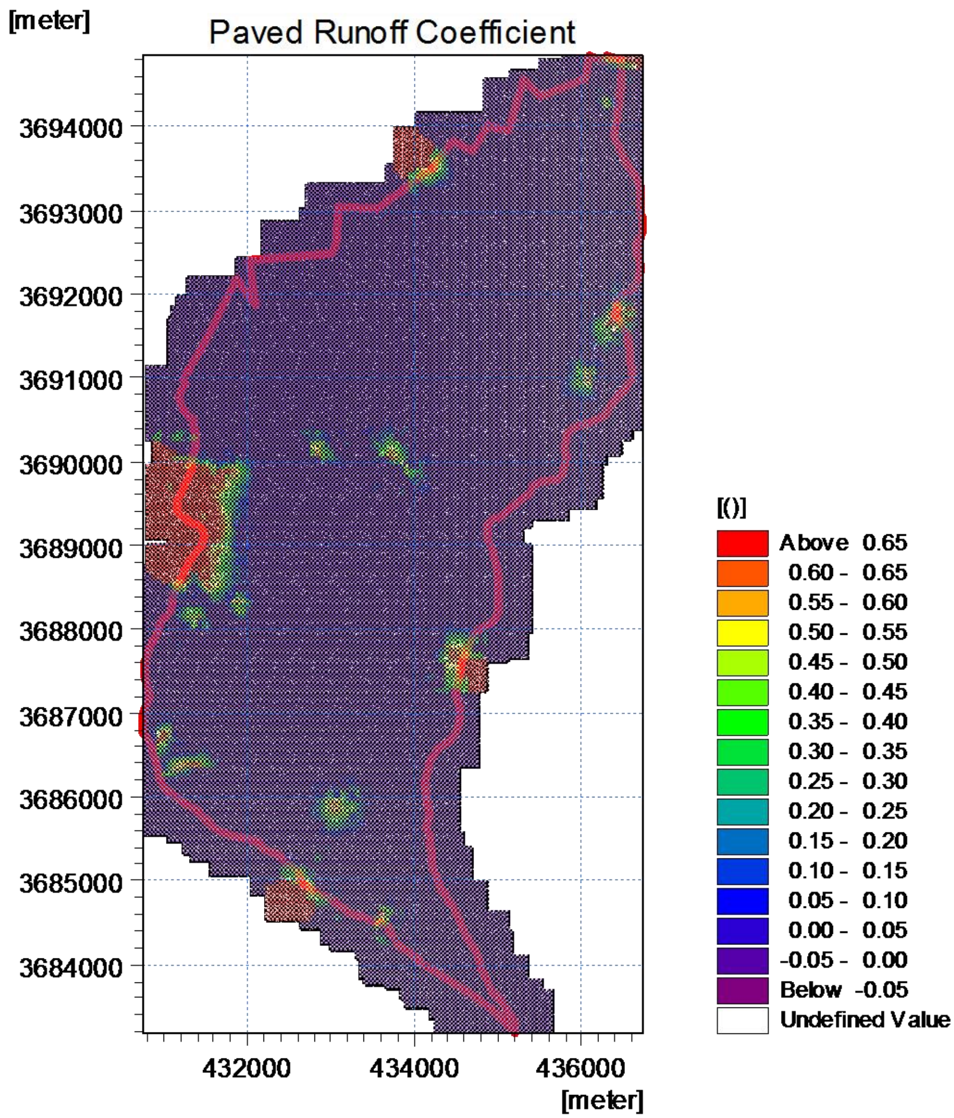

Figure 33. Paved Runoff Coefficient grid file as viewed in MIKE SHE.

Development of Maps & Reports

GIS can also serve as a useful tool in visually displaying research results via maps, graphs and reports which help to enhance the understanding and interpretation of model-derived data and to obtain a perception closer to reality. Several maps of the Tims Branch watershed were created using the ArcGIS mapping interface. Some of these maps can be viewed in APPENDIX B: TIMS BRANCH WATERSHED MAPS.

DEVELOPMENT OF THE FLOW MODEL

A detailed review of previous studies and available data was conducted and reported to the DOE on May 31, 2015. The document entitled "Literature Review for Surface Water Contaminant

Fate and Transport Modeling of Tims Branch", document name "ARC-FIU-2015-800000439-04c-231_final", can be downloaded from our DOE Research website at https://doeresearch.fiu.edu/SitePages/Soil%20and%20Groundwater.aspx. More than 30 SRS-DOE reports and 100 published journals were reviewed. In total, 10 reports and 40 journal articles were relevant to this project. Particular emphasis was given to identify studies exclusively focusing on hydrological modeling efforts for the Tims Branch. ARC researchers (Dr. Mehrnoosh Mahmoudi and Angelique Lawrence) visited SRS on 13-14 April, 2015, and were given a tour of the study area by Dr. Brian Looney and Ms. Thelesia Oliver from SRNL, to gain a better understanding of the hydrology of Tims Branch watershed. The locations visited that are relevant to this study included the A/M Area Air Stripper VOC/Hg treatment system; outfalls A14, A11, A11 LL Hg Sampling Location; the Wetland Treatment System; the outfall tributary; the erosion (rip rap) site upstream of the weir, weir site; and Tims Branch (Beaver Pond 2, Steed Pond). Some of the photos from the visit can be viewed below (Figure 34 - Figure 37). Following the SRS site visit, FIU received further guidance from Dr. Omar Abdul-Aziz from the FIU Department of Civil and Environmental Engineering on the data requirements and approximation of features such as channel geometry and bathymetry in the event that this data was unavailable for developing the surface water model (see APPENDIX C: SUB-PROJECT REPORT FROM DR. OMAR ABDUL-AZIZ). Modifications were made to the hydrological model being developed for Tims Branch with respect to flow, boundary conditions and calibration parameters, to reflect a more realistic account of the topographic and hydrologic phenomena encountered.

Figure 34. Photo of Noosha Mahmoudi (left), Brian Looney (center) and Thelesia Oliver (right) visiting the location of the M-1 Air Stripper at SRS.

Figure 35. Photo of Noosha Mahmoudi (left), Brian Looney (center) and Thelesia Oliver (right) at the A-11 Low Level Mercury Sampling Location at SRS

Figure 36. Photo of Angelique Lawrence at the A-11 Low Level Mercury Sampling Location at SRS.

Figure 37. Photo of Noosha Mahmoudi and Brian Looney exploring Tims Branch.

Model Theoretical Basis

The modeling system consists of MIKE SHE, an integrated 3-dimensional saturated and unsaturated groundwater flow, and 2-dimensional overland flow model. MIKE SHE is a deterministic, physically based and full distributed hydrological modeling system (Abbott and Refsgaard, 1996). It consists of the Water Movement and Water Quality modules. The hydrological processes are described mostly by physical laws (laws of conservation of mass, momentum and energy). The 1-D and 2-D diffusive wave Saint Venant equations describe channel and overland flow, respectively. The Kristensen and Jensen methods are used for evapotranspiration, the 1-D Richards‘s equation for unsaturated zone flow, and a 3-D Boussinesq equation for saturated zone flow. These partial differential equations are solved by finite difference methods, while other methods (interception, evapotranspiration and snowmelt) in the model are empirical equations obtained from independent experimental research. The basic steps for modeling the overland flow include:

1. Modeling of the saturated flow using MIKE SHE.
2. Incorporation of evapotranspiration and unsaturated flow into MIKE SHE.

A 2-D integrated surface and groundwater flow model (MIKE SHE) of Tims Branch Watershed (TBW) was developed for visualization of the overland flow distribution in the SRS area. Historical records derived from the preliminary data search were used as input for model development. Simulations include (but not limited) to seasonal fluctuation of precipitation and extreme flood events. The developed model for TBW offers the ability to input relevant hydrologic parameters to create a watershed model which is capable of simulating flow in the subsurface (saturated and unsaturated zones) and surface sub-domains (overland and river) and contaminant transport and exchange between various sub-domains using an advection-dispersion module. Topography, river networks, flow velocities, precipitation, soils, aquifers, vegetation, and land use are some of the parameters included in the development of the watershed model.

Model Domain

The domain of the project is defined as the Tims Branch (TB) watershed as delineated by SRS. The TB watershed has a drainage area of about 16 km^2 (Batson et al., 1996). The domain was created by utilizing a GIS shapefile of the Tims Branch Watershed. In Figure 38, grid cells inside the model domain are assigned a value of 1 and grid cells on the model boundary are assign a value of 2, as required. This distinction between interior grid cells and boundary cells is to facilitate the definition of boundary conditions. For example, drainage flow can be routed to external boundaries but not to internal boundaries.

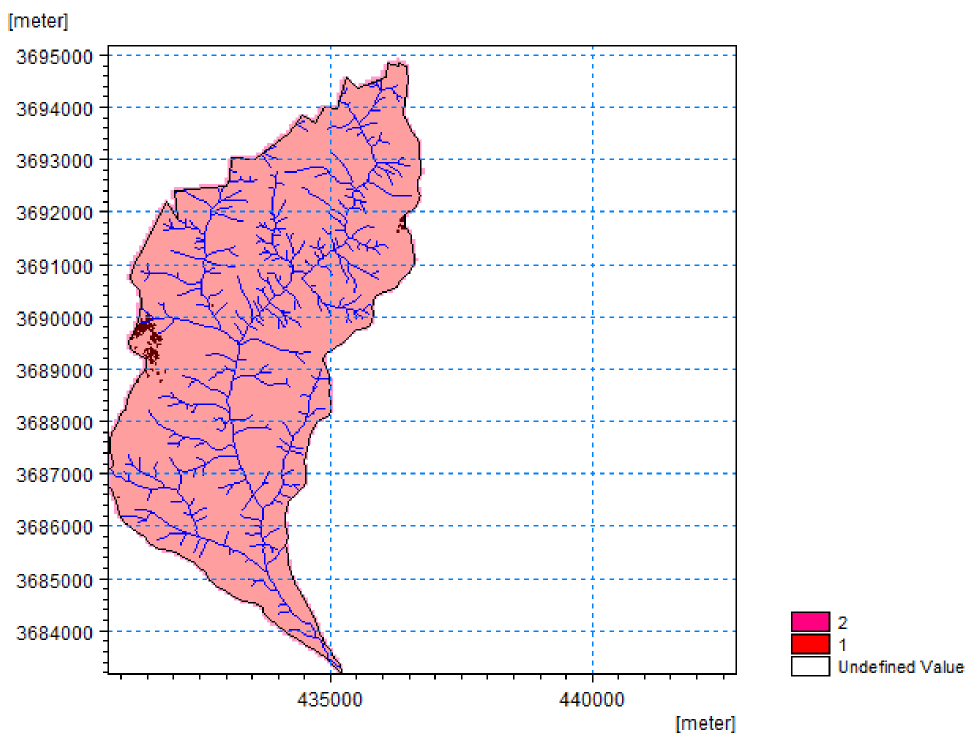

Figure 38. Hydrological model domain.

Topography

The model input for topography was generated by adding a GIS point shapefile derived from LIDAR data provided by SRS to the MIKE SHE model. The model interpolates this via inverse distance weighted (IDW) gapfilling into a gridded surface. This was then exported as a .dfs2 file, which is a native MIKE SHE file format. The .dfs2 file was then used to replace the Point shapefile in the model.

Topography of the site shows the ridge and valley features which run vertically in the graph Figure 39). Another visible feature is the increasing steepness of the Tims Branch valley banks from the upper to the lower reaches of the river; this feature relates to increasing stream flows due to diverging streams and basin flow. The topography ranges from 42 to 126 meters above mean sea level.

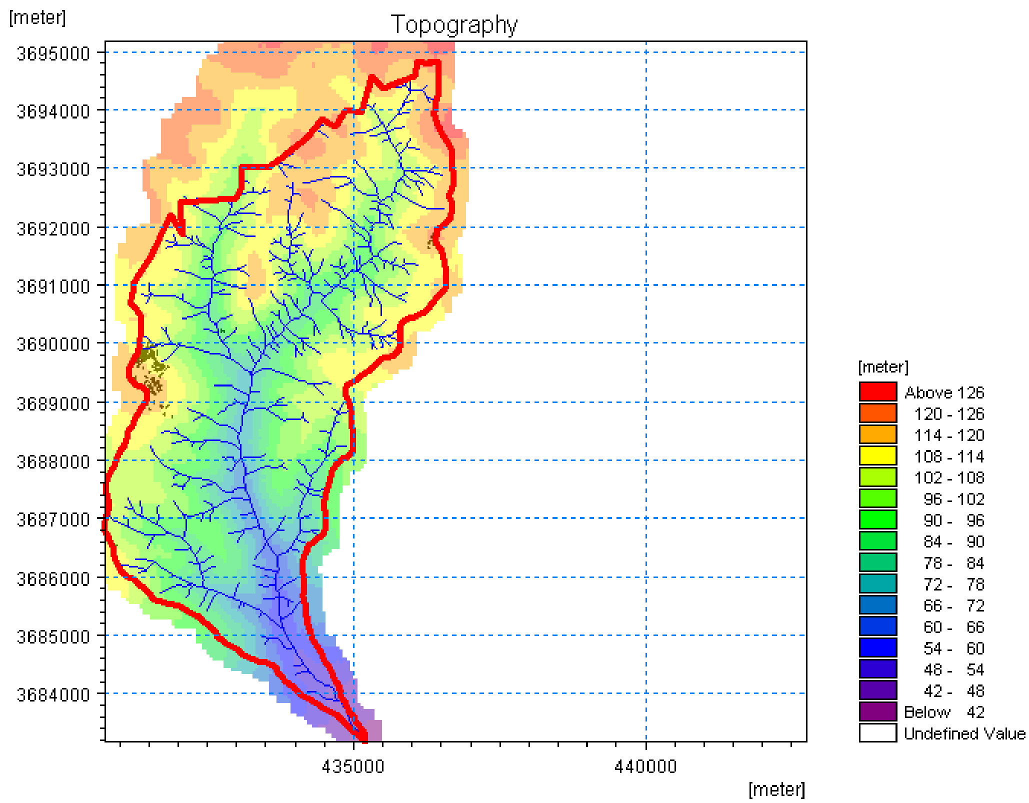

Figure 39. Site topography.

Climate Data

The climate data was acquired from the NOAA climatological dataset compiled for the state of South Carolina. Precipitation data is represented as water equivalent totals and includes liquid and melted frozen precipitation. For the purpose of this research, it is unnecessary to include separate snow melt data, as it is summarized in the precipitation data.

Precipitation

For use in MIKE SHE, the Precipitation Rate can be specified as a rate (e.g., mm/hr) or as an amount (e.g., mm). If an amount is used, MIKE SHE automatically converts this to a rate during the simulation. If a rate is used, then the EUM Data Units must be Precipitation and the time series must be Mean Step Accumulated. If an amount is used, the EUM Data Units must be Rainfall and the time series must be Step Accumulated (see MIKE SHE Manual Volume 2, page 58).

For the model, the precipitation rate time series used a Step Accumulated Rainfall for the Rainfall data in millimeters for the duration of one day. Data has been gathered for approximately 50 years (01/01/1964-09/30/2014); however, MIKE SHE will only use the data within the specified Simulation Period. In this work, the period of 10/01/1993-09/30/1996 was used.

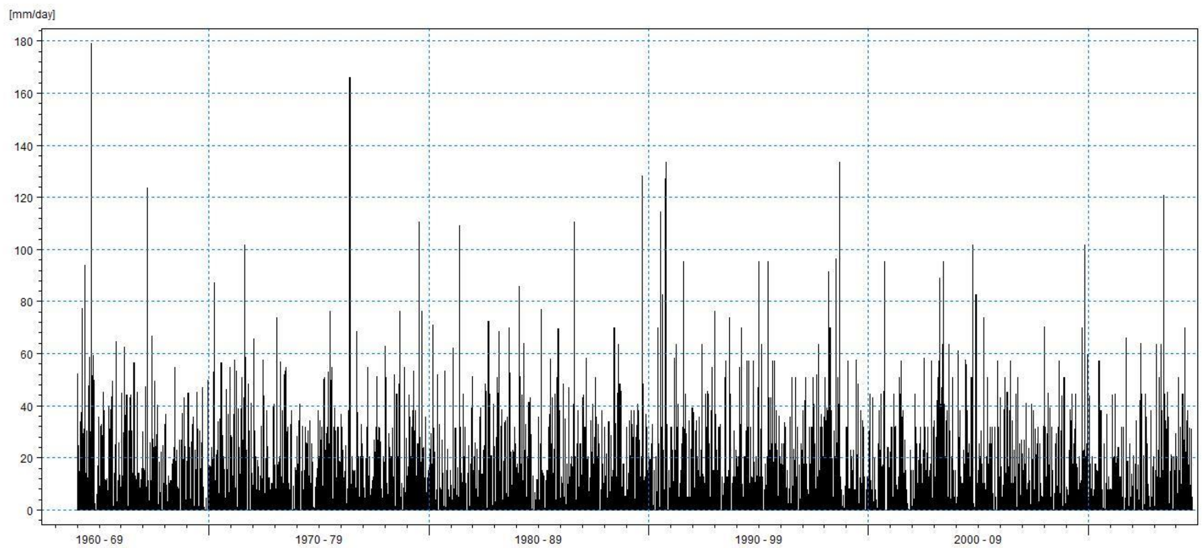

Figure 40. Precipitation at SRS.

Figure 40 depicts rainfall timeseries data in mm/d for the period 01/01/1964 and 09/30/2014.

Precipitation is one of the critical variables in the integrated hydrological model, which determines the surface water flows in the watershed and the dynamics of the groundwater table. The selected time period (10/01/1993-09/30/1996) shows a typical variability of rainfall events within a month and includes the timeseries of discharge recorded by the United States Geological Survey (USGS) station in Tims Branch.

Evapotranspiration

The calculation of evapotranspiration (ET) uses meteorological and vegetative data to predict the total evapotranspiration and net rainfall due to:

- Interception of rainfall by the canopy,
- Drainage from the canopy to the soil surface,
- Evaporation from the canopy surface,
- Evaporation from the soil surface, and
- Uptake of water by plant roots and its transpiration, based on soil moisture in the unsaturated root zone.

MIKE SHE models ET using two distinct methods. The primary ET model is utilizes formulas derived from the work of Kristensen and Jensen (1975). In this model, the actual evapotranspiration and the actual soil moisture status in the root zone is calculated from the potential evaporation rate, along with maximum root depth and leaf area index for the plants.

The 2-Layer Water Balance Method is an alternative to the more complex unsaturated flow process coupled to the Kristensen and Jensen module for describing evapotranspiration. The 2-Layer Water Balance Method is based on a formulation presented in Yan and Smith (1994), the main purpose of which is to calculate actual evapotranspiration and the amount of water that recharges the saturated zone. The module is particularly useful for areas with a shallow ground water table, such as swamps or wetlands areas, where the actual evapotranspiration rate is close to the reference rate. The 2-Layer Water Balance Method includes the processes of interception, ponding, and evapotranspiration, while considering the entire unsaturated zone to consist of two `layers' representing average conditions in the unsaturated zone. The vegetation is described in terms of leaf area index (LAI) and root depth.

At this point in the model setup, only a reference ET is needed for the Climate section. The reference evapotranspiration is the rate of ET from a reference surface with an unlimited amount of water. This value is independent of everything but climate and can be calculated from weather data. Aadland et al. (1995) has reported an annual evapotranspiration of about 32 inches for South Carolina; therefore, a constant Reference ET value of 2.22 mm/day was used. The reference ET will then be adjusted according to the vegetation data (leaf area index and root depth) found in the following section.

Land Use

Land cover data, as previously viewed in Figure 31, was provided by SRNS in the form of a GIS shapefile. This land use file was used to represent the vegetation coverage in the MIKE SHE model. Each classification was assigned Leaf Area Index (LAI) and Root Depth (RD) constant values which were defined in the MIKE SHE Vegetation Database. Table 7 shows the LAI and RD values assigned for each class.

Table 7. Leaf Area Index (LAI) and Root Depth (RD)

Class Name	LAI	RD (mm)	Class Name	LAI	RD (mm)
Bare soil	1.31	4000	Food plot	3.62	1500
Basin	3	2000	Grassland	1.71	1500
Barrow pit with grass	3	2000	Mixed deciduous	5.5	2000
Bottomland hardwood	5.5	2000	Mixed evergreen	5.5	1800
Bottomland scrub shrub	2.08	2500	Other features	2.5	2000
Clear cut	3.62	1500	Other scrub shrub	2.5	2000
Deciduous	5.5	2000	Pond	0	0
Emergent wetland	5	2000	Regeneration scrub	2.5	2000
Evergreen forest	5.5	1800	Research plot	2.5	2000
Facility	1.5	2000	Transportation	1.3	4000
Facility	1.5	2000	Utility	1.3	4000

These parameters are used to spatially adjust the reference evapotranspiration described in the Climate section. In MIKE SHE, the ET process proceeds as follows: a portion of the rainfall is intercepted by the canopy and evaporates, the remainder reaches the soil and adds to runoff or percolates into the upper soil layer, part of the infiltrating water is either transpired by plant roots or evaporated, and the remaining water recharges the groundwater. The various sections where plants intercept the path of water are spatially distributed by the LAI and RD parameters of the vegetation maps.

Saturated Zone (SZ)

Development of site-specific hydrological models requires knowledge of the SRS geology to adequately correlate the composition of soil parent material with soil hydrological properties. Soil geologic properties also provide basic information about factors controlling groundwater flow.

The SRS occupies approximately 800 km^2 and lies in the Atlantic Coastal Plain physiographic province in west-central South Carolina, southeast of the Fall Line which is the boundary between the Coastal Plain and the Piedmont provinces.

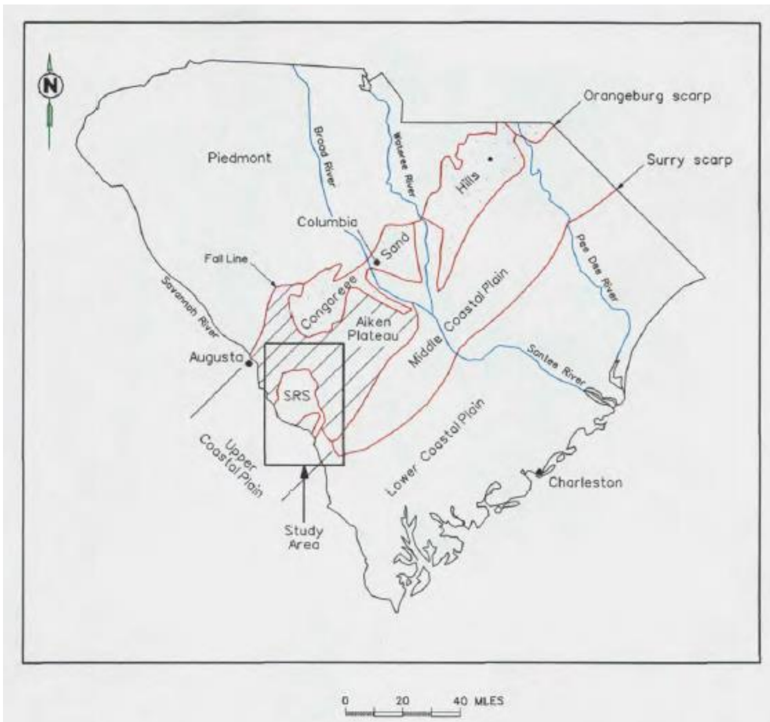

Figure 41. Location of the SRS study area within the Aiken Plateau (Aadland et al., 1995).

The Upper Coastal Plain of South Carolina is divided into the Aiken Plateau and Congaree Sand Hills (Figure 41). The SRS study area is located within the Aiken Plateau, which is bounded by the Savannah and Congaree Rivers and extends from the Fall Line to the Orangeburg scarp. The Coastal Plain is underlain by Piedmont rocks and Triassic-Jurassic sedimentary rocks (Denham, 1999).

Figure 42 shows a USGS physiographic map of South Carolina (downloaded from Central Savannah River Area Geological Society online at http://www.usca.edu/csrags/fall-line.html). The Coastal Plain near the study area consists of about 213 m (700 ft) of Late Cretaceous quartz sand, pebbly sand, and kaolinitic clay, overlain by about 18 m (60 ft) of Paleocene clayey and silty quartz sand, glauconitic sand, and silt. The Paleocene beds are overlain by about 107 m (350 ft) of Eocene quartz sand, glauconitic quartz sand, clay, and limestone grading into calcareous sand, silt, and clay.

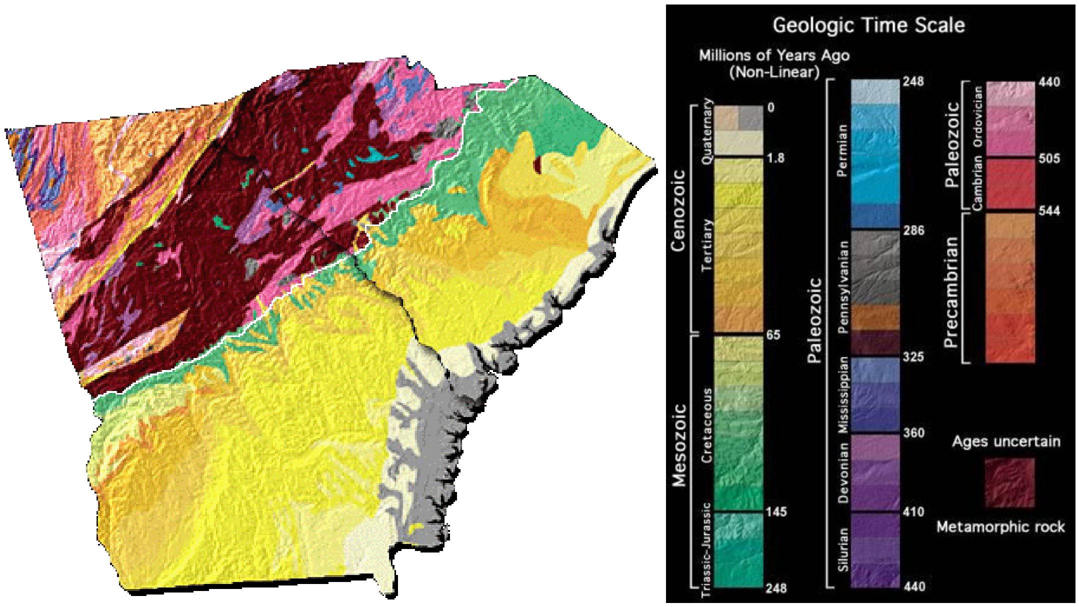

Figure 42. USGS physiographic map of South Carolina (downloaded from Central Savannah River Area Geological Society online at http://www.usca.edu/csrags/fall-line.html).

The Upper Cretaceous region is about 213 m (700 ft) thick near the study area and consists mostly of poorly consolidated, clay-rich, fine- to medium-grained, micaceous sand, sandy clay, and gravel (Faye and Prowell, 1982). Thin clay layers are common; however, clay beds and lenses up to 21 m (70 ft) thick can also be found along with fluvial to prodeltaic depositions. The number and thickness of the clay, sandy clay, and clayey sand layers in each hydrostratigraphic unit were determined from the geophysical logs and drill-core descriptions in a study conducted by the Westinghouse Savannah River Company (WSRC) in collaboration with the South Carolina Department of Natural Resources (SCDNR) in order to better define the lithology of the units.

Figure 43 shows the geological layers GIS shapefile in the Tims Branch Watershed study area provided by the Savannah River Nuclear Solutions (SRNS) Geotechnical Engineering Department, which was derived from the South Carolina Geological Survey (Surface Geology, SCGS 1:24,000). The area along the tributary is dominated by alluvium deposits.

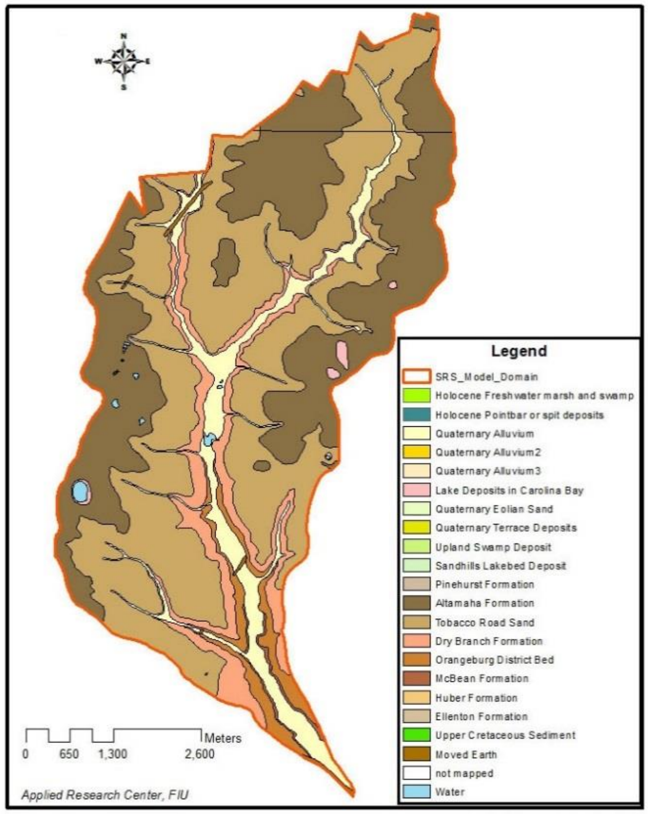

Figure 43. Geologic layers.

The Southeastern Coastal Plain hydrogeologic province in west-central South Carolina and adjacent east-central Georgia is comprised of the Floridan, Dublin, and Midville aquifer systems. The Floridan and Dublin aquifer systems are separated by the Meyers Branch confining system and the Dublin aquifer system is separated from the underlying Midville aquifer system by the Allendale confining system (Aadland et al., 1995). According to Clarke and West (1998), the groundwater and surface water systems interact dynamically in the Savannah River area near SRS.

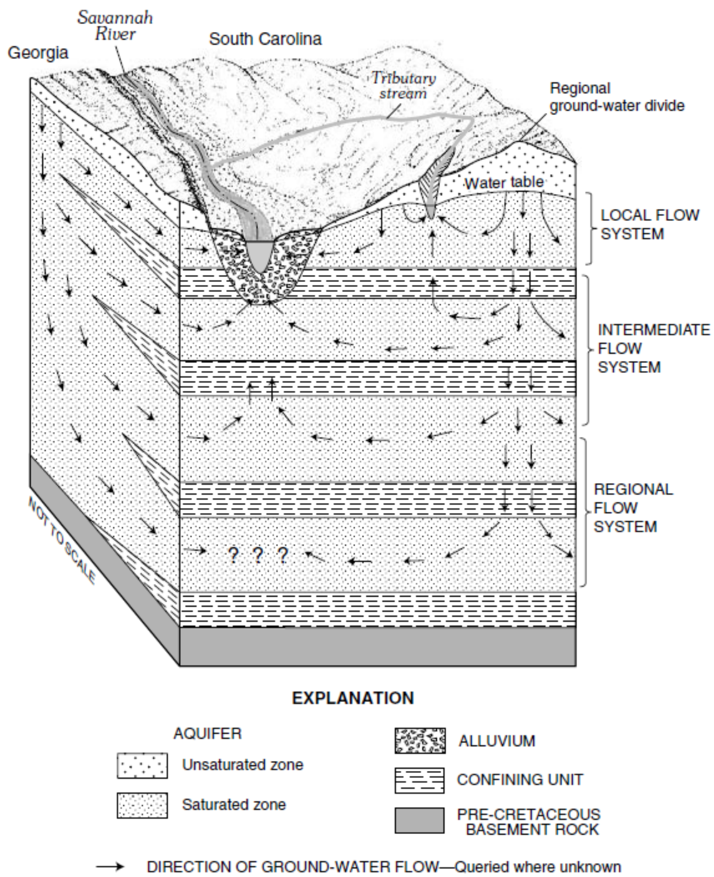

Figure 44. Conceptualized hydrogeologic framework and related groundwater flow in the vicinity of SRS (Clarke and West, 1998).

In an unconfined aquifer, specific yield is defined as the volume of water released per unit surface area of aquifer per unit decline in head. It is a dimensionless characteristic that is used only in transient simulations in cells that contain the water table (see MIKE SHE manual Volume 2 page 114). Specific storage is similar, but is defined as the volume of water released per volume of aquifer per unit decline in head and has units of L^{-1}. A specific yield of 0.2 and a specific storage of 3.048×10^{-5} L^{-1} were used.

MIKE SHE requires a reference system for linking the drainage to a recipient node or cell. The recipient can be a MIKE 11 river node, another SZ grid cell, or a model boundary. Drainage routed downhill based on adjacent drain levels was the option used for all simulations. Whenever drain flow is produced during a simulation, the computed drain flow is routed to the recipient point using a linear reservoir routing technique. The reference system is created automatically by the pre-processor using the slope of the drains calculated from the drainage levels in each cell. Thus, the pre-processor calculates the drainage source-recipient reference system by:

a) Looking at each cell in turn,
b) Looking for the neighboring cell with the lowest drain level, and
c) If this cell is an outer boundary cell or contains a river link, the search stops.

If the cell does not contain a boundary or river link, then the next search is repeated until either a local minimum is found or a boundary cell or river link is located. The result of the above search for each cell is used to build the source recipient reference system. If local depressions in the drainage levels exist, the SZ nodes in these depressions may become the recipients for a number of drain flow producing nodes. This often results in the creation of a small lake at such local depressions. If overland flow is simulated, then the drainage water will become part of the local overland flow system. The drainage level was assumed to be -1.0 m relative to the ground; the drainage time constant was assumed to be 1.0×10^{-6} sec^{-1}.

Unsaturated Flow

Texture types of the soils within the TB study area were identified by investigating SRS soil map units on the basis of geologic formation, geomorphology, and soil parent material. Each soil textural type has certain hydrological properties. The soil literature contains numerous assessments of soil water characteristics and hydraulic conductivity values, which are often not easy to determine experimentally. The van Genuchten (1980) water retention parameter is a simplified widely used approach for the prediction of soil water content as a function of pressure head. This model is represented by the following algorithm:

$$\theta = \theta r + \frac{(\theta s - \theta r)}{[1 + (\alpha h)^N]^M} \tag{10}$$

where: θ = water content; θ_r = residual water content; θ_s = total saturated water content; α = empirical constant, cm^{-1}; N = empirical constant; M = empirical constant; and h = capillary head, cm. The correlation between N and M is as follows:

$$M = 1 - \frac{1}{N} \tag{11}$$

Hydraulic conductivity is expressed by:

$$\frac{K(\theta)}{K_s} = \left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^{\frac{1}{2}} \left\{1 - \left[1 - \left(\frac{\theta - \theta_r}{\theta_s - \theta_s}\right)^{\frac{1}{M}}\right]^M\right\}^2 \tag{12}$$

where $K(\theta)$ is the hydraulic conductivity for a given water content (cm h^{-1}) and K_s is the saturated hydraulic conductivity (cm h^{-1}). Parameters for equation (1) were obtained from the Carsel and Parrish database (1988).

Overland Flow

The overland flow can be calculated using either a semi-distributed method or a finite difference method using the diffusive wave approximation. The finite difference method should be used when calculating detailed overland flow, while the semi-distributed, simplified method should be used for regional applications where detailed overland flow is not required.

The outer boundary condition for the overland flow solver is a specified head, based on the initial water depth in the outer nodes of the model domain. Thus, if the water depth inside the model domain is greater than the initial depth on the boundary, water will flow out of the model. If the water depth is less than the initial depth on the boundary, the boundary will act as a source of water. The domain of the model is a delineated watershed, which should indicate that all of the water that falls within the domain flows to the rivers and out toward Tims Branch. For this reason, all of the overland flow within the domain is treated as a source of water and the Initial Water Depth is set to zero to ensure flow in this direction and not out of the domain. Detention Storage is used to limit the amount of water that can flow over the ground surface. For the model, detention storage is set to zero.

When the net rainfall rate exceeds the infiltration capacity of the soil, water is ponded on the ground surface. This water is available as surface runoff, to be routed downhill towards the river system. The exact route and quantity is determined by the topography and flow resistance, as well as the losses due to evapotranspiration and infiltration along the flow path. The water flow on the ground surface is calculated by MIKE SHE’s Overland Flow Module, using the diffusive wave approximation of the Saint Venant equations, or using a semi-distributed approach based on the Manning’s equation. USGS has described a procedure for estimating the roughness factor (Manning’s number) for densely vegetated flood plains (Arcement Jr. and Schneider, 1989). The n value is determined from the values of the factors that affect the roughness of channels and flood plains. In densely vegetated flood plains, the major roughness is caused by trees, vines, and brush. The n value for this type of flood plain can be determined by measuring the vegetation density of the flood plain.

MIKE SHE assumes a Manning’s number equal to 1/n (Figure 45), inverse of actual n values, for a planar surface of infinite width with uniform rainfall. Precipitation falls on the plane, accumulates on the surface in response to the surface roughness, and flows down the slope in the positive x-direction. In the figure, L is the length of the slope, Y is the local depth of water on the surface at any point along the surface and α is the slope.

$$q = M \cdot y^{5/3} \sqrt{\alpha} \tag{13}$$

Manning’s n units = s/m$^{1/3}$ in software, Manning M units = m$^{1/3}$/s.

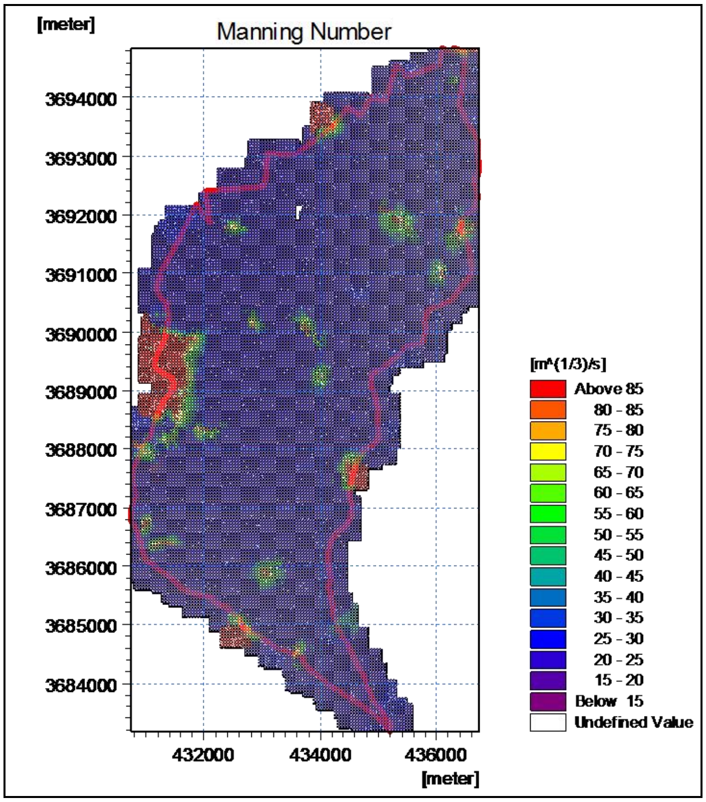

Figure 45. Manning's M (1/*n*) grid file as viewed in MIKE SHE.

Hydrologic Simulations

MIKE SHE simulates the terrestrial water cycle including evapotranspiration (ET), overland flow, unsaturated soil water, and groundwater movements. At this stage of model development, only overland flow has been simulated to determine the response of the watershed as a function of rainfall variability, infiltration capacity of the soil, losses due to evaporation and infiltration along the flow. Simulation of overland flow for a watershed is an important step to understand the different hydrological components and water balance of a watershed system. In the next phase of the modeling framework, simulation of unsaturated and saturated flow (UZ/SZ), as well as evapotranspiration (ET) will be included to understand the different components of the hydrological cycle in the TB watershed. ET is modeled as a function of potential ET, leaf area index (LAI), and soil moisture content using the Kristensen and Jensen (1975) method. The unsaturated soil water infiltration and redistribution processes are modeled using Richard's equation or a simple wetland soil water balance equation. Saturated water flow (i.e., ground water) is simulated by a 3-D groundwater flow model. Channel flows and channel surface water and upland groundwater interactions are controlled by the MIKE 11 model, and by coupling of MIKE SHE and MIKE 11. MIKE 11 is a one-dimensional model that tracks channel water levels using a fully dynamic wave version of the Saint Venant equations. The coupling of MIKE SHE and MIKE 11 is especially important for simulating the dynamics of variable source areas in both the downstream and upland watersheds. In this study, a preliminary simulation was performed for a 2 month period of rainfall from 07/30/2014 to 09/30/2014. Future simulations will be performed for the period 10/01/1993 to 09/30/1996 for which there is measured streamflow/discharge data at TB watershed USGS gage station. Calibration and validation of the hydrological model will be performed in the future modeling framework using the USGS observed streamflow data. The calibration of the model will be performed during the period of 10/01/1993 to 10/01/1995 and model validation will be performed during 10/01/1995 to 09/30/1996. The model will be also tested for various scenarios including extreme rainfall and episodic storm events.

RESULTS

Preliminary Modeling Results

Simulation of overland flow was conducted during high rainfall events in the TB watershed. Figure 46 and Figure 47 are visual illustrations of the MIKE SHE hydrological model outputs. Each figure shows a snapshot of a specific time step during the model simulation.

The model was used to simulate different rainfall conditions to examine the impact of annual and seasonal rainfall on overland flow within the watershed, as well as changes in the infiltration capacity of the soil. Figure 46 shows the preliminary result of an overland flow simulation in the Tim Branch watershed for a high rainfall day (August 11, 2014). The measured rainfall in the watershed on August 11, 2014 was approximately 31.5 mm. This high rainfall event contributed to increased surface runoff/overland flow resulting in a higher streamflow. As depicted in the figures below, there is high discharge in the river system due to increased overland flow. Understanding the seasonal variability of rainfall and the watershed’s response to the subsequent environmental changes assists in modeling the response of the watershed as a function of climate variability, soil infiltration capacity, vegetation cover/land use and other hydrological conditions.

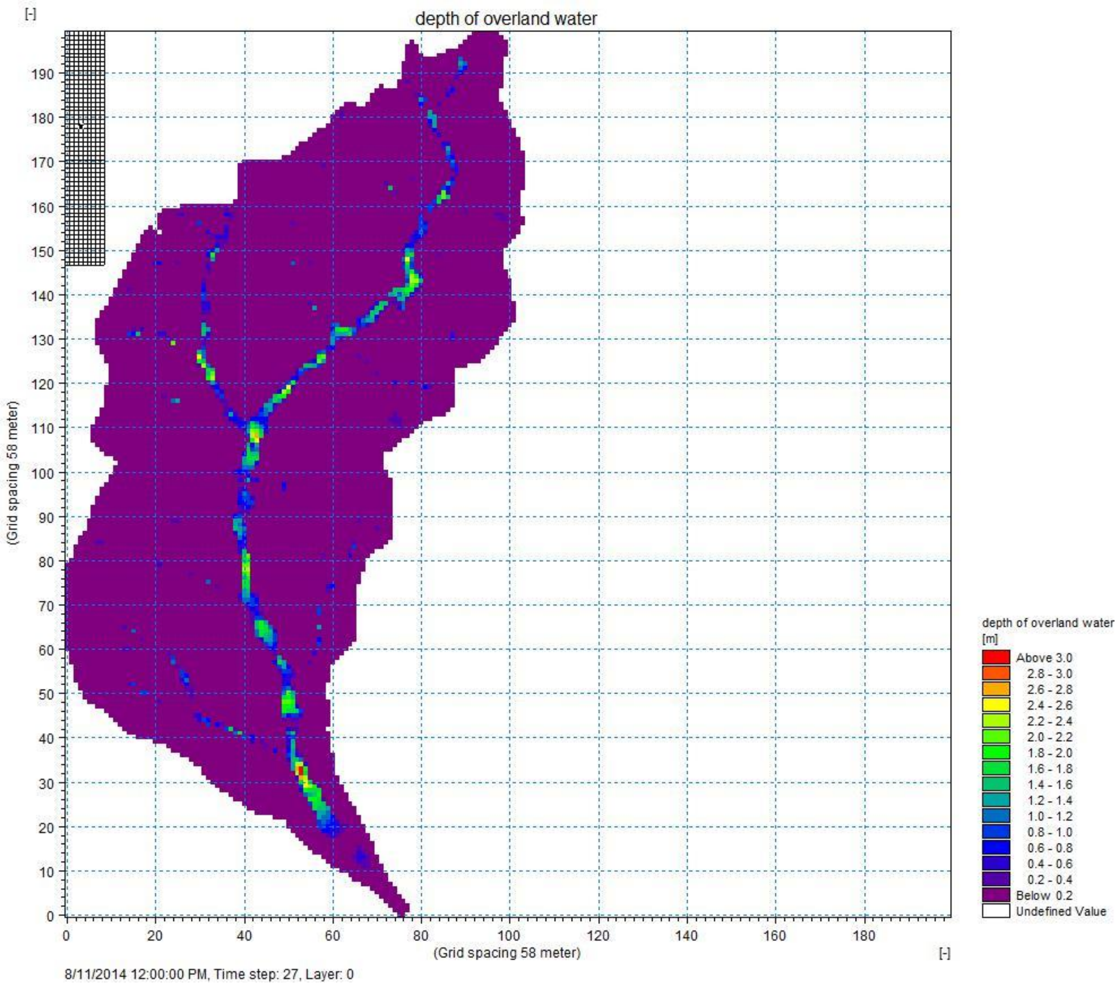

Figure 46. Depth of overland flow during high rainfall day (31.5 mm), August 11, 2014.

Another simulation of overland flow was performed for the year 1993 which coincided with the start-up of the M1 air stripper in the SRS A/M area and the discharge to Tims Branch from the nearby outfalls. Figure 47 is a graph of monthly rainfall in mm/d for the year 1993 which shows two peaks of high precipitation during January and September with some heavy rainfall events in July.

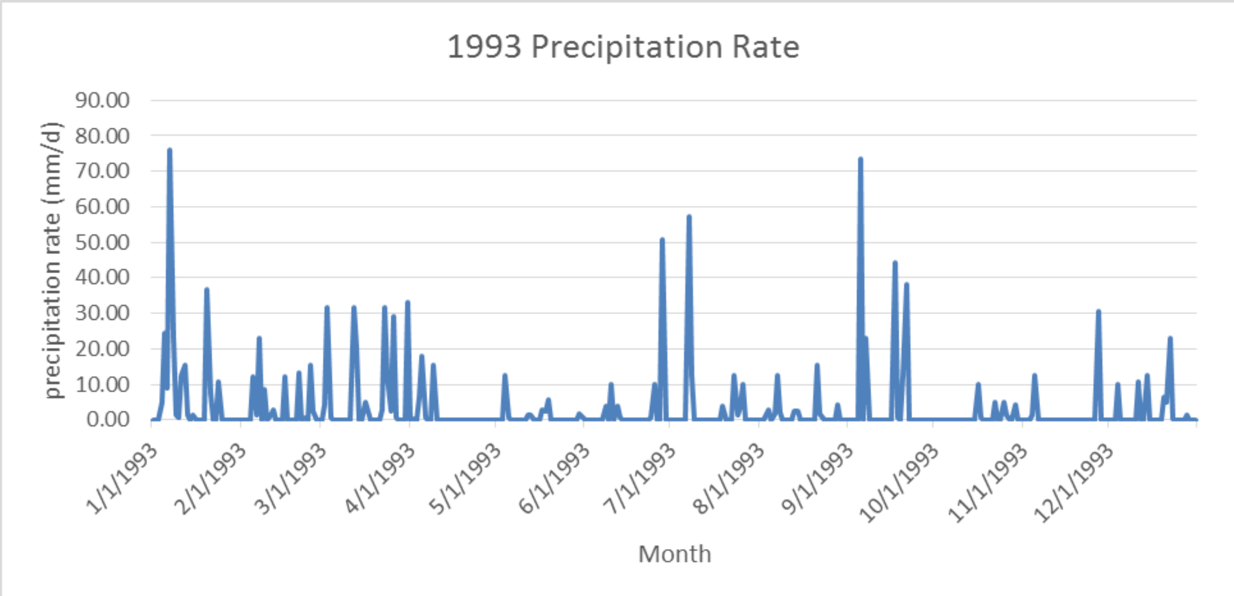

Figure 47. Rainfall for the year 1993.

Figure 48 shows the results of the MIKE SHE simulation for a single year from 1/1/1993 to 1/1/1994. This figure consists of snapshots of overland flow for the months of March, June, September, and December which represent spring, summer, fall and winter respectively.

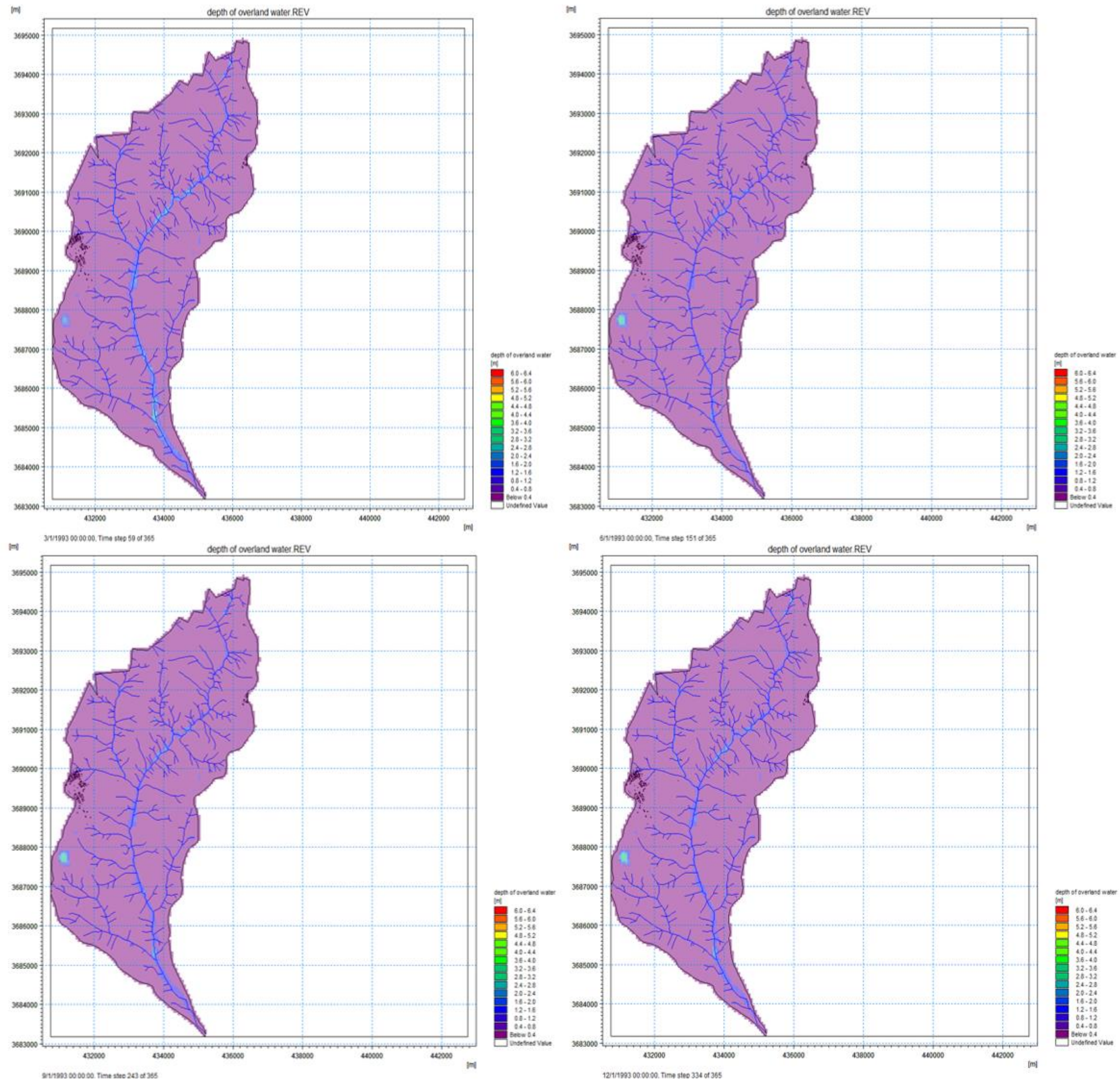

Figure 48. MIKE SHE simulation results of seasonal overland depth of water for year 1993 indicating spring, summer, fall and winter overland flow simulation.

Temporal variation of depth of overland flow during the rainfall in 1993 in two locations is shown in Figure 49. Point 1 is located in the vicinity of Steed Pond and Point 2 is located downstream of TB near the UTR conjunction. The depth pattern in both locations exhibits similar behavior with higher depth of water during rain events and lower depth when low rainfall or no rainfall happens.

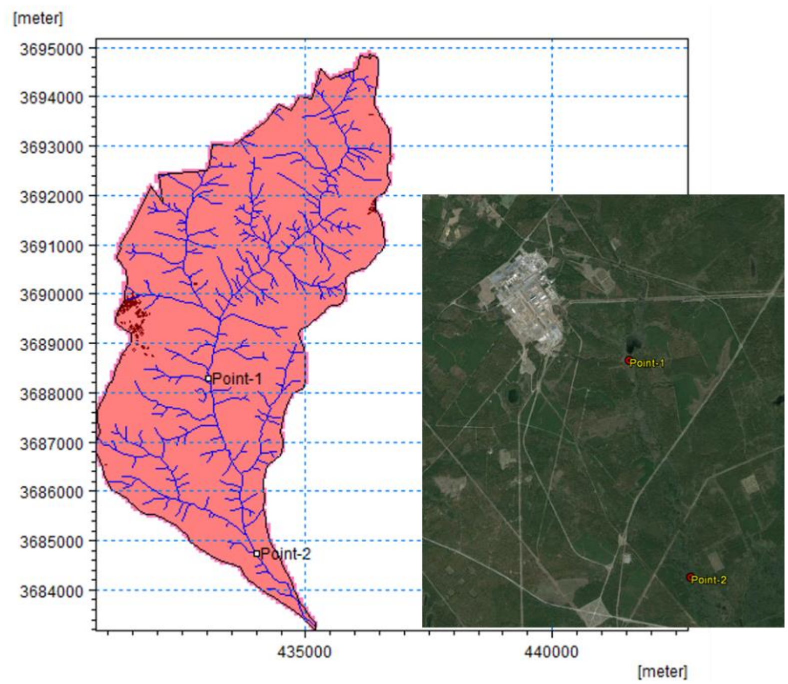

Figure 49. Point 1 and Point 2 locations in the study area (SRS).

Depth of water seems to be lower at point 1 (Steed Pond) than TB downstream which is mostly due to the topographic gradient from north toward south of the study area, vegetation coverage and soil types.

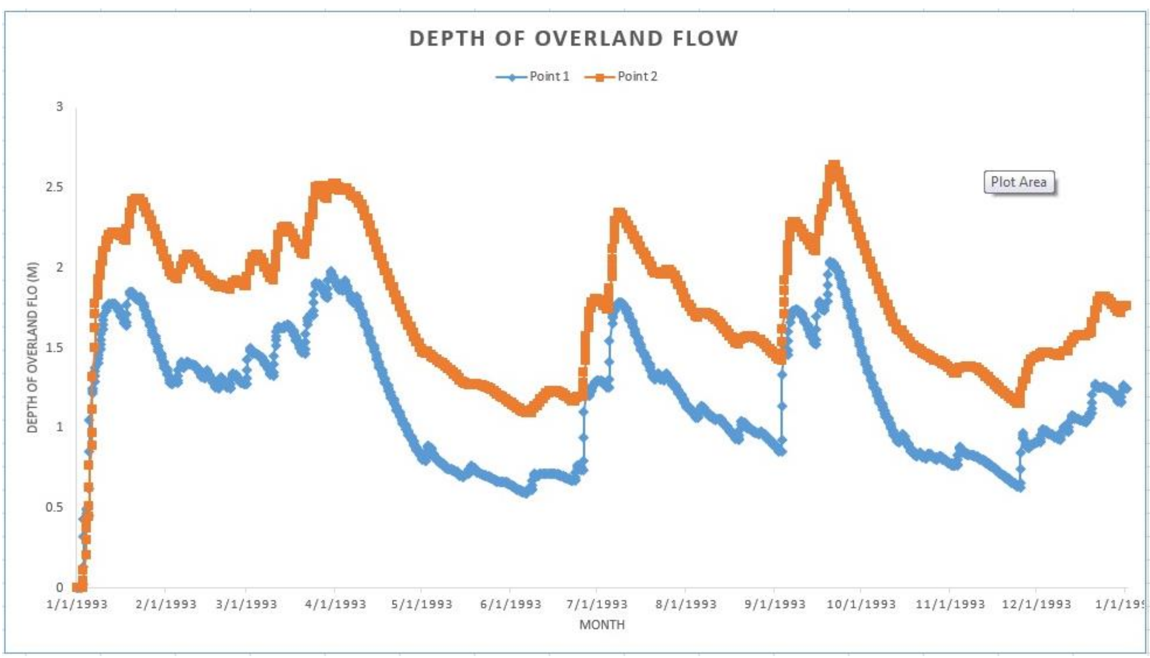

Figure 50. Depth of overland flow at two locations, Point 1 near Steed Pond and Point 2 close to UTR conjunction.

The variation in the depth of overland flow in a watershed, which is the water available as surface runoff to be routed downhill towards the river system, is highly dependent on rainfall intensity and distribution. Comparing the graphs shown in Figure 50, variation in the depth of overland flow highly depends on the amount and distribution of rainfall in the watershed.

CONCLUSIONS

The main purpose of this study was to develop an overland hydrology model using MIKE SHE that is capable of simulating surface flow depth and velocity throughout the Tims Branch Watershed and how climatic variability, particularly extreme rainfall or storm events, can remobilize and redistribute tin within the overland and river sub-domains, increasing the potential for tin methylation. The MIKE SHE modeling package has several advantages over many hydrologic models for estimating watershed runoff: (1) it is a distributed model and most of the algorithms in describing the water movements are based on physical processes, (2) it simulates the overland flow processes commonly found in dry regions, and (3) it has been commercialized and a GIS user interface was built into the system that can directly use geospatial databases for model inputs. Moreover, the model has a strong visualization utility that makes interpretation of modeling outputs much easier. The model developed in this study will be used as a tool to understand the dynamics of the different hydrological components of the Tims Branch Watershed. Preliminary model development has included the simulation of overland flow, which is one of the main components of the MIKE SHE modeling system in hydrological analysis due to the fact that a significant amount of water flows as overland flow/surface runoff that joins streams and waterbodies. Knowledge of the temporal and spatial distribution of overland flow helps to understand flow as a function of climate and catchment characteristics in the land phase of the hydrological cycle. Accurate prediction of overland flow helps to understand the surface water responses to changes in vegetation, climate variability and topography of a watershed. In this study emphasis was placed on understanding the characteristics of overland flow as a function of climate and catchment characteristics and other hydrological processes including evapotranspiration, infiltration and unsaturated and groundwater flow. The seasonal distribution of overland flow helps to understand the flooding and other extreme flow conditions in the watershed. In this study, seasonal (i.e., winter, spring, summer and fall) overland flow was simulated. Model simulation results are preliminary as not all of the hydrological components have been incorporated, and give a general understanding of the watershed as a function of precipitation and other catchment characteristics. The developed surface water model will undergo a considerable calibration and validation process using measured streamflow/discharge data within the target watershed. The calibration of the model will refine the parameter values that will help to fully develop the integrated model for better representation of the watershed. Different statistical evaluation methods will be employed to ensure the accuracy of the calibration results. This calibration and validation exercise will help to improve the predictive capability and reliability of the model.

Future Work

The simulation of the fate and transport of tin in the Tims Branch Watershed (TBW) will continue based on the modeling work scope defined in Figure 51.

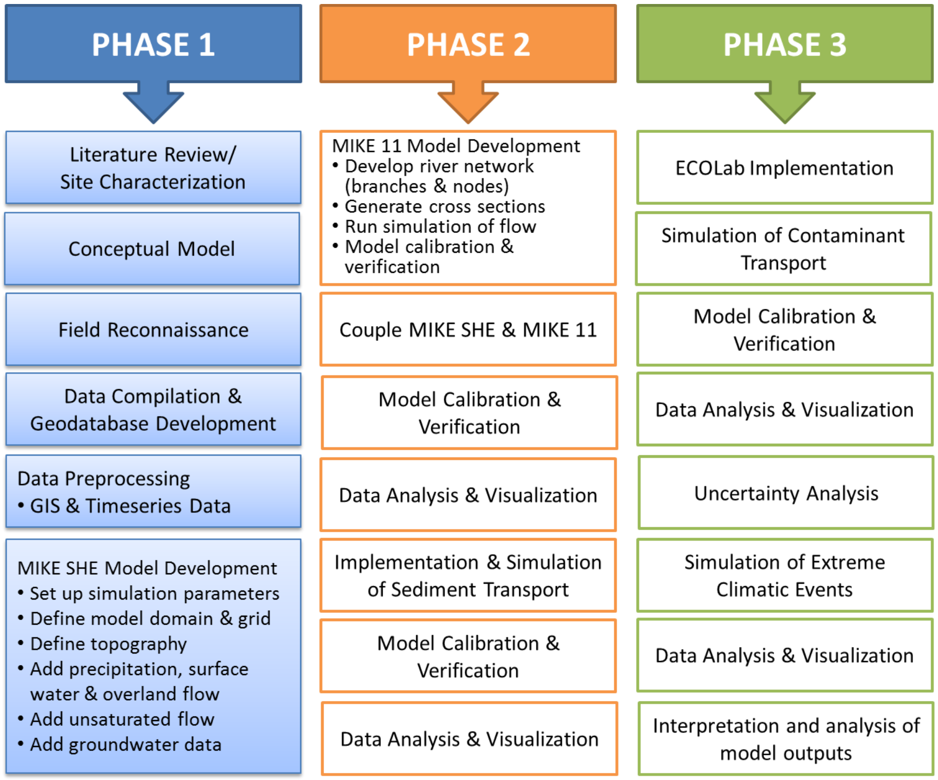

Figure 51. Hydrological modeling phases and detailed future plans.

The future modeling tasks to be performed include:

1. Refinement of the input data for coupling of the surface water/groundwater model to include evapotranspiration (ET) and groundwater parameters.
2. Running the UZ/SZ/ET modules simultaneously within MIKE SHE domain for prediction of the water balance of the TBW.
3. Calibration of the model will be carried out to evaluate and refine parameter values by comparing simulated and observed values in an attempt to develop a model that represents the watershed. Different statistical evaluation methods will be employed to ensure the accuracy of the calibration results. This calibration and validation exercise helps to improve the predictive capability and reliability of the model. The main steps used for model calibration include: identification of calibration parameters, sensitivity analysis and numerical optimization.
4. Developing a 1-D river model using MIKE 11 for TB.
5. Calibrating and validating of the MIKE 11 river model of TB in accordance with the MIKE SHE simulation of the TBW.
6. Coupling the MIKE SHE watershed model and the MIKE 11 river model.
7. Finally, the developed model will then be integrated with the ECO Lab module to simulate contaminant transport in the TBW and stream.

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TASK 3: SUSTAINABILITY PLAN FOR THE A/M AREA GROUNDWATER REMEDIATION SYSTEM

The performance of the M Area groundwater remediation system (GRS) at M Area Savannah River Site (SRS) has been reviewed many times over it lifetime. The M Area GRS consists of a network of extraction wells feeding a central treatment process – the M1 Air Stripper. As pumps and motors have worn out over the 28 years of continuous operation, more efficient commercial ones have replaced them. Various remediation operations such as soil vapor extraction, thermally enhanced extraction (e.g., six phase heating and *in situ* steam stripping) in combination with the M-Area GRS have contributed to a major reduction in the source term of trichloroethylene (TCE) and tetrachloroethylene (PCE) contamination in the vadose zone and saturated zone. The concentrations of TCE from 6 of 12 recovery wells (RWM 1-12) connected to the M1 Air Stripper have dropped by more than a factor of 10 since operations began in 1985. While the concentrations are still higher than regulatory limits in many extraction wells, SRS technical support staff and the South Carolina Department of Health & Environmental Control (SCDHEC) are working together to assess the system performance and develop future plans to finalize the remediation of M-Area groundwater. These planning efforts consider any remaining TCE/PCE sources, potential enhanced attenuation actions using the existing recirculation wells, and the nature and rates of natural attenuation in the plume. The primary objective of the project in 2015 is to collect engineering data for the M1 Air Stripper in August and September 2015 trips to SRS and use the data to complete a Green and Sustainable Remediation (GSR) analysis of the M1 Air Stripper by December 2015. During August and September, SRNL, FIU and DOE EM HQ will work to identify scope for this task for 2016. FIU proposes to analyze mass, distribution and transport of contaminants at SRS M Area to determine if a scaled down remediation system is feasible and perform a GSR for this option. It is postulated that most of the TCE and PCE have been removed from the vadose zone at the M Area of SRS from multiple remediation operations.

This technical report has 4 sections: (1) a primer on Green and Sustainable Remediation analyses, tools and case studies; (2) background on the SRS M Area contamination and its groundwater remediation system containing the M1 Air Stripper and 15 connected recovery wells; (3) FIU's analysis of historical data of TCE and PCE removal from 1987-2012; and (4) a path forward for a more extensive GSR analysis of the M1 Area remediation systems in 2016.

The September meeting at SRS will bring together experts from Savannah River National Laboratory and the site remediation contractors (Savannah River Nuclear Solutions) and is expected to provide information and documentation on the M1 Air Stripper and to provide a setting to discuss possible future remediation options. These in turn will provide necessary information for FIU to do a GSR analysis of the air stripper and pumps by December and a GSR of a potential major transformation of the M Area groundwater remediation system.

INTRODUCTION

Primer on Green and Sustainable Remediation

Definitions for Green and Sustainable Remediation and Green Remediation

There are multiple definitions of "Green Remediation," "Sustainability" and "Green and Sustainable Remediation." For this report, we focus on GSR and Green Remediation as defined by the Interstate Technology & Regulatory Council (ITRC) and the U.S. EPA below.

GSR: The site-specific employment of products, processes, technologies, and procedures that mitigate contaminant risk to receptors while making decisions that are cognizant of balancing community goals, economic impacts, and net environmental effects (ITRC, May 2011).

Green Remediation: Reducing environmental impacts of common investigation and remediation activities (ITRC, May 2011).

Green Remediation: The practice of evaluating all environmental effects of remedy implementation and incorporating options to maximize the environmental footprints of cleanup actions (U.S. EPA, April 2008).

The US EPA identifies **6 core elements** of Green Remediation in its primer (U.S. EPA, April 2008) that are considered when designing and implementing cleanup measures:

- ♦ *Material & Waste*: Reduce material use; source unrefined materials locally and/or from recycled sources; minimize hazardous and non-hazardous waste generated onsite; and recycle waste generated on site.
- ♦ *Land & Ecosystem*: Protection of valuable "ecosystem services" at sites during cleanup (soil erosion control, nutrient uptake and water quality protection, wildlife habitat, etc.).
- ♦ *Water:* Seek beneficial use of extracted/treated water; optimize capture zones of pump and treat (P&T) systems; divert clean water around impacted area; infiltrate diverted storm water for aquifer storage; use less-refined water resources when possible; and manage stormwater runoff.
- ♦ *Energy:* High-efficiency equipment, low-emission vehicles, carpools, local materials and services, DC motors, cogeneration, on-site renewable energy, etc.
- ♦ *Air:* Reduce particulate matter, sulfur oxides, nitrous oxides, and greenhouse gases (GHGs).
- ♦ *Stewardship:* Reduce emissions of greenhouse gases; install renewable energy systems; use passive sampling; solicit community involvement.

Regulatory Drivers for GSR

Regulatory drivers are important for implementing best demonstrated and available technologies (BDATs); fostering the use of best management practices (BMPs); and for achieving a myriad of environmental performance goals such as the cleanup of air, streams, groundwater and more. The following are regulatory drivers to encourage site managers to implement GSR practices and broader sustainability planning and practices:

- Executive Order 13514: Federal Leadership in Environmental, Energy and Economic Performance. Sets sustainability goals for Federal agencies and focuses on making improvements in their environmental, energy, and economic performance.
- DOE Order 436.1: Departmental Sustainability. Requires sustainability principles be integrated into DOE's Strategic Sustainability Performance Plan (SSPP).
- EPA Strategic Plan 2011-2015: Goal 3: Cleaning up communities and advancing sustainable development. Aimed to prevent and reduce exposure to contaminants and accelerate the pace of cleanup across the country.
- EPA OSWER Policy: Principles for Greener Cleanups
    - Protect human health and the environment
    - Comply with all applicable laws and regulations
    - Consult with communities regarding response action impacts consistent with existing requirements
- Superfund managers fit GSR into Superfund framework [e.g., *EPA shall consider the "potential environmental impacts of the remedial action and the effectiveness and reliability of mitigative measures during implementation." (40 CFR 300.415(e)(iii)(E)(3))*]

Benefits of GSR

There are numerous benefits derived from implementing GSR from the concrete saving of monies to the more intangible building of good will and support from community, regulators and other stakeholders. These benefits may vary significantly depending on the specific site characteristics and requirements. The 10 most cited benefits of GSR are (U.S. DOE 2, September 2013) (U.S. DOE, June 2013):

- Reduces energy consumption;
- Contributes to meeting our greenhouse gas (GHG) goals;
- Reduces toxic air emissions;
- Reduces polluting waste water discharges;
- Lessens impact on ecosystems;
- Decreases land use and carbon footprints;
- Reduces waste generation;
- Reflects BMPs and good environmental stewardship;
- Helps achieve public acceptance; and
- Reduces cost.

GSR practices also benefit the surrounding community. Fewer emissions, less waste production, and less natural resource use all help protect public health, and make the community more aesthetically pleasing. In some cases, GSR also translates into shorter cleanup times and reduced disturbance as compared to machinery-intense cleanups (The Horinko Group, February 2014).

When GSR practices include the use of locally sourcing materials, and when cleanup results in the reuse of a site, communities may benefit from economic development, job creation, and increased real estate values.

Recommended Steps for GSR Implementation

Footprint reduction is not as straightforward as the other benefits. In order to reduce land use and carbon footprints, it is important that goals and a common ground are found during the remedy selection and design phase. This can be challenging and so below are several steps to follow to facilitate footprint reductions:

- Develop an accurate conceptual site model (CSM);
- Characterize the source areas and contaminant plumes;
- Determine which sustainability metrics should be considered for the site;
- Establish and apply a methodology to quantify or characterize each metric;
- Obtain consensus regarding how metrics are weighed against each other and against traditional criteria in selecting the remedial approach;
- Identify methods to reduce environmental footprint of remedy components; and
- Prioritize, select, and document what footprint reduction methods should be implemented with consideration of the overall net environmental benefit and available funding.

Perceived "Roadblocks" to Institutionalizing Green Remediation

There are many roadblocks to institutionalizing Green Remediation and GSR practices. Some of these roadblocks are real and others result from the perception of site managers regarding what is possible. The US EPA has done extensive surveys on the perceived roadblocks and below is a prioritized list of them in order of their relevancy:

1. Lack of unified approach, common language, education, communication;
2. Existing mindsets and dis-incentives;
3. Authorization and justification to implement;
4. Funding level and schedule constraints;
5. Measurement of the benefit; and
6. Remedy protectiveness and greenwashing.

Progress in overcoming these roadblocks is evident in publications, conferences, emerging best management practices, regulatory guidelines, and numerous other ways.

Examples of evidence of this change are:

- A growing number of publications, various awards, numerous conferences related to "green remediation," and "sustainability" now available from journals, conferences and the EPA;
- The new ASTM voluntary green cleanup standard practice;
- Incentives for remediation contractors to counterbalance the many dis-incentives for GSR and BMPs;
- A few federal agencies increased use of SITEWISE™ and other GSR tools;

- Small business trainings and the ITRC GSR training; and
- More websites, documents and other information resources on GSR.

EPA Information Resources on GSR

Listed below are some of the key information resources on GSR from the U.S. EPA:

- EPA's "Methodology for Understanding and Reducing a Project's Environmental Footprint"
- Primers
- Guidance documents
- Case studies
- Project profiles
- Technical bulletins
- Fact sheets
- www.clu-in.org/greenremediation
- www.brownfieldstsc.org
- www.triadcentral.org
- www.itrcweb.org/Documents/GSR-1.pdf
- www.sustainableremediation.org/library
- U.S. EPA GSR Contacts is: Carlos Pachon (pachon.carlos@epa.gov) (Interstate Technology & Regulatory Council August 2012)

Implementing GSR

The framework for GSR includes the planning phase and the implementation phase. While implementation is very site specific and relies upon stakeholder involvement, there are established steps to planning GSR and steps for implementing GSR. These are listed below.

Planning GSR steps:

1. Evaluate/update site conceptual model
2. Establish GSR goals
3. Establish strong stakeholder involvement
4. Select metrics, evaluation level, and boundaries
5. Document all GSR activities

GSR implementation occurs during multiple phases of the remediation project. Therefore, it is useful to consider the phases in remediation projects and how GSR may be brought to bear during each of them.

Site remediation steps include:

1. Investigation (GSR applied during planning)
2. Remedy evaluation and selection (best point for implementing GSR)
3. Remedy design (integration of GSR into remedy)
4. Remedy construction (GSR is integral to remedy)
5. Remedy operation, maintenance and monitoring (benefits from GSR accumulate)
6. Remedy optimization (sustainable performance improvements)

7. Close out (support for site reuse, negotiations with regulators may be improved by GSR)
8. Post-closure monitoring, PCM (needed at some sites, allows for GSR framework for PCM)

While progressing through site remediation steps, the GSR steps include:

1. Identify GSR options
2. Evaluate GSR options
3. Implement GSR approaches, and
4. Monitor, track and document all GSR activities.

FIU has created a visual flowchart that will help improve understanding and implementation of GSR (See Figure 52a and Figure 52b below).

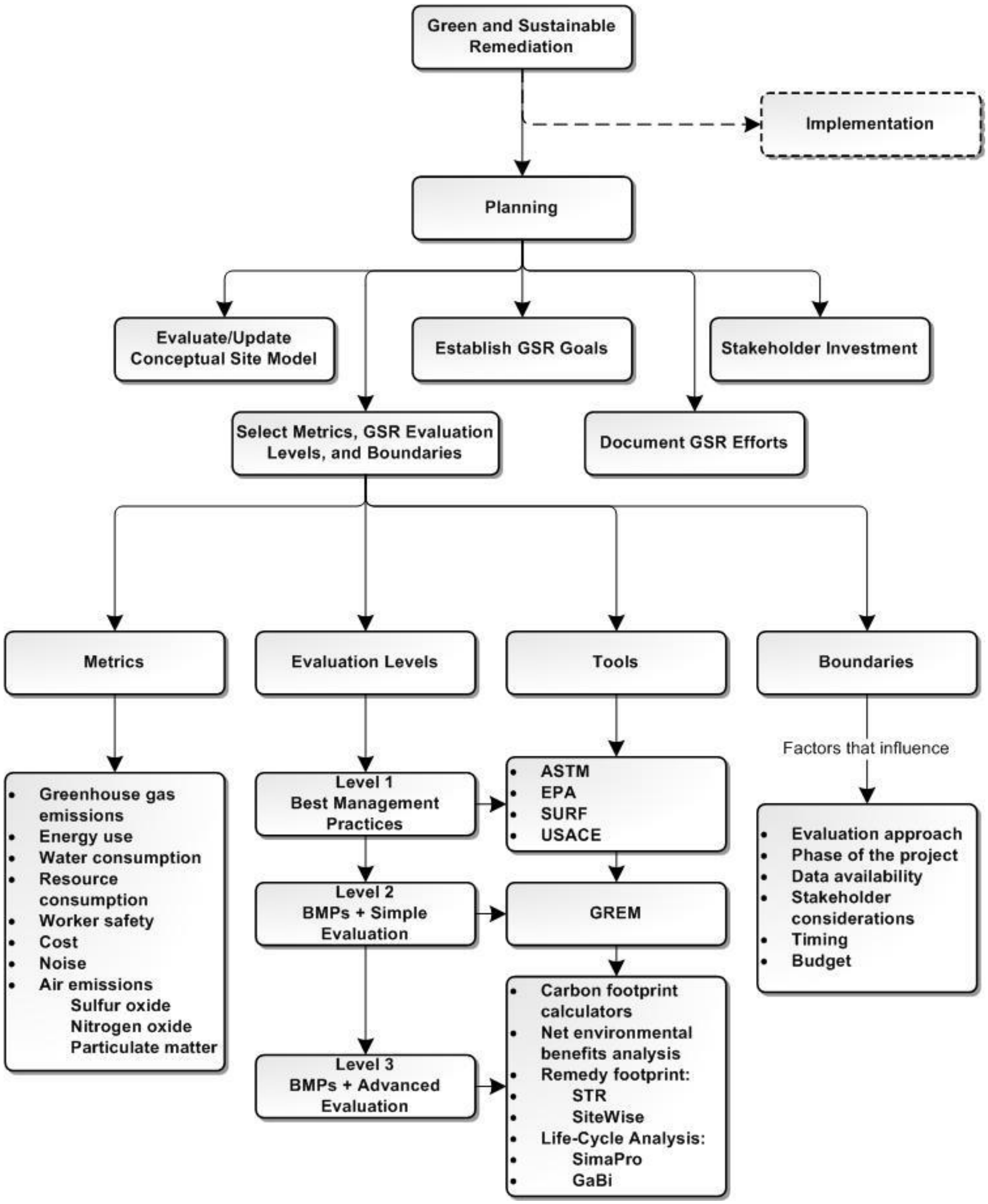

Figure 52a. Flowchart for GSR Planning.

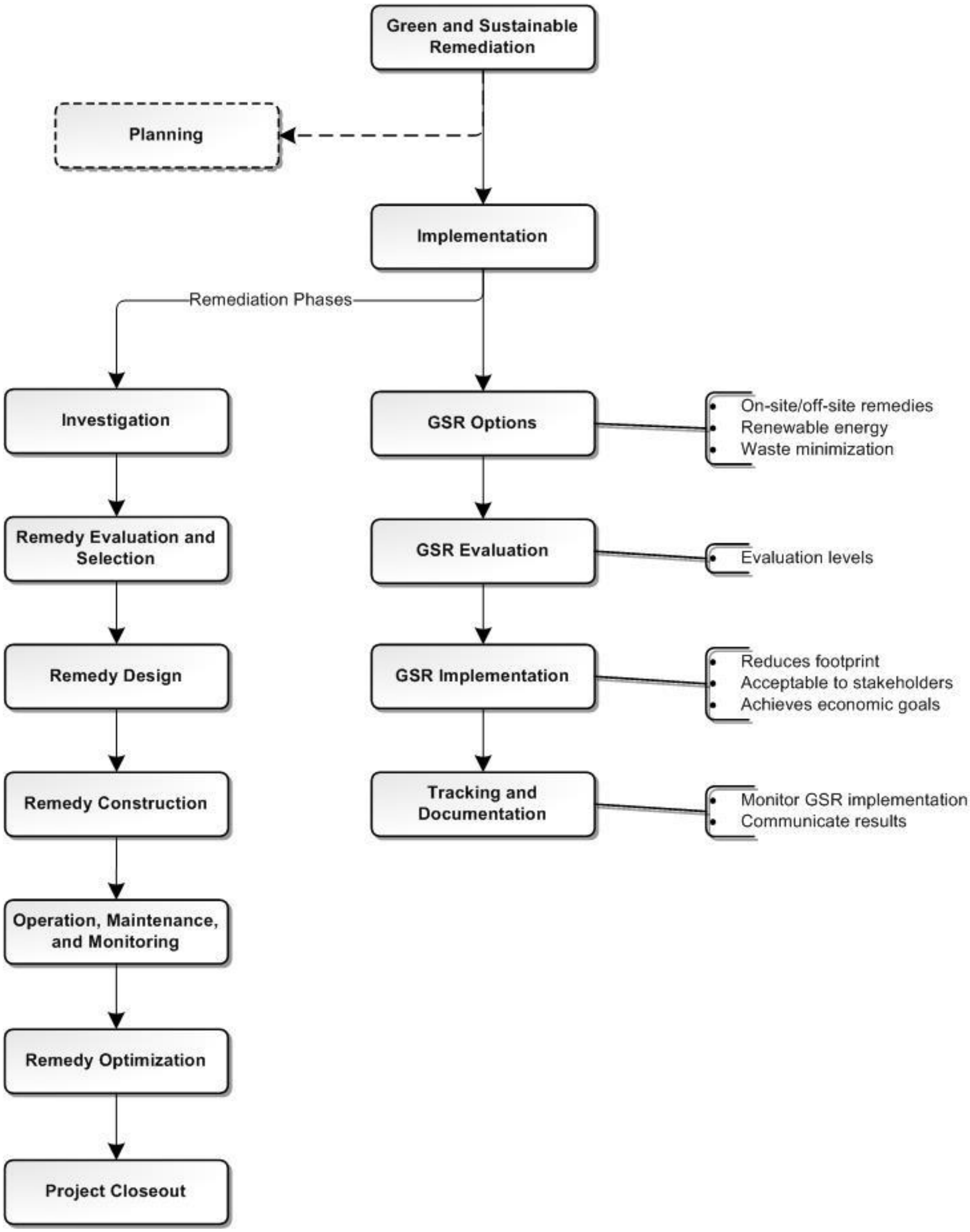

Figure 52b. Flowchart for GSR Implementation.

GSR Metrics

The selection of particular metrics varies among all sites implementing GSR. Since regulators and the local community are involved, some low cost intangible GSR metrics can be developed that bring more trust, potential economic development, and good will that can often result in better technical remedies at a lower cost. The most common metrics assessed for possible implementation include:

- Fresh water consumption
- Biodiversity
- Renewable energy use
- GHG emissions
- Material use
- Community impacts
- Land use
- Waste generation
- Cultural resources
- Carbon footprint
- Capital costs, and
- Employment

Key Lessons from Case Studies of GSR Implementations

While it in not institutionalized or even common practice, there have been many very successful GSR implementations. From the ITRC GSR training document, key lessons learned from several case studies include:

- Flexibility: the GSR process can be applied to a variety of sites, remediation phases and regulatory programs;
- Communication: communication with stakeholders is critical to successful application of GSR;
- Assumptions: because evaluation methods are new, users must understand the assumptions of the tools being used; and
- Holistic: this holistic approach will minimize a project’s life cycle impacts.

GSR Tools and their Selection

There is no certification or industry standard for GSR tools. Important considerations in tool selection include:

- Site specific GSR goals and metrics;
- Scope, budget, schedule and purpose of GSR evaluation;
- Availability of site data;
- Types of remediation technology; and
- Regulatory cleanup program in effect.

GSR Tools include:

- Best Management Practices (BMPs) level 1 (ASTM, EPA, SURF, USACE, EPA fact sheets) *qualitative;*
- Best Management Practices (BMPs) level 2 (CA Green Remediation Evaluation Matrix) *semi-quantitative;*
- Best Management Practices (BMPs) level 3 [carbon footprint calculators; remedy footprint tools (Air Force Sustainable Remediation Tool; Navy, USACE SITEWISE™); Net environmental benefits analysis tools; and Life Cycle Assessment tools] *quantitative.*

Background of the SRS M Area Contamination and the M1 Air Stripper System

The Savannah River Site (SRS), located in Aiken, Allendale, and Barnwell Counties in South Carolina, is a nuclear production facility operated for the U.S. Department of Energy (DOE). SRS contains 36,000 acres of wetlands and an additional 5,000 acres of bottomland soils subject to flooding. By the 1950's, the SRS facility was focused on nuclear weapons production and power production. These operations led to the release to the environment of major quantities of contaminants. Like many defense operations sites in the 1970's and 1980's, trichloroethylene (TCE) and tetrachloroethylene (PCE) were the main solvents used in degreasing and other industrial operations. In the 1980's, major operations were initiated to remediate the contaminated soil and groundwater which continues today. This first major environmental cleanup operation at SRS saw the world's first air stripper designed, built and installed to treat contaminated groundwater, and soil vapor extraction units for removal of contaminants from air pulled from soil in the vadose zone (above the water table). PCE and TCE are categorized as dense non-aqueous phase liquids (DNAPLs), semi-volatile, and hazardous chemical compounds.

Since 1985, groundwater in the A/M Area on the northern part of SRS has been treated to reduce concentrations of chlorinated solvents. This treatment system consists of groundwater wells from which groundwater in the area is pumped to the M1 Air Stripper, which removes chlorinated solvents. The treated groundwater is discharged to a stream of Tims Branch, a small stream ecosystem also in the northern portion of SRS.

Just upstream of the air stripper, the pumped groundwater is altered with tin (II) chloride ($SnCl_2$ or stannous chloride), which reacts with mercury in the water to reduce it to elemental mercury. The groundwater enters the M1 Air Stripper and the elemental mercury, which is more volatile than dissolved mercury, is stripped from the water along with the chlorinated solvents. The mercury concentration in the untreated groundwater is initially approximately 250 ng/L (parts per trillion) and the treatment system reduces the concentration of mercury in the treated groundwater to approximately 10 ng/L.[1]

Since the DOE SRS A/M Area groundwater remediation system is expected to operate continuously for the foreseeable future, any 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. Increased contaminant recovery will reduce the overall time necessary to meet regulatory requirements. Options for improved contaminant recovery include restoring well efficiency and redistributing pumping within the existing network. Information compiled in the baseline analysis will be used to identify opportunities to increase contaminant recovery using existing wells.

The M1 Air Stripper has operated continuously for over 27 years at an average electrical load of 150kW and flow rate of 420 gpm. This represents an average of 1,247,000 kW-hr of electricity consumed per year and 209,714,000 gallons pumped per year. The influent TCE concentration to the air stripper has decreased exponentially from 25,200 µg/L in 1986 to 2,230 µg/L by the end of 2012. This concentration decrease is common for groundwater remediation systems that use groundwater pumping. The M1 Air Stripper at SRS removed 33,231 pounds of TCE during its first full year of operation and removed 2,092 pounds of TCE during its 26^{th} year of operation while consuming the same amount of electricity and removing the same amount of water in both years. The pumping and overall electrical energy efficiency (per 1 pound of TCE removed and destroyed) has decreased to 6% of the initial year of operation. That is, it now requires 15.9 times more energy and groundwater to remove 1 pound of TCE in the 26^{th} year of operation than it did in the first year of operation. PCE was used early at SRS and operations switched to TCE in the 1970's due to the perceived hazard of PCE. PCE is many times less soluble and less volatile than TCE. For these reasons, recovery for the first 25 years has been dominated by TCE recovery and will be dominated by PCE recovery for the next 25 years. Already, PCE recovery equals or exceeds TCE recovery in 7 of 12 recovery wells. Reducing the environmental costs of the A/M groundwater remediation system will reduce the overall cost to SRS to operate the system through improved mass recovery and reduced use of energy and other site resources.

Recovery wells in the A/M Area groundwater remediation system have been operated with constant speed pumps since the system began operation. The constant speed pumps produce line pressures that range from 35 – 95 psig. In some cases, the pumps may be producing excess pressure that is not required and as a result are continuously consuming energy that is not necessary for operation. The piping diagram and operating pressure throughout the system will be studied to identify wells which may be able to operate using a smaller pump while still maintaining the same flow rate.

The overall objective of the A/M Area groundwater remediation system is to provide hydraulic containment of the most contaminated portion of groundwater until regulatory requirements are met. The M1 Air Stripper has operated at a constant air/water ratio since it began operation. The air/water ratio was set to treat the prevailing influent contaminant concentrations existing at start-up. Contaminant concentrations have decreased an order of magnitude during the first 27 years of operation and, as a result, the air/water ratio can likely be decreased. The water flow rate is set by the hydraulic containment objective and is not considered to be an option for improvement. The air flow rate, however, is based on the influent contaminant concentration. It is believed that the air flow rate can be reduced and still meet the discharge limits at the outfall receiving effluent from the M1 Air Stripper. Reducing the air flow rate would significantly reduce the energy demand since the M1 Air Stripper operates continuously.

Figure 53 contains the spatial locations of the groundwater recovery wells, soil vapor extraction units, and dynamic underground stripping wells. Note that the M1 Air Stripper draws groundwater from recovery wells RWM-1 – RWM-12. The injection of steam for 4 years as part of the dynamic underground stripping remediation process was very successful in removing and destroying TCE and PCE in the nearby M Area settling basin. The increased ground temperature has mobilized DNAPL and resulted in increased recovery in several of the RWM 1-12 wells at this DNAPL location. Soil temperatures have been cooling since steam injection ended in 2009, but the elevated temperatures will continue for another decade and continue to enhance removal of TCE and PCE.

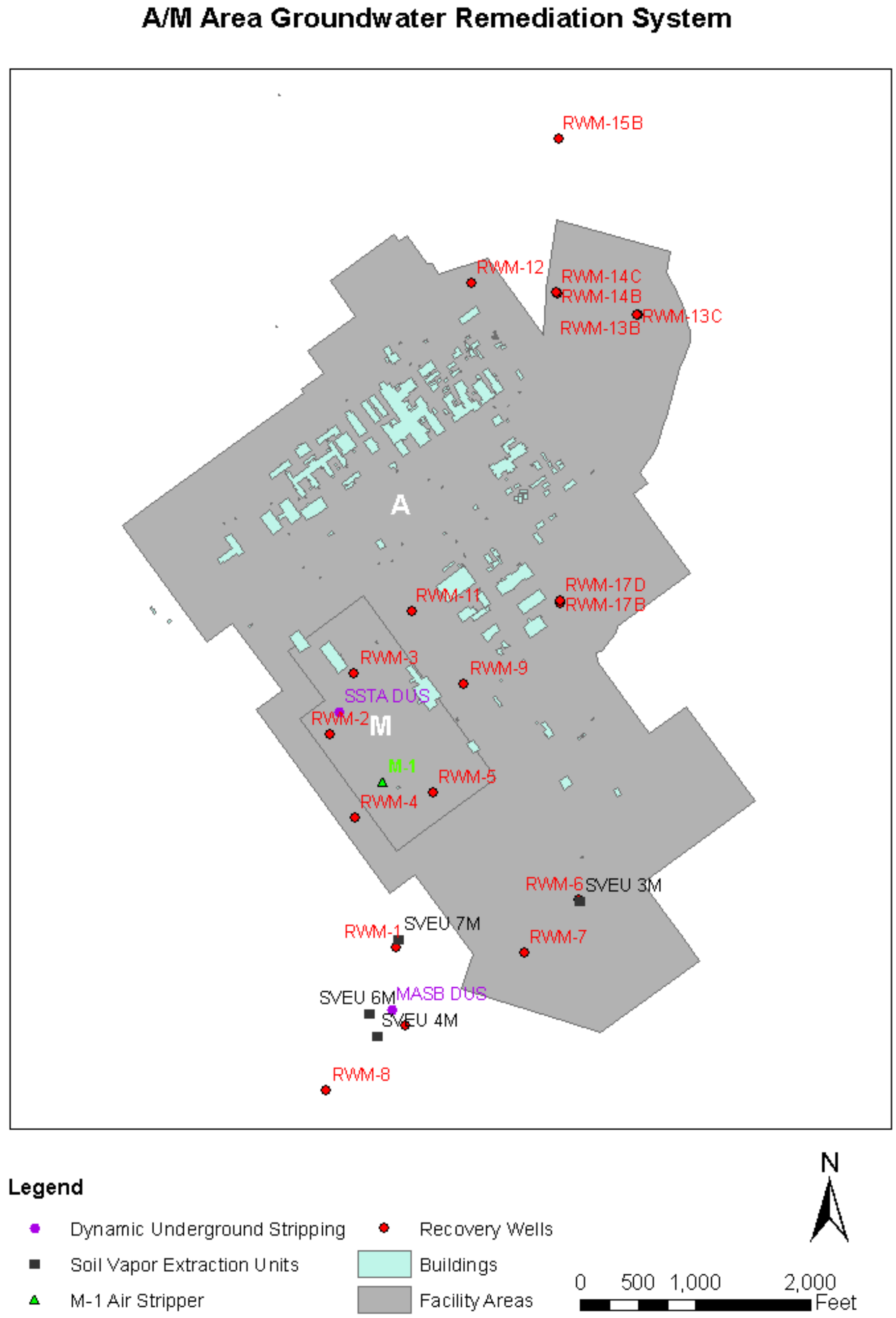

Figure 53. Spatial location of buildings, groundwater wells, soil vapor extraction units, and Dynamic Underground Stripping wells for steam injection in A and M areas.

Background - Air Stripping Process

The air stripping process is a mass transfer operation that provides contact between air and water, encouraging the volatile organic compounds (VOCs) to move from the water to the air. There are different types of air strippers which should be selected based on the conditions of each site. The most common one is the packed column air stripper which consists of a counter-current flow of water and air through a packing material in a large tower. The packing material is usually plastic, ceramic, or steel with different shapes and sizes that allow a higher surface-to-volume ratio and provide the necessary transfer surface to permit volatile components to move from the liquid stream to the air stream. In the packed column stripper, the contaminated water comes from an aeration nozzle at the top of the tower, and the air is blown from the bottom (Figure 54).[2] Optimal conditions for the packed column air stripper and what parameters need to be taken into account to design it and optimize it will be analyzed more in depth in this report.

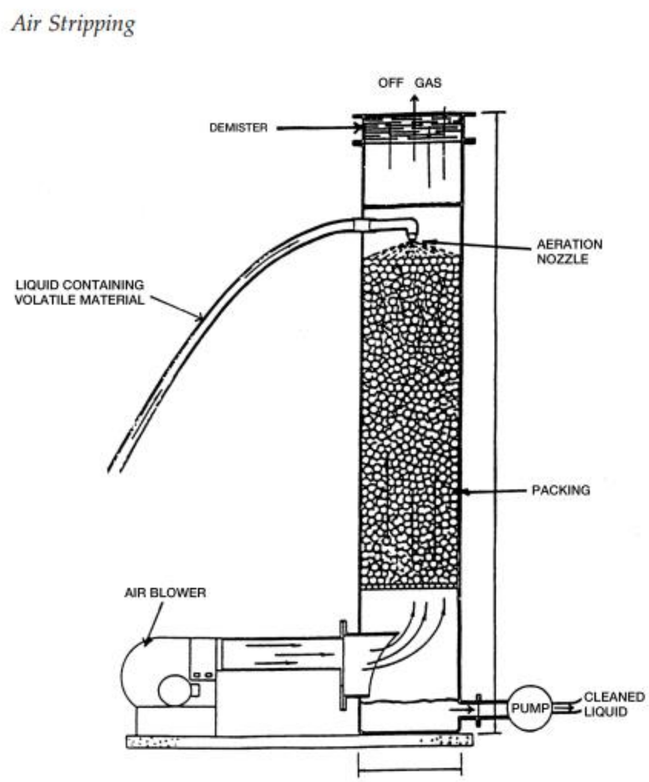

Figure 54. Schematic diagram of an air stripping tower.

Since the air stripping process involves association between air and water, we need to know the solubility of the gas in the liquid to determine under what conditions the stripper will work adequately, and how easily the contaminant will be removed. This ratio of the contaminant at equilibrium in the liquid phase to the contaminant in the gaseous phase is a relationship called Henry's Law in which at equilibrium, as air molecules pass into the water, an equivalent number of molecules of the solvents in the liquid leave the water phase and become part of the vapor.

Under equilibrium conditions, the partial pressure of a gas above a liquid is proportional to the concentration of the chemical in the liquid:

$$P_g = H\,C_L$$

Where: P_g is the partial pressure of the gas
H is Henry's constant
C_L is the concentration of the chemical in the liquid

Design[3, 4]

When designing an air stripper, many factors come together. The height of the packed tower will affect the removal efficiency of the contaminant. The desired rate of flow of the liquid will determine the diameter of the air stripping column. The type of packing material, its size and shape, will impact the mass transfer rate. The packing material provides the air-to-water interfacial area which will determine the efficiency of the stripping process. The air-to-water flow ratio will control the removal rate of the contaminant. If this ratio increases, usually it results in a greater removal rate. Although, if the entrance of the liquid goes through the air flow, the result is a spike increase in the air pressure drop, causing what is called flooding. The usual pressure drop in the tower should be between 200 - 400 N/m^2.

A key aspect in the proper operation of every machine is its maintenance. In the case of packed column air strippers, this relates to the fouling of the packing material. Due to the size of the towers on column air strippers, it is difficult to clean the packing material. If the packing material is not cleaned frequently enough, mineral deposits like calcium will concentrate on the packing, reducing the surface area. This will result in a lowering of the mass transfer process, thus preventing an efficient stripping. Also, routine blower and pump maintenance is required for optimum performance of the stripper.

RESULTS AND DISCUSSION

Analysis of Historic Data of TCE and PCE removal from 1987-2012

The monthly rainfall at SRS from 1987 through 2012 was collected from the USGS and is plotted below in Figure 55. Data from wet and dry periods were compared to TCE and PCE monthly removal rates without any correlations obvious via simple inspection of the data.

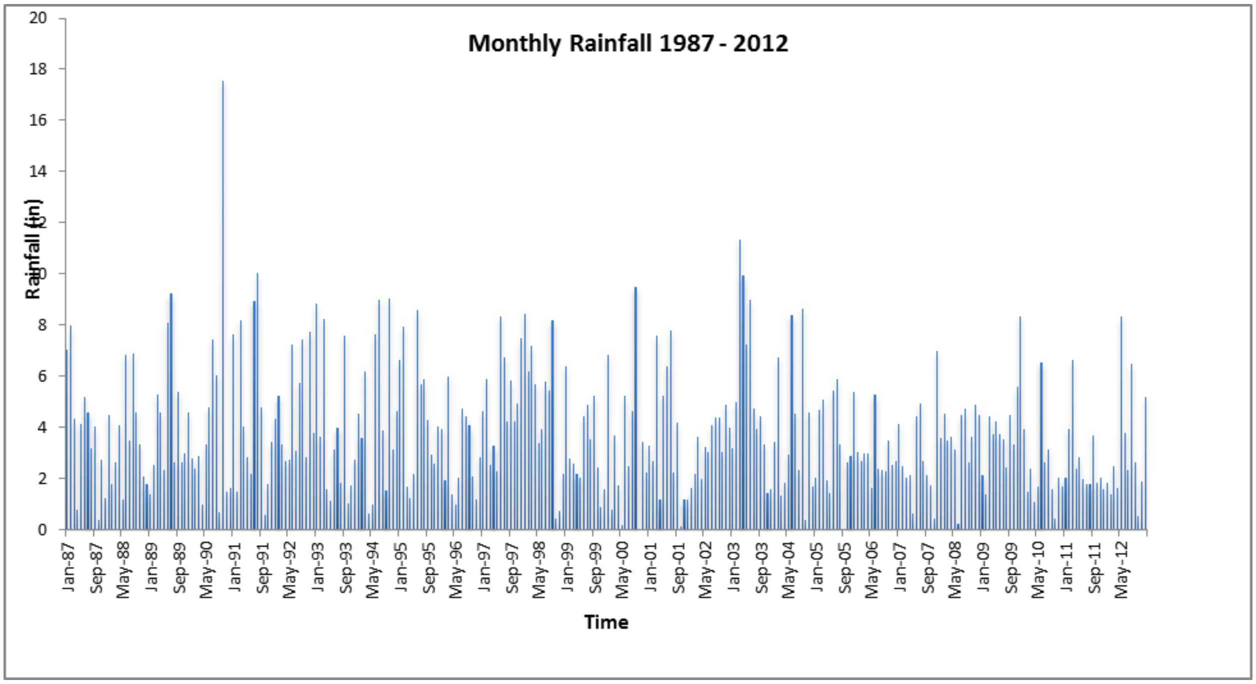

Figure 55. Monthly Rainfall at SRS from 1987-2012.

TCE and PCE monthly recovery rates, as well as pumping flow rates for this period from SRS sources, had many months of missing data. SRS did have the total monthly removal rates of all wells combined for this period. FIU sifted through numerous historical site documents to identify missing data as well as specific months when specific wells were not operational.[5-14]

A significant amount of data was found in the following reports:

- 1990 M-Area Hazardous Waste Management Facility Post-Closure Care Permit Groundwater Monitoring and Corrective Action Program.
- Fourth Quarter 1992 and 1992 Summary M-Area Hazardous Waste Management Facility Groundwater Monitoring Report, Volume I.
- Fourth Quarter 1994 M-Area Hazardous Waste Management Facility Groundwater Monitoring and Corrective-Action Report.
- Third and Fourth Quarters 1995 M-Area Hazardous Waste Management Facility Groundwater Monitoring and Corrective-Action Report.
- Third and Fourth Quarters 1996 M-Area and Metallurgical Laboratory Hazardous Waste Management Facility Groundwater Monitoring and Corrective-Action Report, Volume I.
- Third and Fourth Quarters 1997 M-Area and Metallurgical Laboratory Hazardous Waste Management Facility Groundwater Monitoring and Corrective-Action, Volume I.
- Third and Fourth Quarters 1999 Annual M-Area and Metallurgical Laboratory Hazardous Waste Management Facility Groundwater Monitoring and Corrective-Action Report, Volume I and II.

- Annual 2010 M-Area and Metallurgical Laboratory Hazardous Waste Management Facilities Groundwater Monitoring and Corrective Action Report, Volume I.
- Annual 2011 M-Area and Metallurgical Laboratory Hazardous Waste Management Facilities Groundwater Monitoring and Corrective Action Report, Volume I.

This missing data and the months when wells were not operational have been added to an Excel file of all the contaminant recovery data.

The monthly removal rate and the cumulative mass removed for TCE and PCE in the 12 recovery wells (RWM-1 through RWM-12) are plotted on the next 6 pages. These plots use all of the monthly well data collected to date. For the several remaining months when wells were operating but for which there is still missing data, FIU will apportion the total recovery from 12 wells per month to each well according to its relative contribution to recovery rates prior to that month.

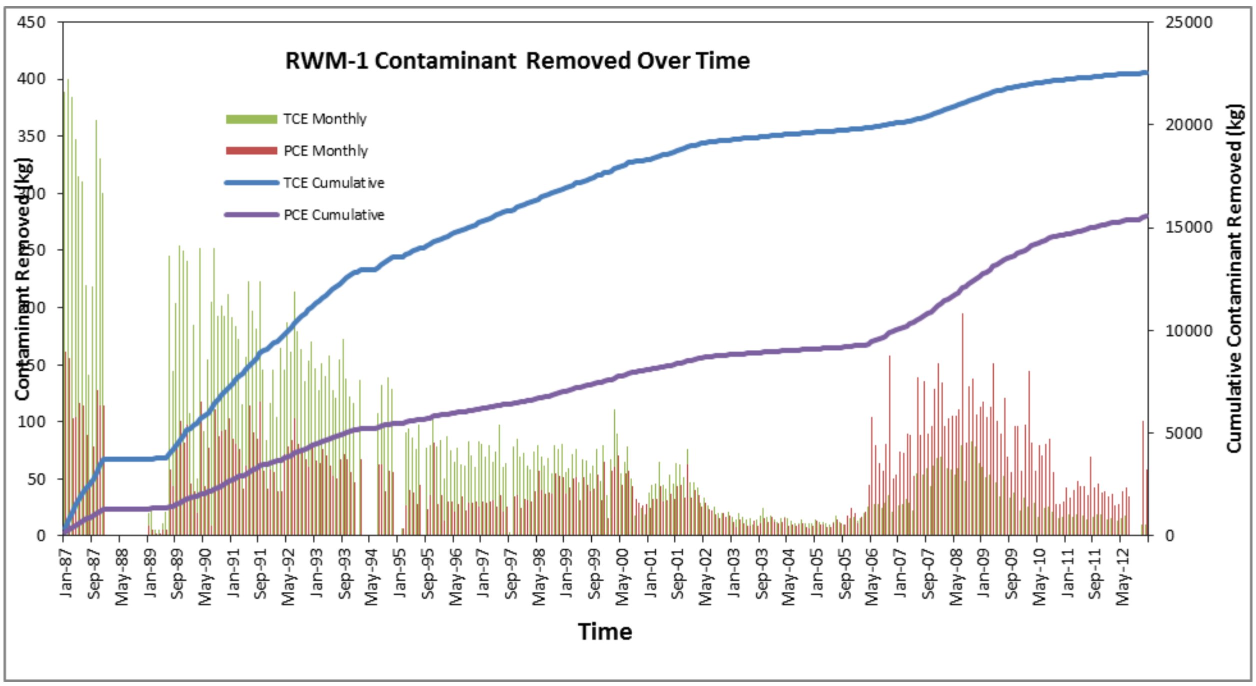

Figure 56. TCE and PCE removed per month and cumulative from 1987-2012 for RWM-1.

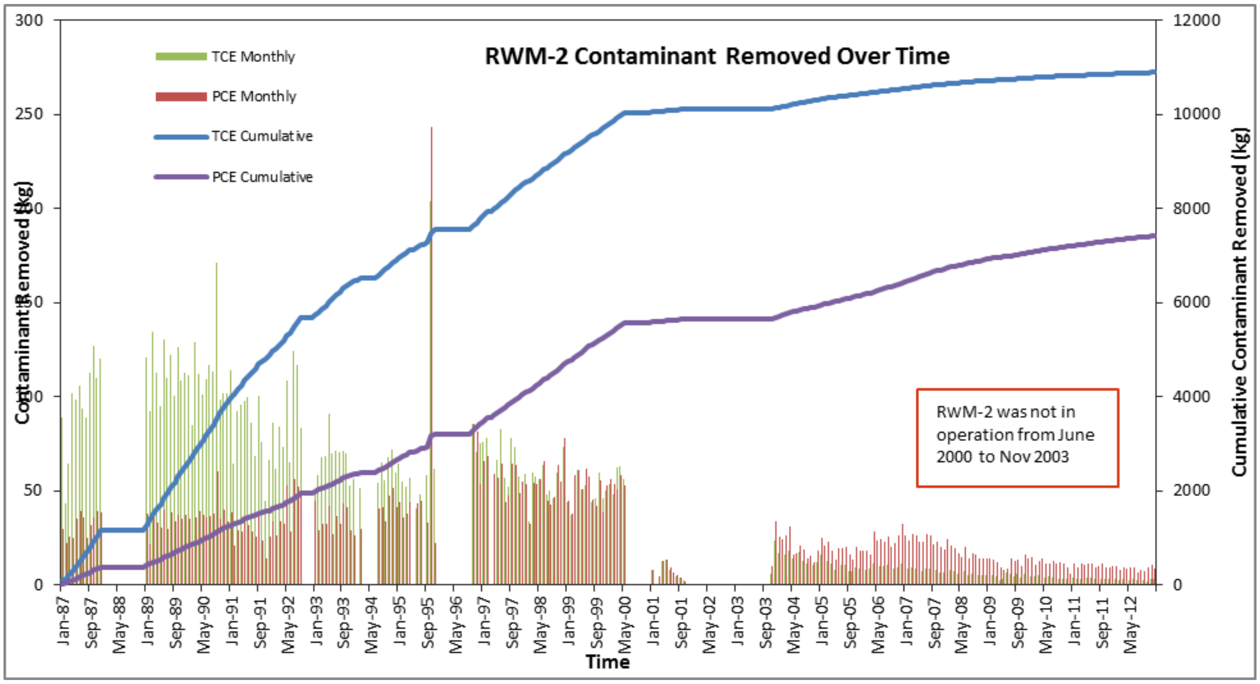

Figure 57. TCE and PCE removed per month and cumulative from 1987-2012 for RWM-2.

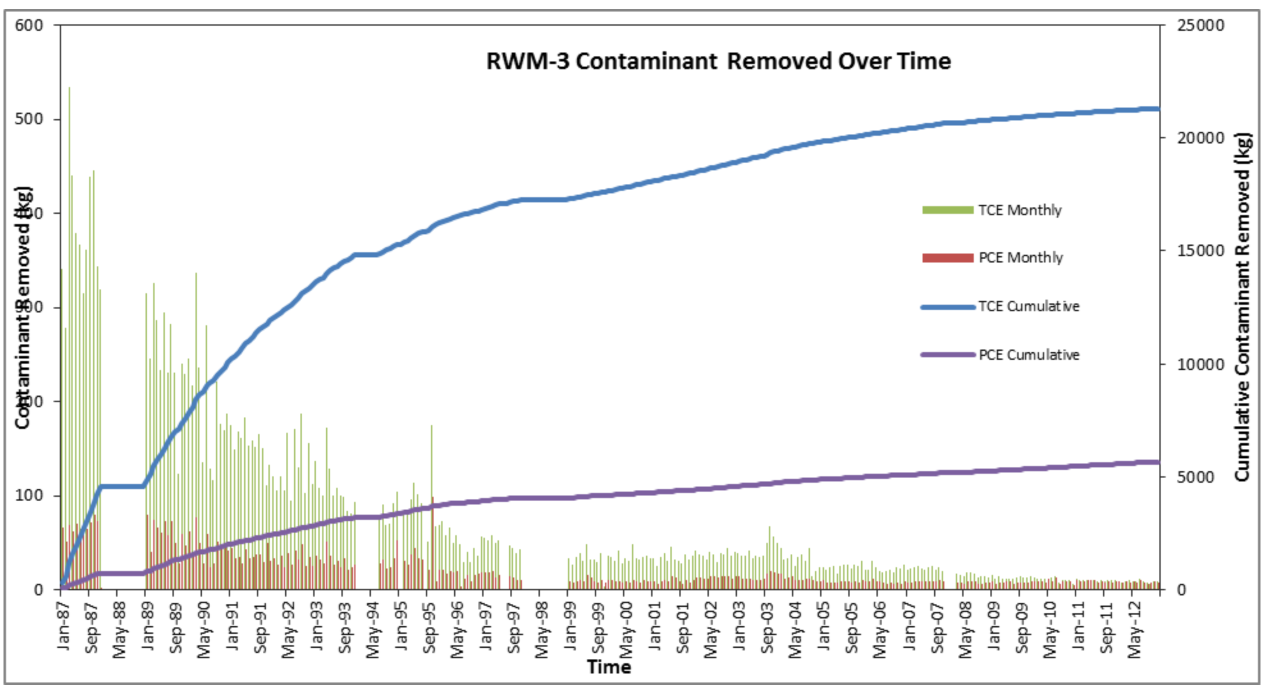

Figure 58. TCE and PCE removed per month and cumulative from 1987-2012 for RWM-3.

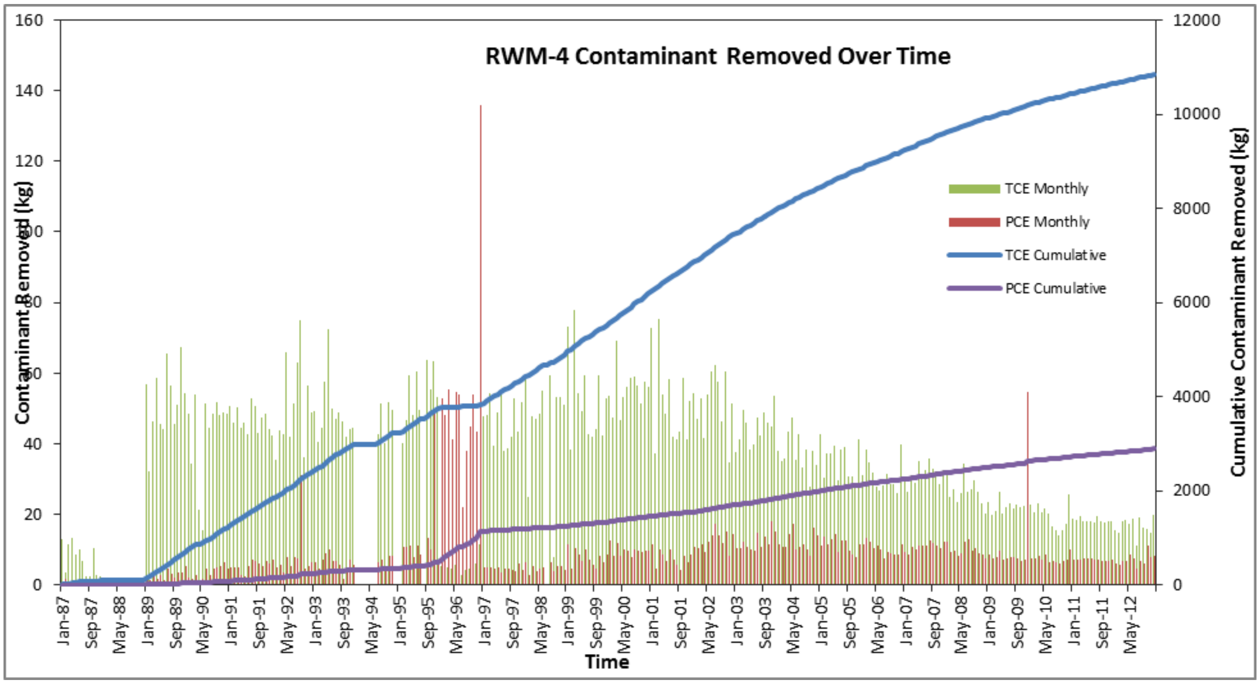

Figure 59. TCE and PCE removed per month and cumulative from 1987-2012 for RWM-4.

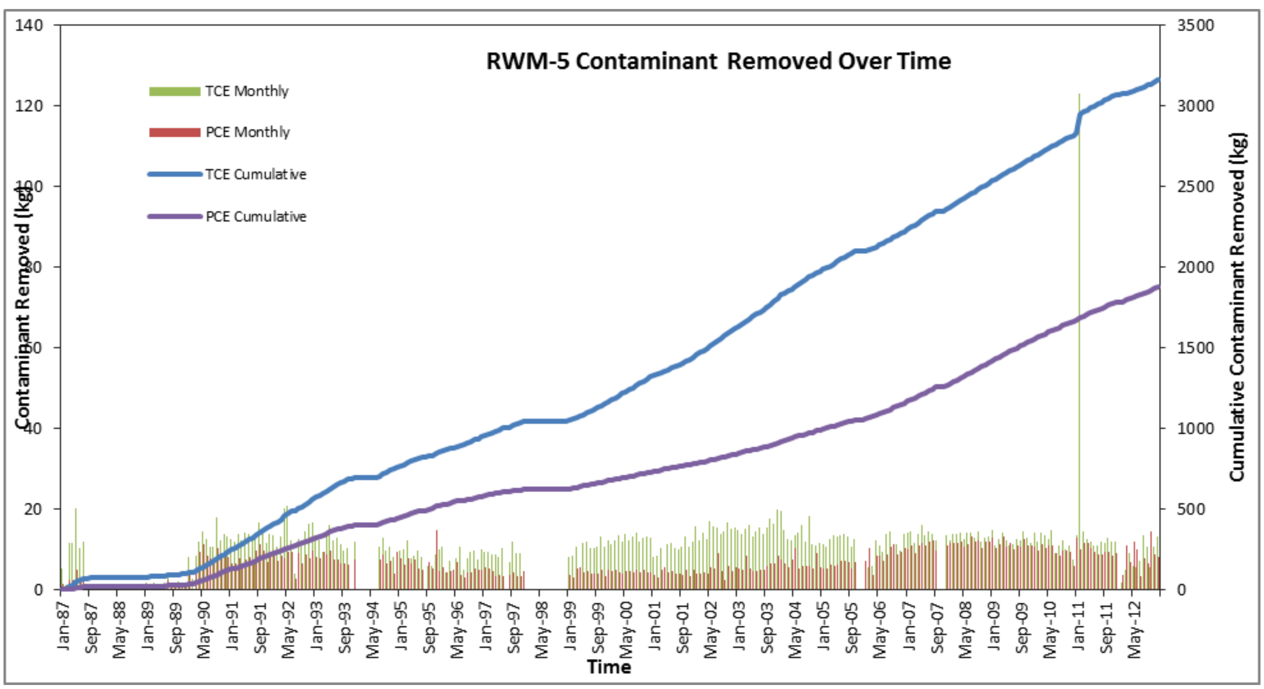

Figure 60. TCE and PCE removed per month and cumulative from 1987-2012 for RWM-5.

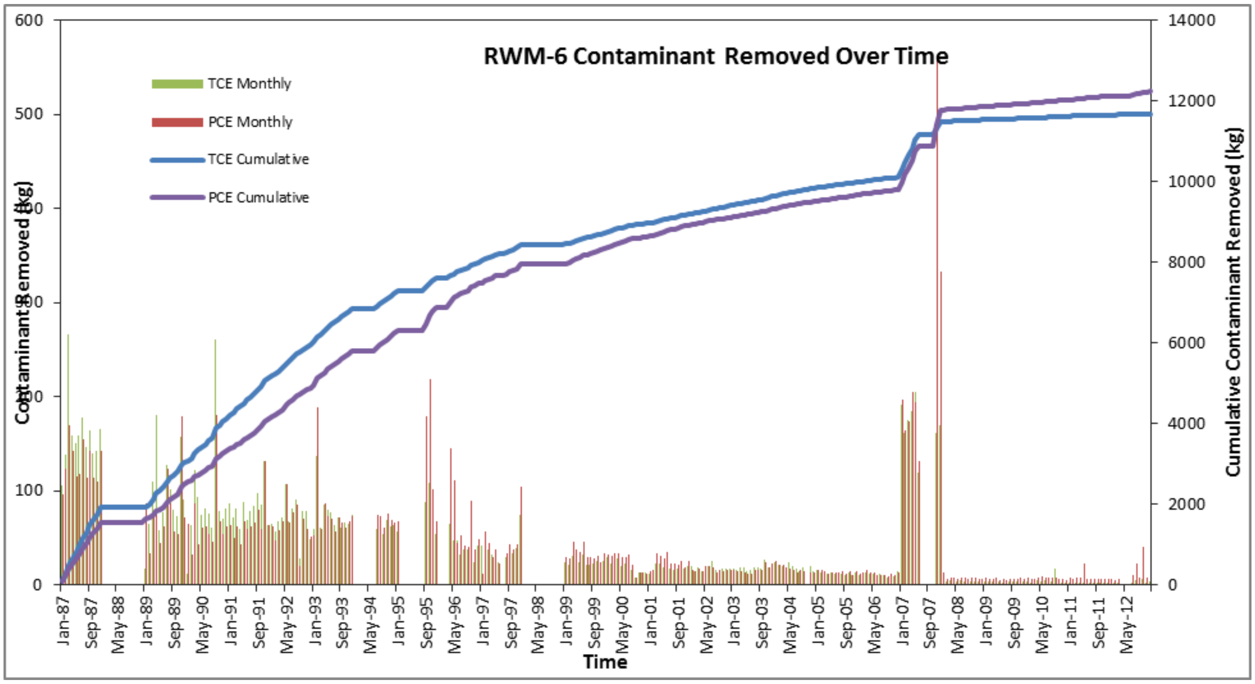

Figure 61. TCE and PCE removed per month and cumulative from 1987-2012 for RWM-6.

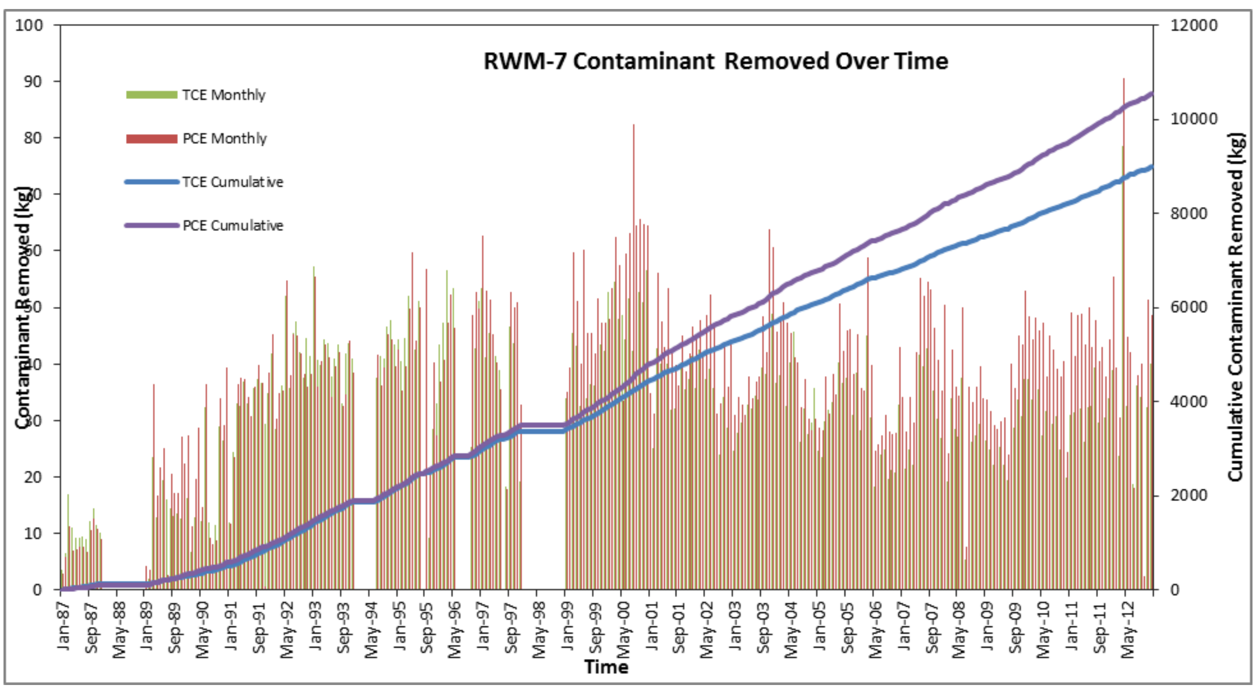

Figure 62. TCE and PCE removed per month and cumulative from 1987-2012 for RWM-7.

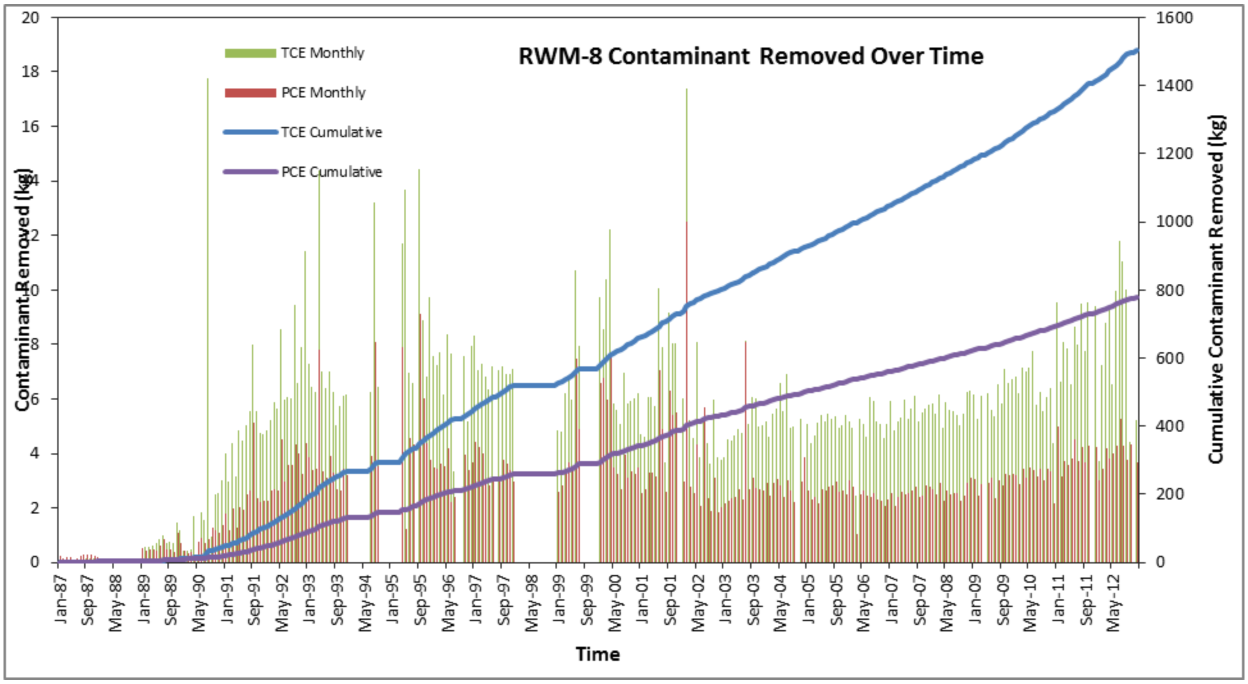

Figure 63. TCE and PCE removed per month and cumulative from 1987-2012 for RWM-8.

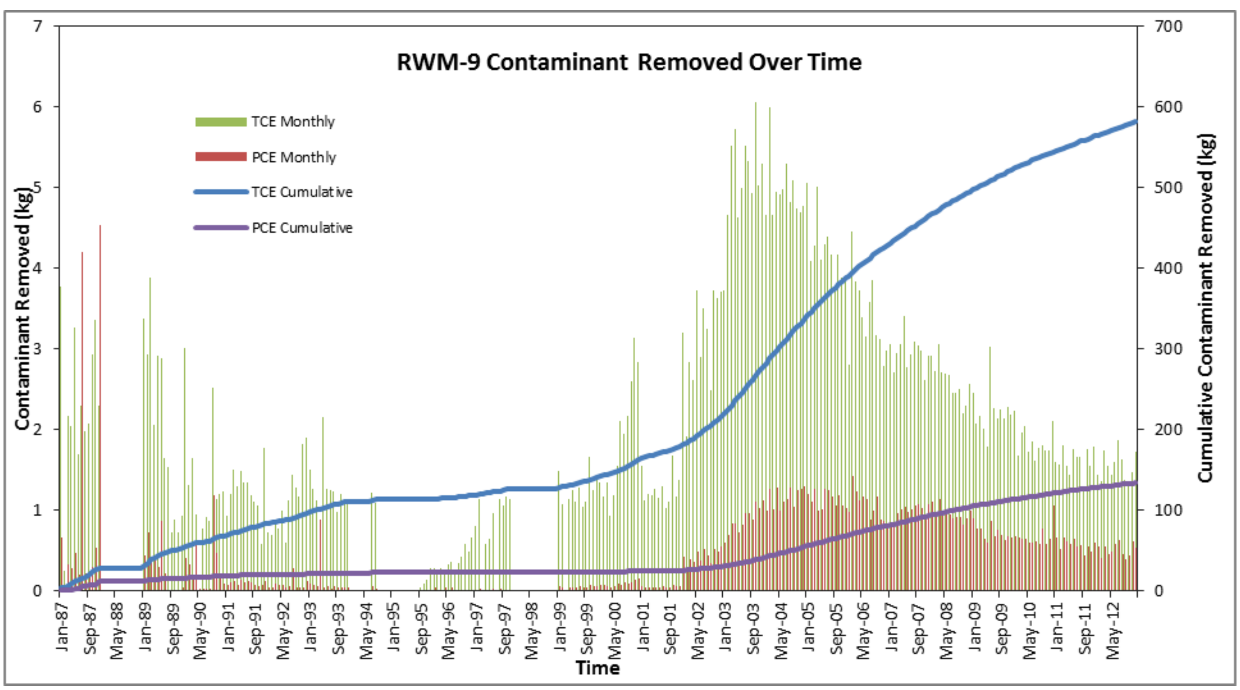

Figure 64. TCE and PCE removed per month and cumulative from 1987-2012 for RWM-9.

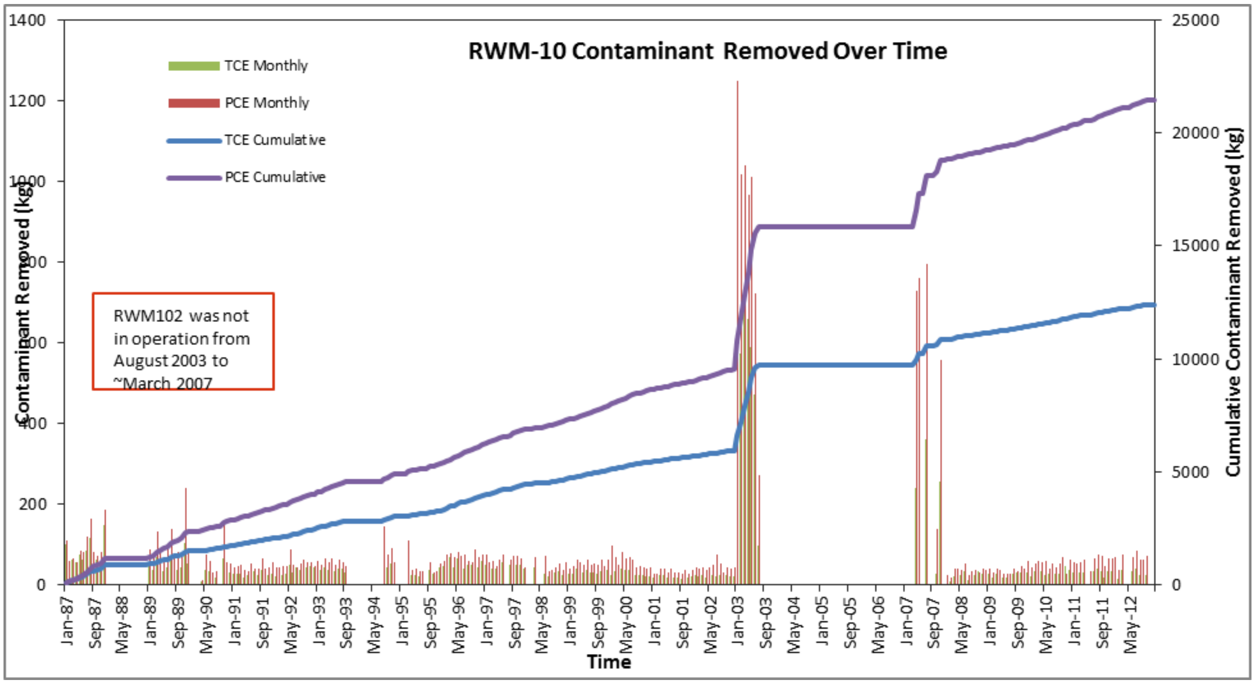

Figure 65. TCE and PCE removed per month and cumulative from 1987-2012 for RWM-10.

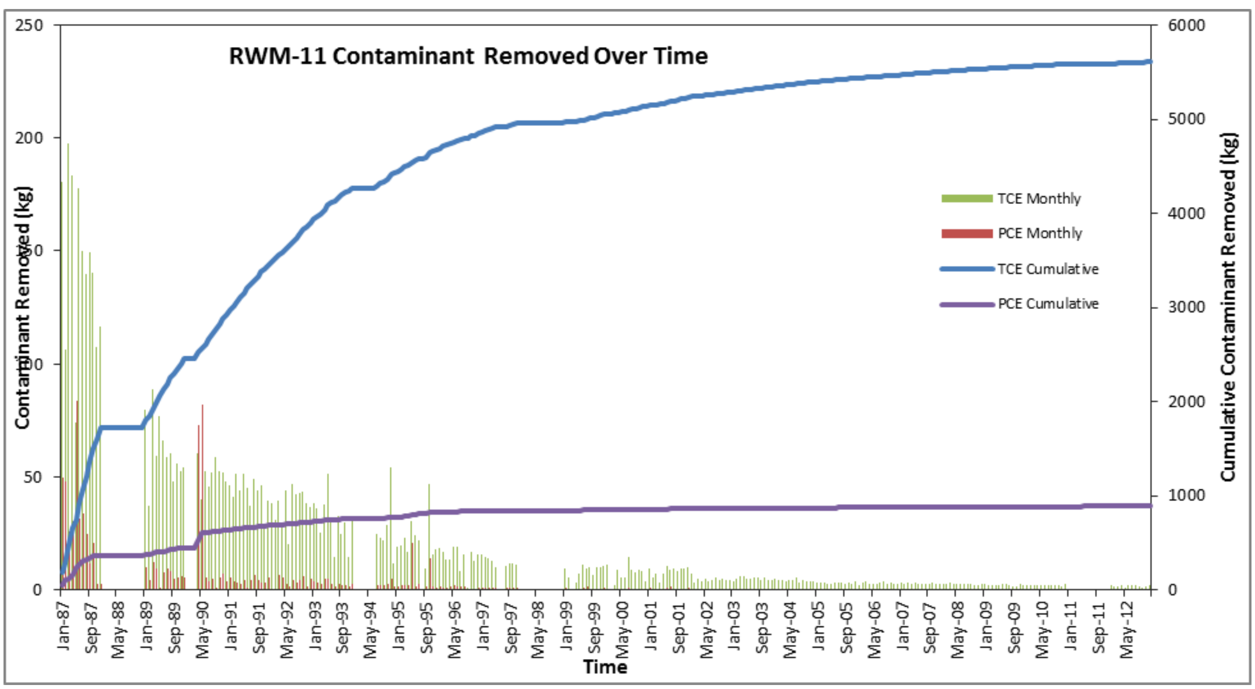

Figure 66. TCE and PCE removed per month and cumulative from 1987-2012 for RWM-11.

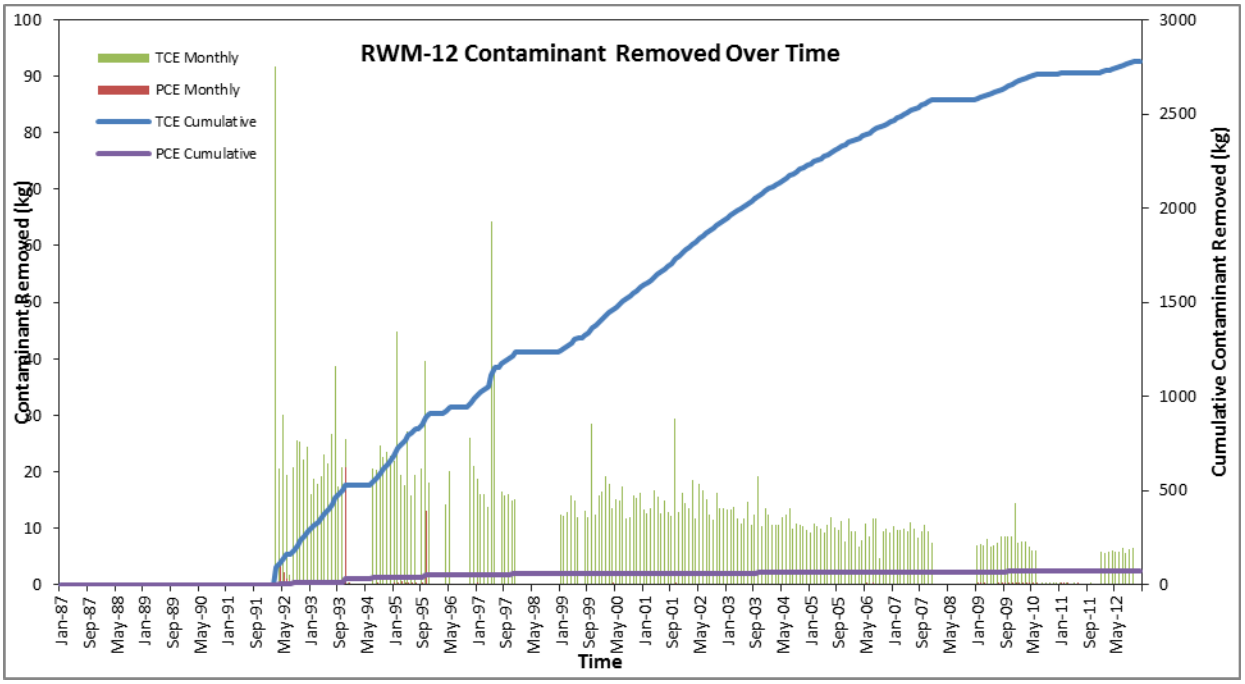

Figure 67. TCE and PCE removed per month and cumulative from 1987-2012 for RWM-12.

Table 8. Comparison of Contaminant Removal from 1987 to 2012

Well ID RWC-	TCE				PCE			
	Jan. '87 removal (kg/mo.)	Dec. '12 removal (kg/mo.)	Jan. '87 H_2O Intensity, kg/MGal	Dec. '12 H_2O Intensity, kg/MGal	Jan. '87 removal (kg/mo.)	Dec. '12 removal (kg/mo.)	Jan. '87 H_2O Intensity, kg/MGal	Dec. '12 H_2O Intensity, kg/MGal
1	389.00	10.57	243	26.9	161.35	58.76	101	149
2	89.09	3.00	98.2	3.24	29.43	8.68	32.4	9.39
3	341.37	8.94	116	3.89	66.55	7.53	22.7	3.27
11	180.52	2.18	69.6	.931	49.59	0.16	19.1	0.0665
4	12.96	19.64	23.1	10.0	0.00	8.13	0.00783	4.15
5	5.29	13.35	5.32	6.57	1.43	8.26	1.44	4.07
7	3.48	40.15	7.32	23.8	2.90	48.72	6.10	28.9
8	0.09	5.20	0.129	2.66	0.22	3.67	0.305	1.88
10	101.16	24.89	52.0	18.5	111.05	70.67	57.1	52.4
6	105.00	2.90	73.7	2.70	95.94	7.58	67.3	7.04
12	91.76	6.39	39.3	3.11	0.05	0.06	0.0196	0.03.13
9	3.77	1.73	3.23	9.08E-07	0.67	0.53	.571	.278

The interesting features of TCE and PCE recovery for each well are discussed below as well as the trends, connections to remediation operations and contaminant mobility considerations.

For the RWM-1 recovery well (see Figure 56), PCE recovery significantly surpasses TCE recovery from early 2006 until Dec. 2012. This trend of more PCE than TCE recovery is seen in 7 of the 12 wells and will be the case in all wells by 2024 or soon thereafter. This is an expected phenomenon. TCE was used initially at SRS and replaced by PCE in the 1970's. TCE is more than 4 times as soluble in groundwater compared to PCE and it is also more volatile. For these reasons, TCE recovery dominates that of PCE for years before PCE recovery ultimately surpasses TCE. Data of monthly removal from each well is missing for 1988. The total removal of TCE and PCE from all wells combined is documented. FIU will apportion the amount removed in 1988 to these 12 wells based upon the removal rate immediately prior to the missing year.

The rate of recovery in this well and other wells were affected by steam injection remediation operations at SRS to remove source term and mobilize contaminants for removal. There were 2 remediation programs targeted to the M-Area Settling Basin area dense non-aqueous phase liquid (DNAPL) source which is not too distant from the area being treated by the M1 Air Stripper and RWM-1 through RWM-12. The steam injection was part of a treatment process known as "dynamic underground stripping." The pilot-scale remediation removed 32 tons of DNAPL contamination during its year of operation ending in September 2001. The major steam injection remediation campaign began in August 2005 and ended in September 2009. There are clear increases in TCE and PCE removal in this well during the months of steam injection. The heating of the ground to over 100°C by August 2009 has been cooling slowly since and will remain higher than background soil temperatures for several more years. The TCE removal rate has dropped in RWM-1 to near its level in 2005 prior to the steam injection since much of the contaminant has been removed. The PCE removal rate is still well above its rate in 2005 prior to the steam injection.

In RWM-2 (see Figure 57), the pump was not operated from June 2000 through November 2003. The steam injection campaign from 2005-2009 did not enhance the mostly depleted TCE but did significantly enhance the PCE removal. The spike in TCE and PCE removal in many of the wells during October 2005 is not understood. It is speculated that it might be a calibration error from the lab analyses.

The TCE and PCE removal rates in well RWM-3 (see Figure 58) appear small in the graph above but its relative size is not small compared to other wells. It appears small due to the large scale for the Y-axis. Note that all graphs are scaled to display the highest monthly recovery rate as near full scale on the Y-axis.

The removal rate data for TCE and PCE in well RWM-4 (see Figure 59) for the year 1996 seems to have been switched. The TCE removal rate dropped by about a factor of 7, matching the PCE removal data in 1995 and 1997. Similarly, the PCE removal rate increased by a factor of 7 to match the TCE data in 1995 and 1997.

There is a major increase in TCE and PCE removal in well RWM-6 (see Figure 61) for the year 2007 and a huge drop in recovery from 2008 to the present.

The recovery of TCE and PCE in well RWM-9 (Figure 64) shows a major increase beginning in 2002 and continuing to the present.

Recovery in RWM-10 (see Figure 65) had an enormous increase for both TCE and PCE in 2003 about 1 year after the pilot-scale remediation program ended. Since the recovery rates were so large (over 1000 kg per month) in 2003, the well was not operational from mid-2003 to mid-2007.

Recovery of TCE and PCE is very low since 2002 in well RWM-11 (see Figure 66).

The removal of TCE and PCE after 26 years is presented in Table 8. Mass of contaminant removed per month in January 1987 is compared to that for December 2012. In addition, the mass of contaminant removed per 1000 gallons of water pumped are compared. Certain wells exhibited similar trends over the past 26 years; for example, wells 1, 2, 3, and 11 exhibit exponential decay in contaminant removal. Wells 4, 5, 7, 8, 10, and 13 exhibit steady concentrations. Wells 6 and 12 exhibit linear decreases and well 9 has a unique, anomalous trend. The Green and Sustainable Remediation analyses underway seem very relevant given the trends and inefficiencies in the current remediation system.

Overall, the process of data analysis and validation was as expected. Increased monthly recovery rates related to heating of the subsurface was expected as was the transition from more TCE recovered during the first 20 years to more PCE recovered than TCE after many years of pump and treat and source term reduction.

FIU has located missing data for many monthly recovery rates of TCE and PCE for recovery wells RWM-1 through RWM-12 and input the data into a more complete database. FIU searched through volumes of SRS documents to locate the data. The more complete monthly data for all wells allows for several types of analyses. The spatial and temporal removal rates can be correlated to spatial and temporal data of contaminant disposal (source locations) and remediation operations. Graphs for the monthly recovery of TCE and PCE were analyzed, showing the effects of remediation on removal rates. In Table 8 there is a comparison of the remediation progress over 26 years. More importantly, there are groups of wells that have contaminant removal rates that are decreasing exponentially and others are decreasing linearly and still others are somewhat constant. Finally, there is one well with anomalous results. Figure 68 below graphically presents the data in Table 8, that is, the change in contaminant removal and gallons of water pumped per kilogram of contaminant removed for year 1 and year 26.

The pumping and overall electrical energy efficiency (per 1 pound of TCE removed and destroyed) has decreased to 6% of what it was during the initial year of operation. That is, it now requires 15.9 times more energy and groundwater to remove 1 pound of TCE in the 26th year of operation than it did in the first year of operation. The next phase of this project will identify options that will offer significant opportunities for improved efficiencies related to electrical energy, water usage, human labor, and the use of other resources.

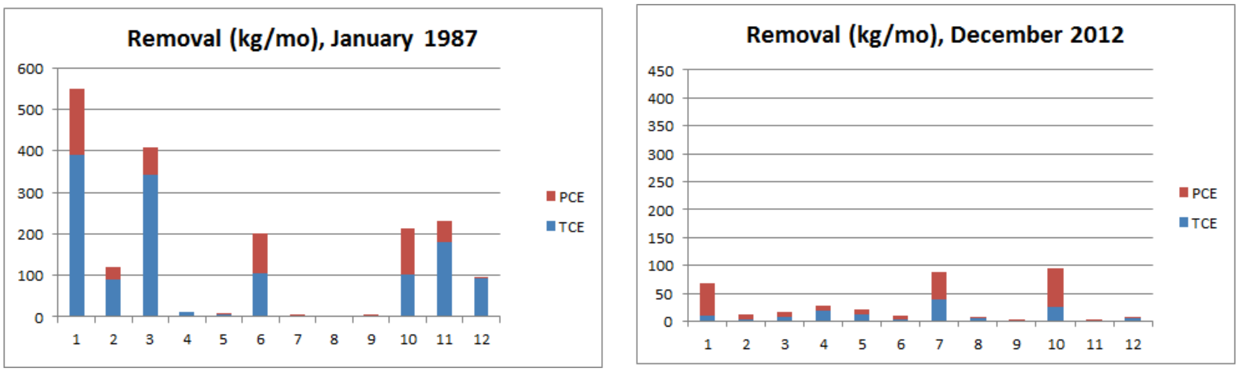

Figure 68. TCE and PCE Removal for 1987 and 2012.

Findings show that 7 of 12 recovery wells have transitioned to more PCE removal than TCE removal. This was an expected result. This is important to our GSR analyses and future remediation options since PCE is much more difficult to mobilize and remove due to its much lower solubility in water than TCE.

The injection of steam for 4 years as part of dynamic underground stripping remediation process was very successful in removing and destroying TCE and PCE in the nearby M Area settling basin area. The increased ground temperature has mobilized DNAPL and resulted in increased recovery in several of the RWM 1-12 wells at this nearby but separate DNAPL location. Soil temperatures have been cooling since steam injection ended in 2009 but the elevated temperatures will continue for another decade and continue to enhance removal of TCE and PCE.

FIU is developing 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. A schedule of reduced hours of operation for the treatment system and specific component replacements for old, inefficient components are recommendations under analysis. 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 Dept. of Energy EM-12/EM-13 Sustainable Remediation (SR) program and will be executed in coordination with the SR program lead. The effort is also referred to as “green and sustainable remediation (GSR)” or “green remediation” in the literature and in various implemented programs [10].

CONCLUSIONS

Path Forward for a GSR of the M1 Air Stripper in 2015 and MNA in 2016

GSR Analysis for the M1 Air Stripper

The improved understanding obtained from modeling and data analysis will allow for GSR options for optimizing system effectiveness by modifying operational variables (e.g., pump rates from each well) and proposing system hardware modifications (e.g., improved packing material for stripper column). There is more information in the next section on the analysis and modeling to optimize pumping and contaminant containment and removal efficiency. Below we discuss the optimization of air strippers which will allow us to propose design modifications and component improvements in order to best achieve system performance while ensuring site goals are met.

Optimization of Air Strippers

In order to provide a proper analysis and optimization for the M1 Air Stripper design and operation, one needs to focus on the goals for the stripper (e.g., the actual treatment goal, which is never 100% efficiency in removal of all contaminants). Design and operational parameters such as: the air to water ratio (which is defined by Henry's constant); the water temperature; the inlet concentration and desired outlet concentration of the contaminants; the diameter of the tower; the flow rate; the current packing material; the power of the blower; the discharge pump power; the head pressure; the height of the tower; and the use of other ancillary equipment, all affect the effectiveness of the stripping process. A very important factor in tower air stripping is the packing material. One of the benefits of tower air strippers is the low energy usage due to the low overall pressure drop, but a huge disadvantage is the fouling of the packing material. For minimizing operating costs of the stripping, the air flow rate is the most important factor, and is mainly affected by blower power consumption.

The removal efficiency of contaminants by packed towers involves many parameters. Economic considerations determine a desired balance between the volume of the tower and the air-to-water ratio as a function of pressure drop and the packing. Because the tower volume affects the costs of the process, minimizing the volume of the tower at a pressure drop to reduce energy consumption is one way to optimize the process in the design of the stripper. In any given application, the most favorable liquid rate packing height, and air-to-water ratio will depend on specific characteristics of the site's water quality, the required and ideal efficiency, and economic considerations. The site stakeholders would be briefed on the complex interdependence of the acceptable window of operating conditions, design modifications and system performance. In **Table 9**, different parameters are modified and the effects on the operations and cost are shown (assuming no changes in the tower design), as well as the effects on the tower design (assuming no change in removal efficiency). For example, for a given tower design (keeping the packing, diameter and height fixed), by increasing the water pumping rate to meet water demands, liquid loading will increase. This causes a decrease in the air-to-water ratio, resulting in a decrease in removal efficiency and an increase in operating costs due to the greater volume of air required to meet the target removal efficiency [15].

Table 9. Parameters Important to Packed Tower Design

Parameter	Effect of Increasing (↑) Parameter on Operations and Cost, Assuming no Change in Tower Design	Effect of Increasing (↑) Parameter on Tower Design, Assuming Removal Efficiency is Maintained
Liquid Loading Rate	↓ Removal Efficiency ↑ Cost	↑ Tower Height (HTU)
Air/Water Ratio (AWR)	↑ Removal Efficiency ↑ Cost	↓ Packing Volume
Water Temperature	↑ Removal Efficiency ↑ Heating Cost ↑ Henry's Constant	↓ Packing Volume
Henry's Constant	↑ Removal Efficiency	↓ Packing Volume ↓ AWR
Packing Type and Size	↑ the Size ↓ Removal Efficiency	↑ the Size ↑ Packing Volume ↓ Pressure Drop
Pressure Drop / Depth	↑ Removal Efficiency ↑ Pump/Blower Cost	↑ AWR

Pumping rates, packing material, and air blower design and operation will all be analyzed as part of the mechanical design optimization studies.

Current influent concentrations will be used with published design guidelines for air strippers to determine the minimum air flow rate that would meet treatment specifications. A new blower strategy will be recommended based on the outcome of the air stripper analysis. In particular, it will allow for correlations between hydraulic flow rates and contaminant mass flow rates, and between airflow rates and contaminant removal rates.

Detailed baseline mass flow charts for each well, loading rates and removal efficiencies, all as a function of time are shown earlier in this report. Statistical analysis of the baseline data allows for the development of correlations between system performance and operating parameters. Excel, OCTAVE, R, and analytical and numerical tools for data analysis, well drawdown calculations and system optimization will be performed.

Understanding these correlations, energy efficiencies and remediation system efficiency, and working with key SRS stakeholders, will allow FIU and SRNL to propose performance metrics for the operation of each well and for the entire system and propose performance targets. These metrics will permit analyses to evaluate potential areas of improvement based on the proposed performance targets and based on the statistical correlations.

The next steps include:

- Collection of all documentation required for this GSR analysis during a trip to SRS in Sept. 2015;
- Analyze design basis, system performance and "as-built" diagrams of current air stripper system components in Oct. 2015;
- Complete a GSR of the air stripper based upon design improvements and use of improved components that would enhance overall system performance.

The effort to investigate operational strategies to increase system performance by optimizing the hydraulic loads, pumping rates, contaminant mass flow rates and well drawdown levels will be completed in 2016 and may broaden (based upon SRS and DOE EM HQ approval) to look at contaminant migration and the potential for future MNA.

POSSIBLE PATH FORWARD FOR 2016

Future effort on this project may involve quantifying the attenuation processes in the plume which will help support future incorporation of monitored natural attenuation (MNA), as appropriate, into the "combined remedies" for the M-Area. Such modeling can also support strategic decisions on the operation of the M-Area GRS. For example, modeling may help address whether remediation goals can be achieved with fewer recovery wells, fewer gallons pumped per day, or a smaller air stripper, using a fraction of the electrical energy of the current system.

The proposed, detailed GSR analysis is planned for 3 phases: (1) optimization and correlation of contaminant removal and pumping rates for all recovery wells; (2) 1-dimensional analysis of groundwater flow and contaminant migration to the SRS boundary; and (3) a more in depth 2-D modeling of contaminant transport and oxidation (only if the 1-D modeling results show great promise for MNA and DOE EM and SRS stakeholders agree that incorporating some level of MNA in the combined remedies at SRS M1 Area in the next decade is possible.

For Phase I, the optimization and correlation of contaminant removal and pumping rates for all recovery wells, FIU will:

- Investigate operational strategies to increase system performance by optimizing the hydraulic loads, pumping rates, contaminant mass flow rates and well drawdown levels;
- Determine a set of metrics which will correlate the pumping rates, the cone of depression, and the interaction between the wells with the contaminant mass flow rates; and
- Determine the best set of operating parameters that will ensure overall steady increase of performance between the optimal well pumping rates and greatest mass flow rates of contaminants.

For Phase II, 1-D groundwater flow and contaminant transport of TCE and PCE to the SRS boundary, FIU will work with SRNS remediation contractors and SRNL to set up, calibrate and run simulations of the contaminant migration. As a first step, no *in situ* destruction of TCE or PCE will be assumed. Based upon the results of this analysis, DOE will decide if there is significant potential for the M1 Air Stripper and associated network of recovery wells to be greatly scaled back in terms of pump rates, number of wells and blower power requirements, or eliminated entirely.

The proposed extended GSR analysis will be discussed at the September 2015 meeting at SRS between the remediation contractors, SRNL and FIU. The scope of work for this task for the next year will be developed with agreement between these parties and documented in FIU's Project Technical Plan.

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OVERALL PROJECT CONCLUSIONS

This project has provided research at various DOE sites in surface and groundwater modeling; subsurface contamination; aqueous chemistry of metals; reactive transport of metals and VOCs; chemical thermodynamics of mercury species; and variable density modeling. FIU researchers have used conventional engineering methodologies (as developed by EPA, USACE, and USGS) in combination with latest scientific software (1D/2D/3D numerical flow and transport models integrated with reaction kinetics and thermodynamic software) to provide an integrated solution for understanding the mobility and impacts of contaminants at the Oak Ridge Reservation and other DOE sites, reducing costs and environmental footprints. Modeling efforts conducted also support the development of total maximum daily loads (TMDLs) to estimate source loading and evaluate loading capacities that meet water quality standards. TMDLs may be used to develop controls for reducing pollution from point and nonpoint sources to restore and maintain water quality.

Geographic information systems (GIS) technology was also employed to support the modeling work conducted by providing a structured, coherent and logical computer-support system for centralized storage, backup and management of hydrological model data. GIS tools were used to perform geoprocessing tasks to prepare the spatial and timeseries data being used for model development.

Project research also focused on the use of state-of-the-practice tools to conduct an analysis of sustainable and green remediation alternatives needed to reduce environmental and social impacts of remedial cleanup and closure activities at DOE sites in a cost-effective way. Assessments of this nature help contribute 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. It also helps to achieve public acceptance, reduce life-cycle costs, and demonstrates performance in achieving environmental sustainability goals. The building block approach being employed will reduce redundancy in sustainability evaluation and facilitate identification of specific activities with greatest environmental footprints. The methodology employed will provide a decision matrix for remedy selection, design, or implementation and allows for a remedy optimization stage as well.

Future work will continue in collaboration with Savannah River National Laboratory (SRNL), utilizing and building upon the capabilities developed under Project 3 in the area of soil and groundwater remediation and treatment technology to apply these approaches to similar environmental challenges at the Savannah River Site. The new tasks are 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 to support environmental remediation; 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.

APPENDIX A. ArcGIS DIAGRAMMER DATA REPORT

ArcGIS Diagrammer

Report Creation	
Date	Friday, May 01, 2015
Author	Lawrence/ARC-2481F4A8 on ARC-2481F4A8
System Information	
Operating System	Microsoft Windows NT 6.1.7601 Service Pack 1
.Net Framework	2.0.50727.5477
Diagrammer	10.0.1.0
Geodatabase	
Workspace Type	File Geodatabase
File	G:\DOE_Project3\SRS_DATA\GIS\SRS_TimsBranch_GeodB\SRS_TimsBranch_GeodB.gdb

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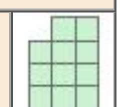
Data Report

ObjectClass Name	Type	Geometry	Subtype	Total	Extent	Snapshot
Admin_FC						
SavannahRiver_Tile_Layout5k	Feature Class	Polygon	-	11	425000 440000 3680000 3700000	
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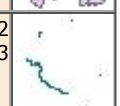
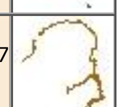
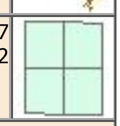
VGIS_BD_SRS_LINE_MEANDER	Feature Class	Polyline	-	1	422558.678800002 457132.343500003 3653704.0584 3696226.3696	
VGIS_BD_SRS_LINE_MONMNT	Feature Class	Polyline	-	1	422561.7654 459782.053099997 3653704.0584 3696226.3696	
VGIS_GD_USGS_QUAD_AREA	Feature Class	Polygon	-	4	418506.420599997 441962.053800002 3679193.1661 3707076.8547	
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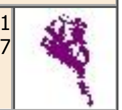
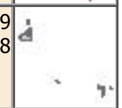
VGIS_FA_TES_SURVEY_AREA_SRS	Feature Class	Polygon	-	15	429282.7589 439738.627 3681375.1678 3689242.6089	
Buildings_FC						
VGIS_BG_BLDG_AREA_SRS_EXIST	Feature Class	Polygon	-	408	428936.980599999 439073.234700002 3682554.8745 3694379.5232	
VGIS_BG_BLDG_AREA_SRS_HIST	Feature	Polygon	-	0	No Extent	-

	Class					
VGIS_BG_BLDG_AREA_SRS_SLAB	Feature Class	Polygon	-	130	430917.611400001 438229.777800001 3682719.6901 3689837.9162	
Contaminants_FC						
soil_pollution_isoline_line	Feature Class	Polyline	-	158	420182.976300001 463525.929399997 3627602.9623 3697798.366	
VGIS_EH_GROUNDWATER_PLUME_I	Feature Class	Polygon	-	15	430356.490699999 439316.502099998 3681729.4108 3689044.2623	
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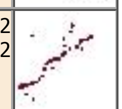
VGIS_EH_RAD_BISMUTH_LINE_1991	Feature Class	Polyline	-	2	427147.046800002 454710.122900002 3672771.9164 3696246.38	
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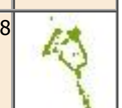
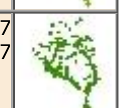
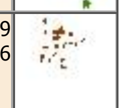
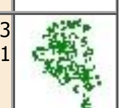
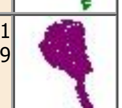
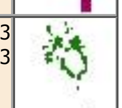
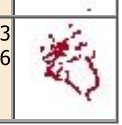
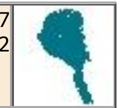
VGIS_EH_RAD_CESIUM_LINE_1986	Feature Class	Polyline	-	0	No Extent	-
VGIS_EH_RAD_CESIUM_LINE_1991	Feature Class	Polyline	-	8	426678.031999998 461918.3763 3627932.9551 3692629.6357	
VGIS_EH_RAD_CESIUM_LINE_1998	Feature Class	Polyline	-	10	421089.495399997 460325.316699997 3643919.5224 3697475.3544	
VGIS_EH_RAD_COBALT_LINE_1991	Feature Class	Polyline	-	8	427071.415899999 459261.215899996 3638131.5585 3690052.3501	
VGIS_EH_RAD_COBALT_LINE_1998	Feature Class	Polyline	-	8	421015.569300003 461076.170400001 3643868.0309 3697755.3221	
VGIS_EH_RAD_GROSS_LINE_1991	Feature Class	Polyline	-	10	421210.122400001 463310.873599999 3627920.4882 3696556.7359	
VGIS_EH_RAD_GROSS_LINE_1998	Feature Class	Polyline	-	14	420845.124700002 461128.2029 3643864.4219 3697782.3376	
VGIS_EH_RAD_MANMADE_LINE_1991	Feature Class	Polyline	-	9	426386.369900003 460520.811800003 3628302.6972 3695430.353	
VGIS_EH_RAD_MANMADE_LINE_1998	Feature Class	Polyline	-	13	421327.786700003 459252.686399996 3644073.4342 3696669.8163	

VGIS_EH_RAD_NATURAL_LINE_1991	Feature Class	Polyline	-	10	421217.369099997 463322.626900002 3627920.2418 3696556.7367	
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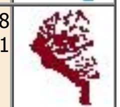
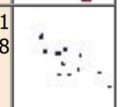
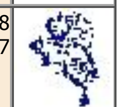
VGIS_EH_RAD_POTASS_LINE_1998	Feature Class	Polyline	-	7	420812.251199998 461081.583700001 3643861.2452 3697740.0839	
VGIS_EH_RAD_PROTACT_LINE_1991	Feature Class	Polyline	-	9	422356.832800001 457840.740199998 3669221.9669 3692639.856	
VGIS_EH_RAD_PROTACT_LINE_1998	Feature Class	Polyline	-	9	421187.368699998 460862.214199997 3643874.7775 3697772.6551	
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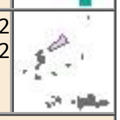
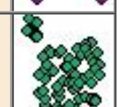
VGIS_EH_RAD_URANIUM_LINE_1991	Feature Class	Polyline	-	8	426432.770499997 460107.640100002 3632070.35 3695823.351	
VGIS_EH_RAD_URANIUM_LINE_1998	Feature Class	Polyline	-	11	420745.711999998 461083.750299998 3643863.5831 3697794.5893	
VGIS_EH_WASTE_AREA_SRS_FILL	Feature Class	Polygon	-	179	428756.855300002 440748.545900002 3682264.6597 3694514.9635	
Geology_FC						
SRS_Geology	Feature Class	Polygon	-	298	421583.3063 441908.5843 3679234.1359 3706997.0255	
vgis_ge_borehole_bedrock_pt	Feature Class	Point	-	13	430831.0696 438819.9988 3683163.1743 3689805.8712	
vgis_ge_borehole_pt_24K	Feature Class	Point	-	75	428690.8855 439039.1504 3682760.6345 3696069.2868	
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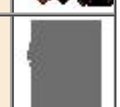
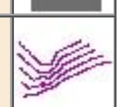
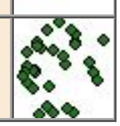
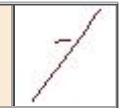
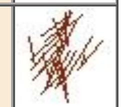
VGIS_GE_DEPTH_BEDROCK_AREA	Feature Class	Polygon	-	3597	427917.1137 439317.0984 3682408.0931 3697208.2747	
vgis_ge_depth_to_basement_line	Feature Class	Polyline	-	5	413736.7059 469393.0501 3677509.9987 3711097.1928	
vgis_ge_fault_control_pt	Feature Class	Point	-	31	430094.2179 439020.0538 3682539.6221 3692941.3938	

vgis_ge_fault_line_1995	Feature Class	Polyline	-	2	427163.9171 436616.098 3681857.5808 3694820.7009	
vgis_ge_fault_line_1996	Feature Class	Polyline	-	4	429963.26 446415.6531 3682116.159 3693485.6486	
vgis_ge_fault_line_am_csand	Feature Class	Polyline	-	41	429014.0004 434332.3707 3684635.1191 3691380.3603	
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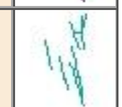
vgis_ge_fault_line_am_langsyne	Feature Class	Polyline	-	13	429014.0004 431983.1567 3684635.1191 3691388.8608	
vgis_ge_fault_line_am_warley	Feature Class	Polyline	-	11	429014.0004 431950.6568 3684635.1191 3691380.3603	
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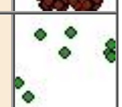
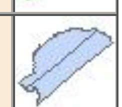
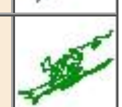
vgis_ge_gravity_line_csra	Feature Class	Polyline	-	17	414503.8678 463616.8396 3676008.1145 3708996.7283	
vgis_ge_gravity_line_reg	Feature Class	Polyline	-	4	404494.4665 499986.5352 3657532.1747 3731196.6914	
vgis_ge_gravity_pt_csra	Feature Class	Point	-	169	428804.0649 439028.7113 3682549.4076 3696766.6221	
vgis_ge_gravity_pt_reg	Feature Class	Point	-	8	428946.4305 436357.0069 3691560.0701 3696765.1228	
vgis_ge_lithology_santee	Feature Class	Polygon	-	2	422558.6751 453991.6273 3669978.2279 3696226.3676	
vgis_ge_magnetic_line_csra	Feature Class	Polyline	-	8	397466.6511 463727.3468 3664560.5181 3717858.2522	
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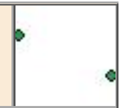
vgis_ge_seismic_pt_csra	Feature Class	Point	-		2	431535.0851 436788.7245 3687474.9253 3689843.1034	
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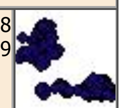
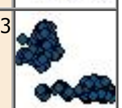
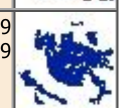
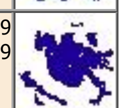
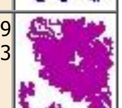
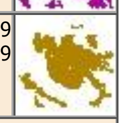
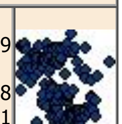
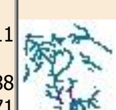
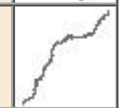
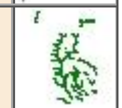
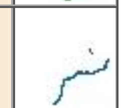
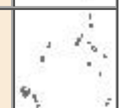
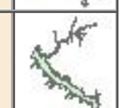
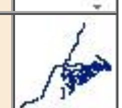
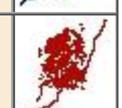
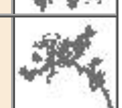
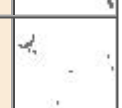
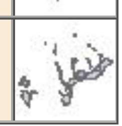
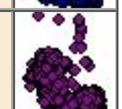
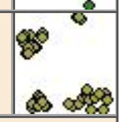
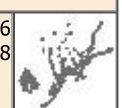
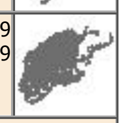
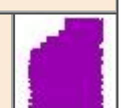
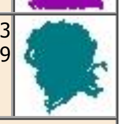
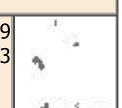
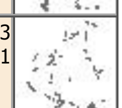
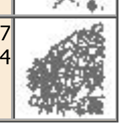
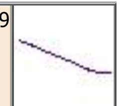
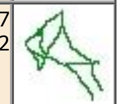
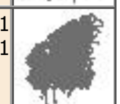
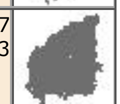
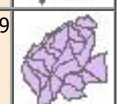
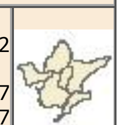
vgis_ge_sub_transect_pt	Feature Class	Point	-		41	436095.5283 439211.863 3682558.9199 3684253.9208	
vgis_ge_surf_area_kb_us	Feature Class	Polygon	-		3	245343.7144 504417.365 3573165.4918 3746677.0555	
VGIS_GE_SURF_AREA_SRS_48K	Feature Class	Polygon	-		28	422586.4252 454349.953 3661683.7633 3696232.3696	
GW_FC							
vgis_hy_piezometer_pt_1998	Feature Class	Point	-		419	428758.945299998 439226.295699999 3682537.6598 3690636.851	
vgis_hy_piezometer_pt_2003	Feature Class	Point	-		537	428759.071900003 439225.989 3682537.1598 3690637.1044	
vgis_hy_water_tbl_line_1995	Feature Class	Polyline	-		13	406498.037799999 476861.531199999 3651125.7645 3714381.5763	
vgis_hy_water_tbl_line_1998	Feature Class	Polyline	-		26	406498.037799999 476861.531199999 3651125.7645 3714381.5763	
vgis_hy_water_tbl_line_2002	Feature Class	Polyline	-		21	421910.565099999 457110.413000003 3661394.4473 3696894.6983	
vgis_hy_water_tbl_line_2003	Feature Class	Polyline	-		26	406498.037799999 476861.531199999 3651125.7645 3714381.5763	
HydrographyNet_FC							
HYDRO_NET_Junctions	Simple Junction	Point	-		159	- 81.7691861835179 - 81.6225707170788 33.2750604150171 33.4295984814439	
NHDFlowline	Simple Edge	Polyline	ArtificialPath CanalDitch Coastline Connector Pipeline StreamRiver Underground Conduit	18 0 0 1 0 125 0	144	- 81.7692713168511 - 81.6225707170788 33.2750604150171 33.4295984814439	
NHDWaterbody	Feature Class	Polygon	Estuary Ice Mass LakePond Playa Reservoir SwampMarsh	0 0 23 0 13 32	68	- 81.7847445834938 - 81.5896733837965 33.2431518150666 33.4194666814596	
Hydrology_FC							

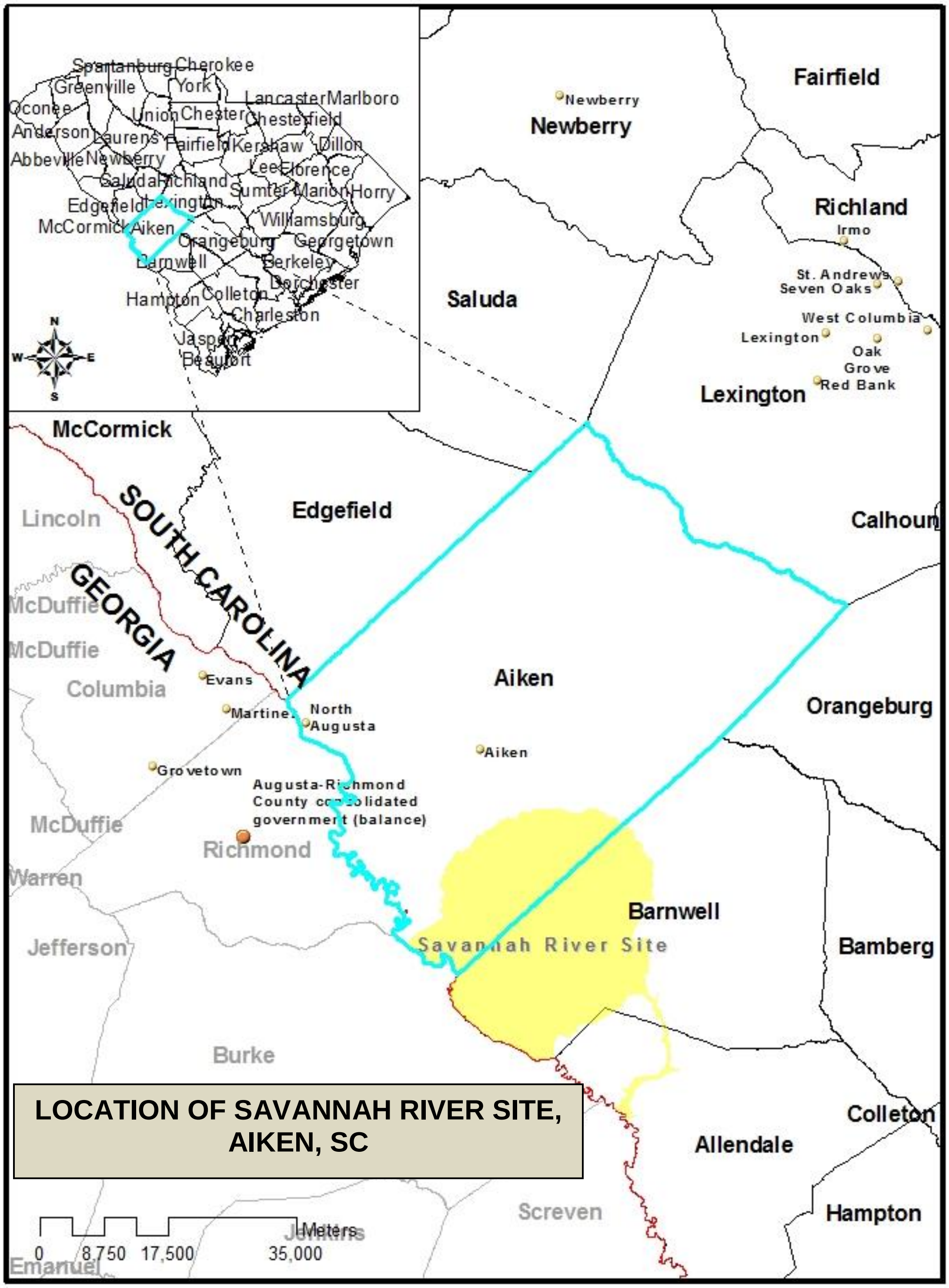
ponds_and_lakes	Feature Class	Polygon	-	7	431095.1329 438265.2051 3682512.0758 3696397.8468	
Rivers	Feature Class	Polygon	-	1	432990.9899 440178.8895 3679386.1679 3687164.3285	
Single_line_drains	Feature Class	Polyline	-	142	428542.9099 439316.1561 3682334.8459 3698075.5112	
Stream_centerlines	Feature Class	Polyline	-	20	432219.0503 439278.1627 3682318.6905 3689915.3078	
Stream_connectors	Feature Class	Polyline	-	80	428644.6993 439254.3735 3682787.3375 3697074.5347	
vgis_hy_carolina_bay_area	Feature Class	Polygon	-	36	428907.0473 438546.9981 3682488.1141 3692628.1909	
vgis_hy_carolina_bay_pt	Feature Class	Point	-	36	428953.2603 438511.7445 3682541.1142 3692571.1901	
vgis_hy_flood_level_point	Feature Class	Point	-	0	No Extent	-
vgis_hy_flood_zone_area_1995	Feature Class	Polygon	-	1	427054.3263 459782.0531 3653687.3118 3696013.3592	
vgis_hy_flood_zone_area_1998_1	Feature Class	Polygon	-	1	421424.2786 455247.5537 3651500.8203 3696219.1153	
vgis_hy_flood_zone_area_1998_2	Feature Class	Polygon	-	1	432531.492 456361.6478 3658986.3194 3690475.3653	
VGIS_HY_STREAM_LINE_CSRA	Feature Class	Polyline	-	272	418749.6262 439634.7725 3687384.2084 3706422.3689	
VGIS_HY_STREAM_LINE_SRS	Feature Class	Polyline	-	974	427562.3225 443669.9347 3677460.1095 3696203.3703	
VGIS_HY_WETLAND_AREA_NWI	Feature Class	Polygon	-	295	426986.0366 439700.2611 3681156.3535 3697310.7847	
VGIS_HY_WETLAND_AREA_SRS_1951	Feature Class	Polygon	-	200	422597.8918 458600.8853 3662632.3762 3695637.2394	
VGIS_HY_WTRBDY_AREA_CSRA_24K	Feature Class	Polygon	-	22	427909.0698 436039.1025 3691838.0942 3697766.5366	
VGIS_HY_WTRBDY_AREA_SRS_24K	Feature Class	Polygon	-	37	428345.9843 440752.2966 3681168.6093 3690856.6743	

vgis_im_dam_area_srs	Feature Class	Polygon	-	3	433424.2338 433559.8872 3686656.381 3686742.636	
LandUse_FC						
VGIS_LS_LNDCOV_AREA_SRS	Feature Class	Polygon	-	1407	424956.0009 448707.583499998 3673877.4067 3695857.9808	
Monitoring_Stations						
LandmarkCurves	Feature Class	Point	-	14066	429158.2697 439229.6307 3682535.1473 3697134.4793	
LandmarkData	Feature Class	Point	-	5062	428756.9099 439246.4952 3682529.9242 3697134.4793	
LandmarkPicks	Feature Class	Point	-	21938	429158.2697 439226.787 3682535.1473 3697090.1519	
SampleStations	Feature Class	Point	-	4640	428756.9099 439246.4952 3682531.4258 3696055.123	
vgis_cl_rain_gauge_pt	Feature Class	Point	-	4	431322.1777 436775.1299 3683150.9091 3693666.1905	
VGIS_EH_SW_DISCHRG_PT_SRS	Feature Class	Point	-	58	430716.535 439158.3442 3682624.0834 3691665.3581	
Soils_FC						
VGIS_SO_AREA_HYDRIC_AREA	Feature Class	Polygon	-	310	427427.729099996 444805.608599998 3678481.6346 3694610.4049	
VGIS_SO_AREA_NRCS_AREA	Feature Class	Polygon	-	626	426935.289999999 449736.462499999 3677543.5145 3696227.6096	
Topography_FC						
contours	Feature Class	Polyline	-	10607	428002 439998 3682002 3697000.0513	
vgis_lf_contour_10ft_usgs	Feature Class	Polyline	-	595	424533.994900003 444454.339699999 3676863.1418 3699410.1442	
Transportation_FC						
VGIS_TR_PARKING_AREA	Feature Class	Polygon	-	67	430755.332699999 439344.643200003 3682404.6284 3694805.6837	
VGIS_TR_ROAD_AREA_SRS_PAV_OP	Feature Class	Polygon	-	129	428286.945600003 438552.378600001 3682359.1608 3694934.1946	
VGIS_TR_ROAD_AREA_SRS_UNPAV_OP	Feature Class	Polygon	-	2333	428112.988399997 439731.281900004 3682152.153 3695816.7584	

VGIS_TR_ROAD_LINE_SRS_PRIM	Feature Class	Polyline	-	4	436506.292199999 439800.7553 3693632.2132 3694838.3119	
VGIS_TR_ROAD_LINE_SRS_SEC_OP	Feature Class	Polyline	-	48	427862.008199997 445408.101800002 3674383.1972 3694828.135	
VGIS_TR_ROAD_LINE_SRS_TERT_OP	Feature Class	Polyline	-	470	427426.7333 448197.666299999 3679563.1695 3695733.3969	
Vegetation_FC						
vgis_fl_fire_area_burn	Feature Class	Polygon	-	90	427081.700999998 453402.821099997 3666910.2376 3695983.5261	
vgis_fl_fire_area_wild	Feature Class	Polygon	-	51	428697.045599997 439140.9745 3682550.6612 3695381.1793	
vgis_fl_flora_study_area	Feature Class	Polygon	-	119	429786.239399999 439995.507700004 3682504.4025 3694837.9752	
vgis_fl_forest_stand_area	Feature Class	Polygon	-	1192	427418.359200001 441832.758000001 3678662.3608 3695981.7347	
VGIS_FL_HABITAT_1999_AREA	Feature Class	Polygon	-	15325	427652.049999997 440882.008100003 3680023.1212 3695983.2783	
vgis_fl_tmbr_compart_area	Feature Class	Polygon	-	20	427008.375399999 443828.386 3678030.8807 3695983.5261	
VGIS_FL_TMBR_MGT_AREA	Feature Class	Polygon	-	3	422518.925700001 456336.6787 3661764.7626 3696232.8696	
Watershed_FC						
WBDHU12	Feature Class	Polygon	-	6	- 81.9208042416162 - 81.5148515005797 33.1574324026997 33.5154340198523	
Stand Alone ObjectClass(s)						
_VBEIDMS_SAMPLE_STATIONS	Table	-	-	29848	No Extent	-
DHI_Branches	Table	-	-	0	No Extent	-
DHI_CrossSections	Feature Class	Polyline	-	0	No Extent	-
DHI_IDManager	Table	-	-	0	No Extent	-
DHI_MetaData	Table	-	-	0	No Extent	-
DHI_MetaDoubles	Table	-	-	0	No Extent	-
DHI_Nodes	Feature Class	Point	-	0	No Extent	-
DHI_Reaches	Feature Class	Polyline	-	0	No Extent	-
DHI_TAFCLookUp	Table	-	-	0	No Extent	-
DHI_Timeseries	Table	-	-	0	No Extent	-
DHI_TSGroups	Table	-	-	0	No Extent	-
DHI_TSType	Table	-	-	0	No Extent	-
DHI_TSValues	Table	-	-	0	No Extent	-

MIKE_SHE_dfs0_PPTN_data	Table	-	-	18535	No Extent	-
NHDFeatureToMetadata	Table	-	-	320642	No Extent	-
SRS_rainfall_data_1964_2014	Table	-	-	18533	No Extent	-
SRS_temp_C_data_1964_2013	Table	-	-	18474	No Extent	-
SRS_temp_F_data_1964_2013	Table	-	-	18474	No Extent	-
Tims_Branch_GIS_Data_FileName_Key	Table	-	-	34	No Extent	-

APPENDIX B: TIMS BRANCH WATERSHED MAPS



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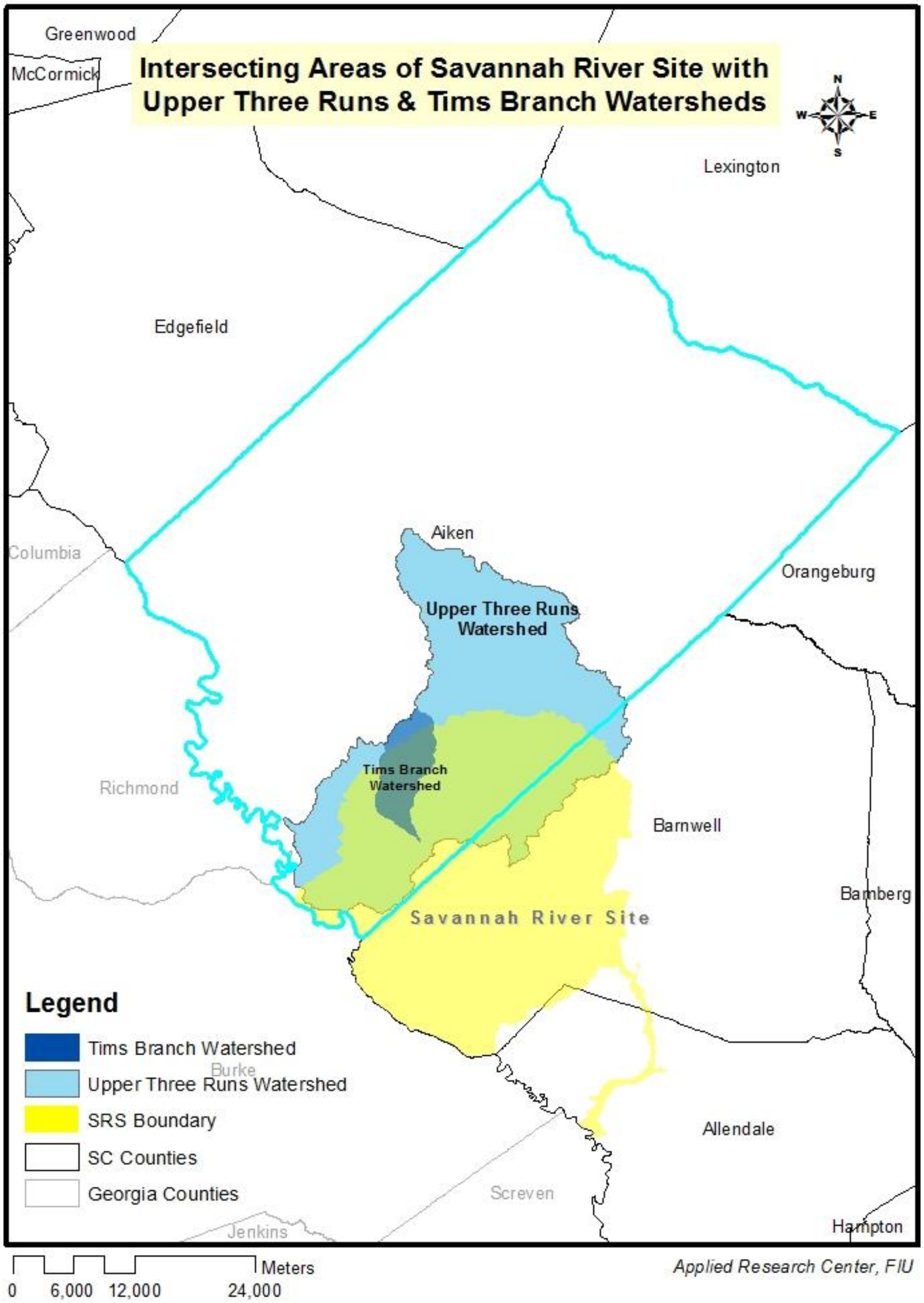
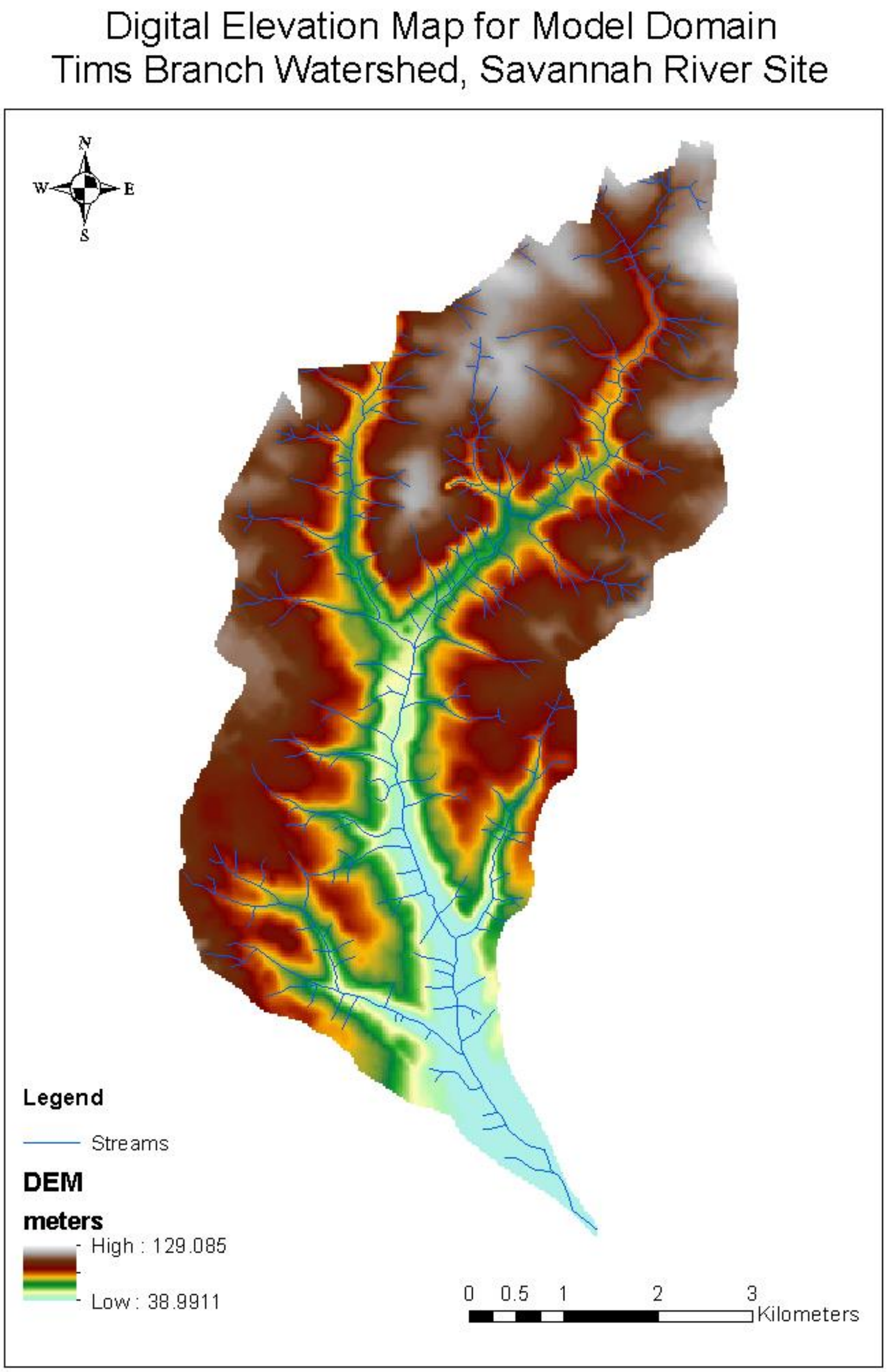
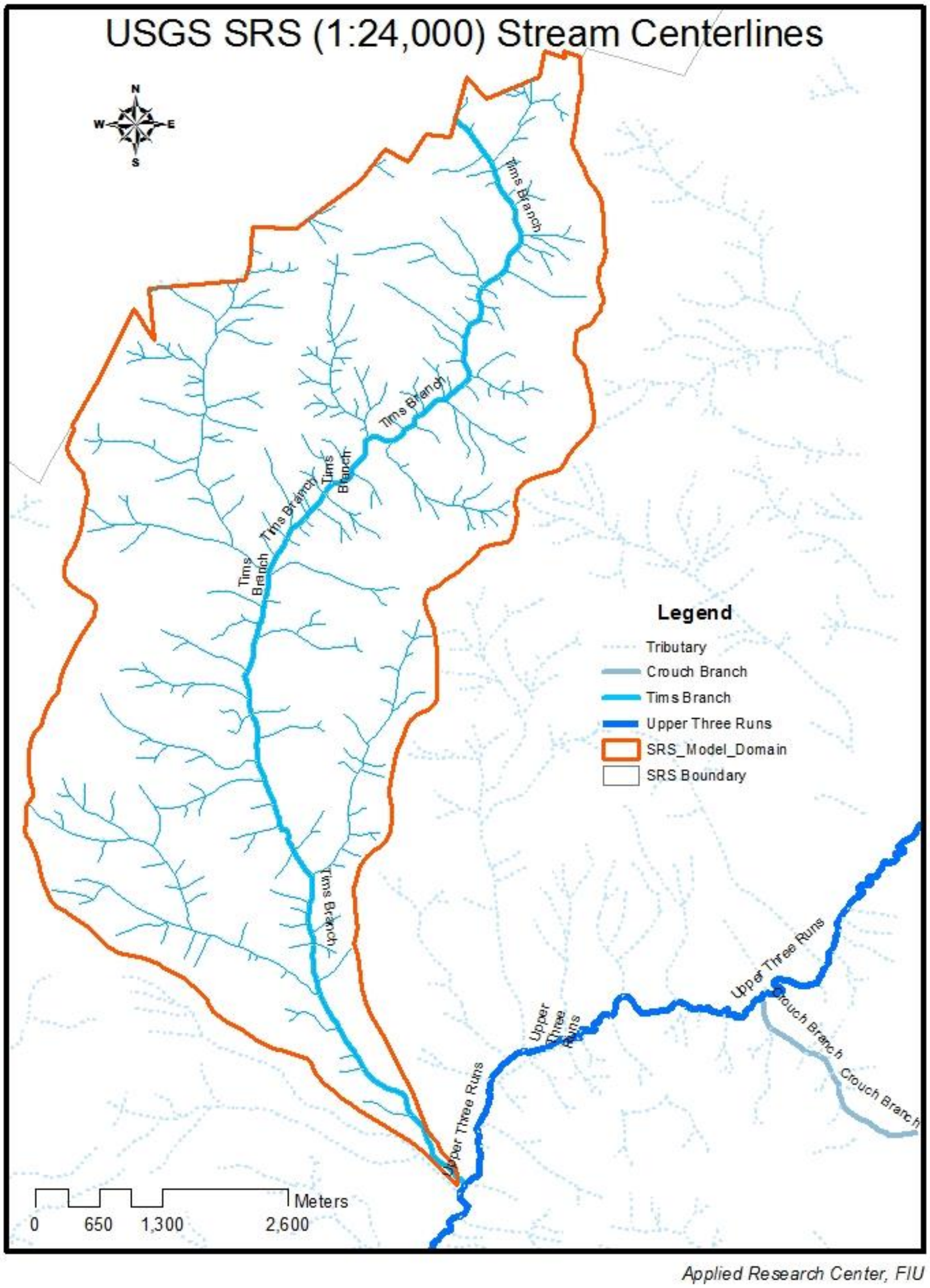

Intersecting Areas of Savannah River Site with Upper Three Runs & Tims Branch Watersheds
N
W
E
S
Greenwood
McCormick
Lexington
Edgefield
Aiken
Columbia
Orangeburg
Upper Three Runs Watershed
Tims Branch Watershed
Richmond
Barnwell
Bamberg
Savannah River Site
Legend
Tims Branch Watershed
Upper Three Runs Watershed
SRS Boundary
SC Counties
Georgia Counties
Burke
Allendale
Screven
Jenkins
Hampton
0 6,000 12,000 24,000 Meters
Applied Research Center, FIU


Digital Elevation Map for Model Domain
Tims Branch Watershed, Savannah River Site
N
W
E
S
Legend
Streams
DEM
meters
High : 129.085
Low : 38.9911
0 0.5 1 2 3
Kilometers


USGS SRS (1:24,000) Stream Centerlines
N
W
E
S
Tims Branch
Tims Branch
Tims Branch
Tims Branch
Tims Branch
Tims Branch
Legend
Tributary
Crouch Branch
Tims Branch
Upper Three Runs
SRS_Model_Domain
SRS Boundary
Upper Three Runs
Upper Three Runs
Upper Three Runs
Crouch Branch
Crouch Branch
0 650 1,300 2,600 Meters
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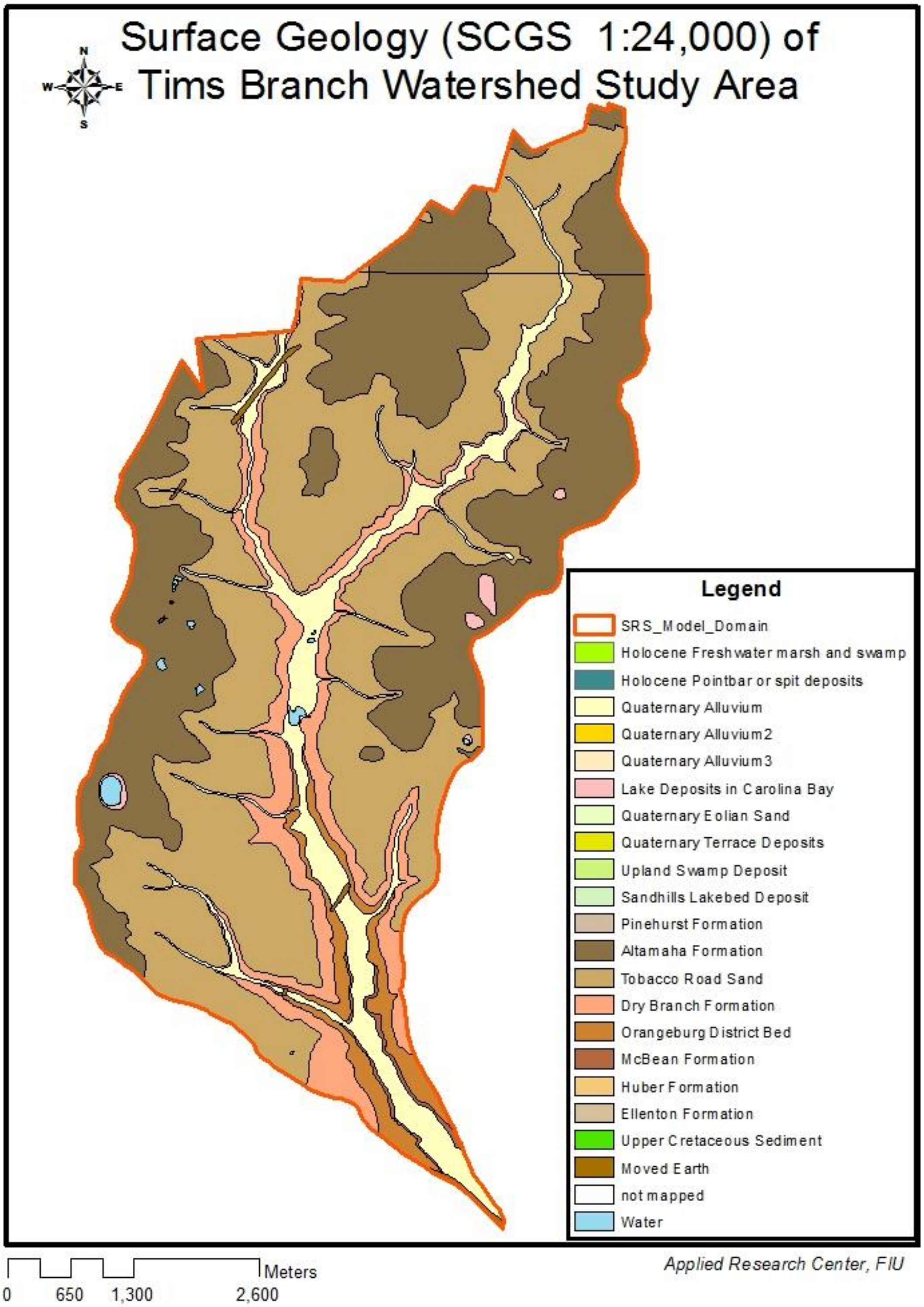
Surface Geology (SCGS 1:24,000) of Tims Branch Watershed Study Area
N
W
E
S
Legend
SRS_Model_Domain
Holocene Freshwater marsh and swamp
Holocene Pointbar or spit deposits
Quaternary Alluvium
Quaternary Alluvium2
Quaternary Alluvium3
Lake Deposits in Carolina Bay
Quaternary Eolian Sand
Quaternary Terrace Deposits
Upland Swamp Deposit
Sandhills Lakebed Deposit
Pinehurst Formation
Altamaha Formation
Tobacco Road Sand
Dry Branch Formation
Orangeburg District Bed
McBean Formation
Huber Formation
Ellenton Formation
Upper Cretaceous Sediment
Moved Earth
not mapped
Water
0 650 1,300 2,600
Meters
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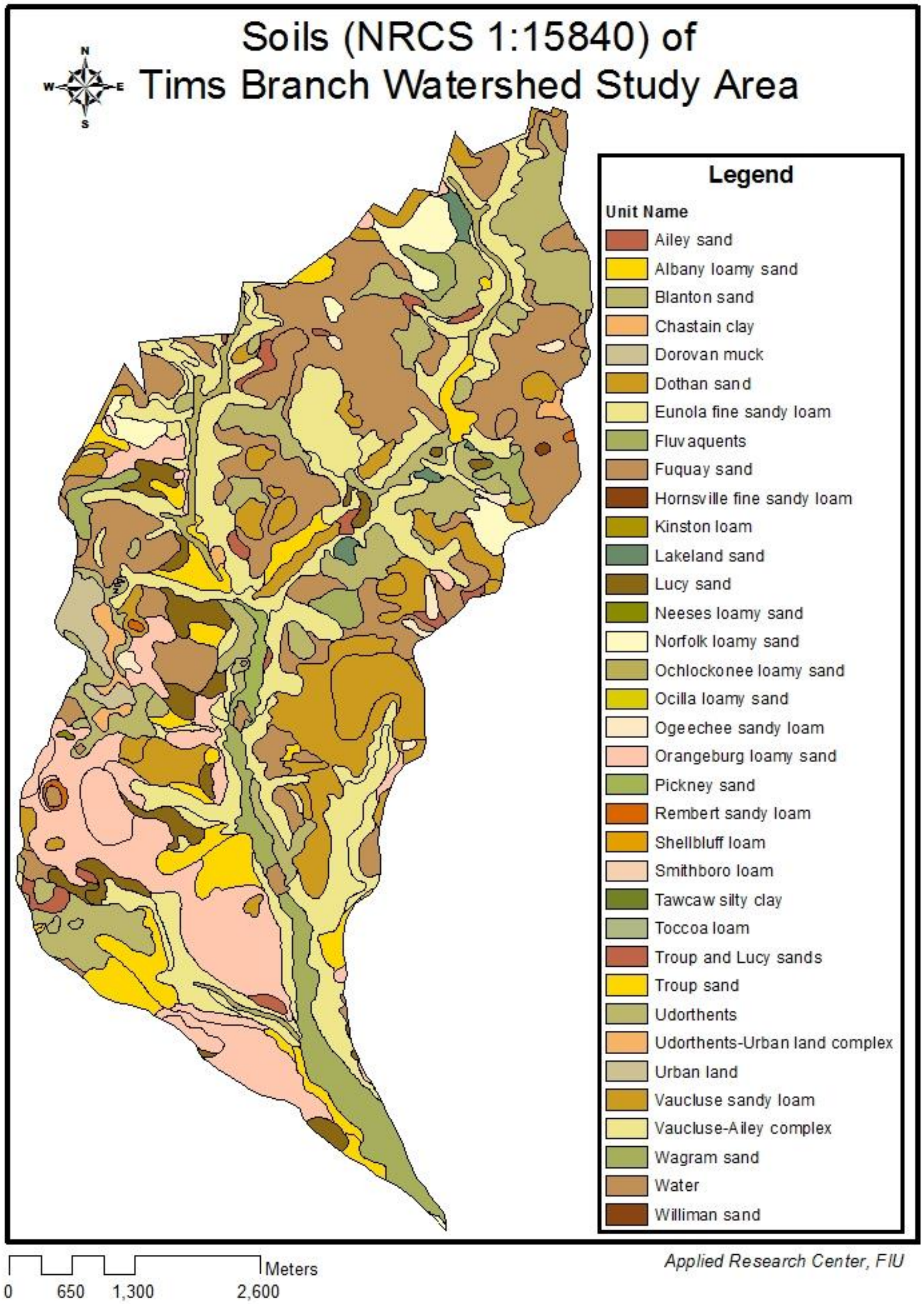
Soils (NRCS 1:15840) of
Tims Branch Watershed Study Area
N
W
E
S
Legend
Unit Name
Ailey sand
Albany loamy sand
Blanton sand
Chastain clay
Dorovan muck
Dothan sand
Eunola fine sandy loam
Fluvaquents
Fuquay sand
Hornsville fine sandy loam
Kinston loam
Lakeland sand
Lucy sand
Neeses loamy sand
Norfolk loamy sand
Ochlockonee loamy sand
Ocilla loamy sand
Ogeechee sandy loam
Orangeburg loamy sand
Pickney sand
Rembert sandy loam
Shellbluff loam
Smithboro loam
Tawcaw silty clay
Toccoa loam
Troup and Lucy sands
Troup sand
Udorthents
Udorthents-Urban land complex
Urban land
Vaucluse sandy loam
Vaucluse-Ailey complex
Wagram sand
Water
Williman sand
Meters
0
650
1,300
2,600
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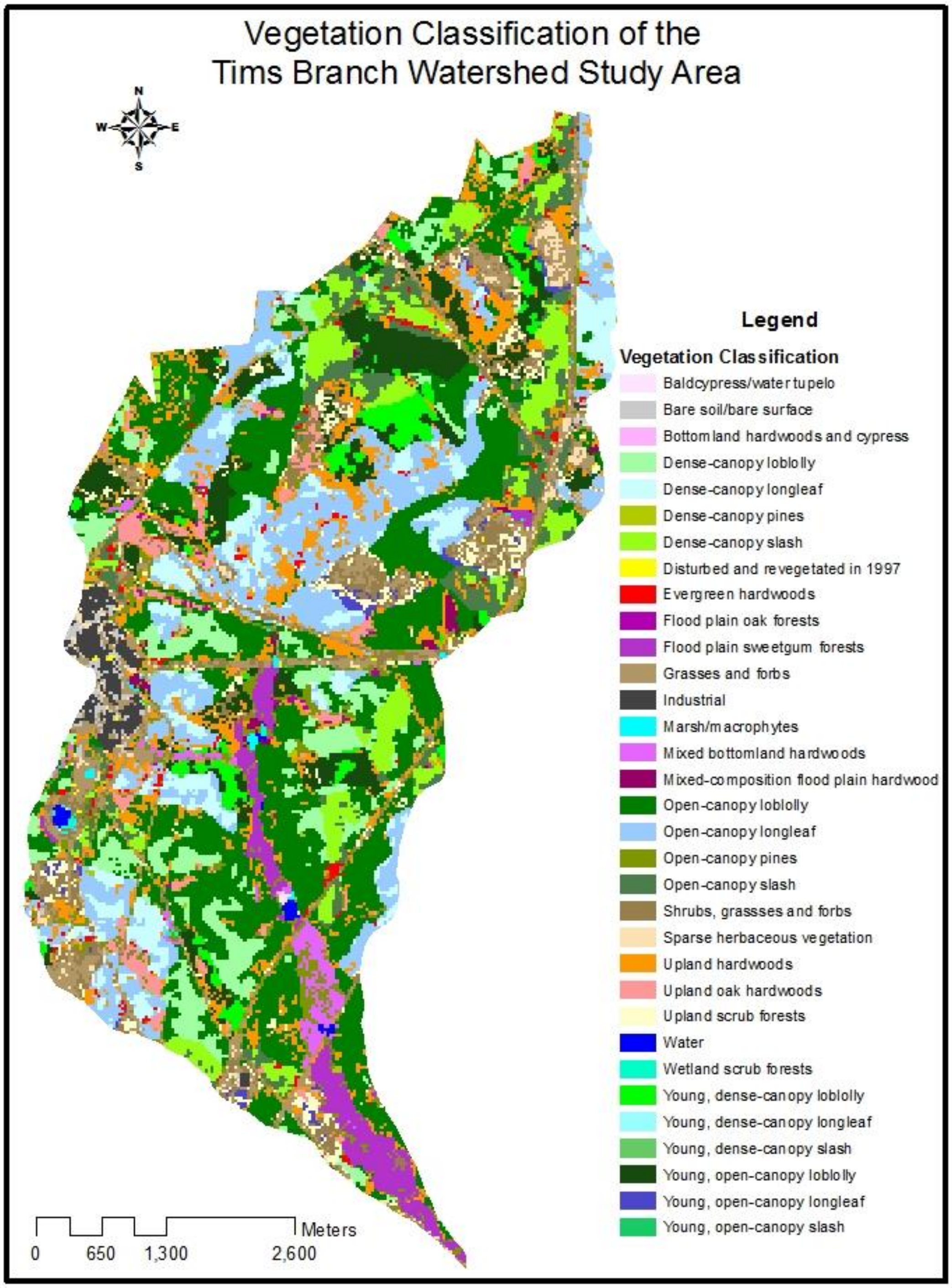

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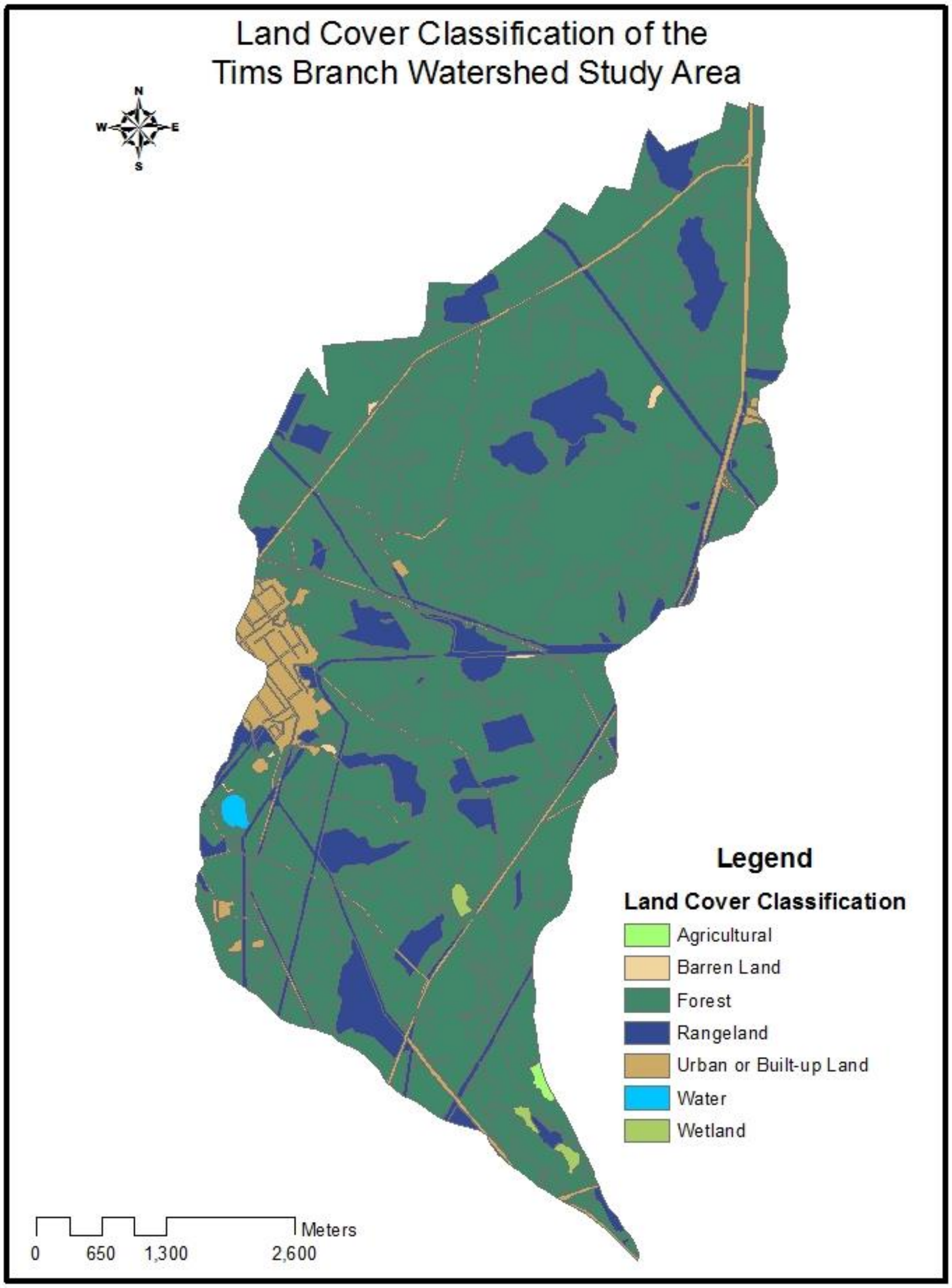

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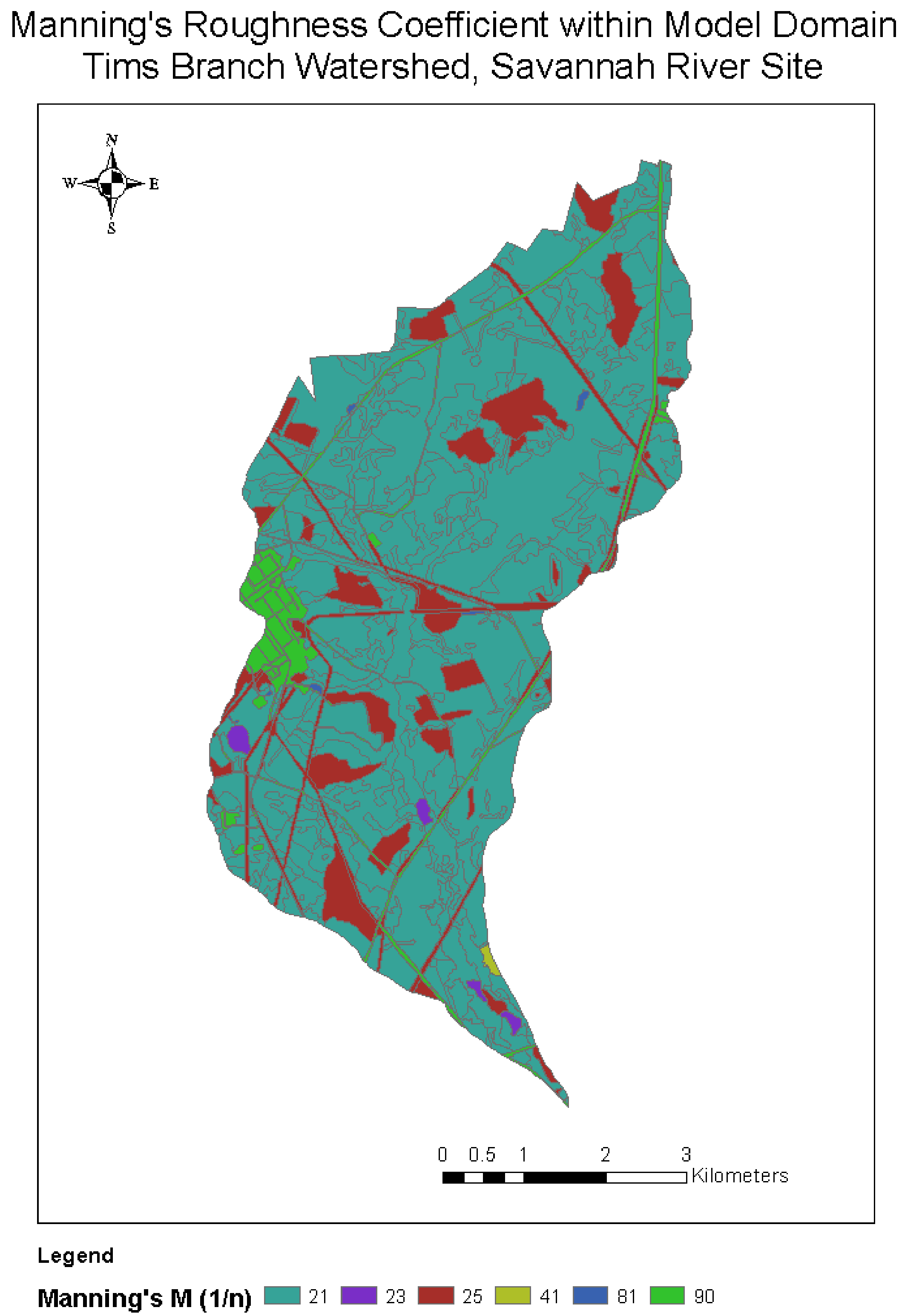
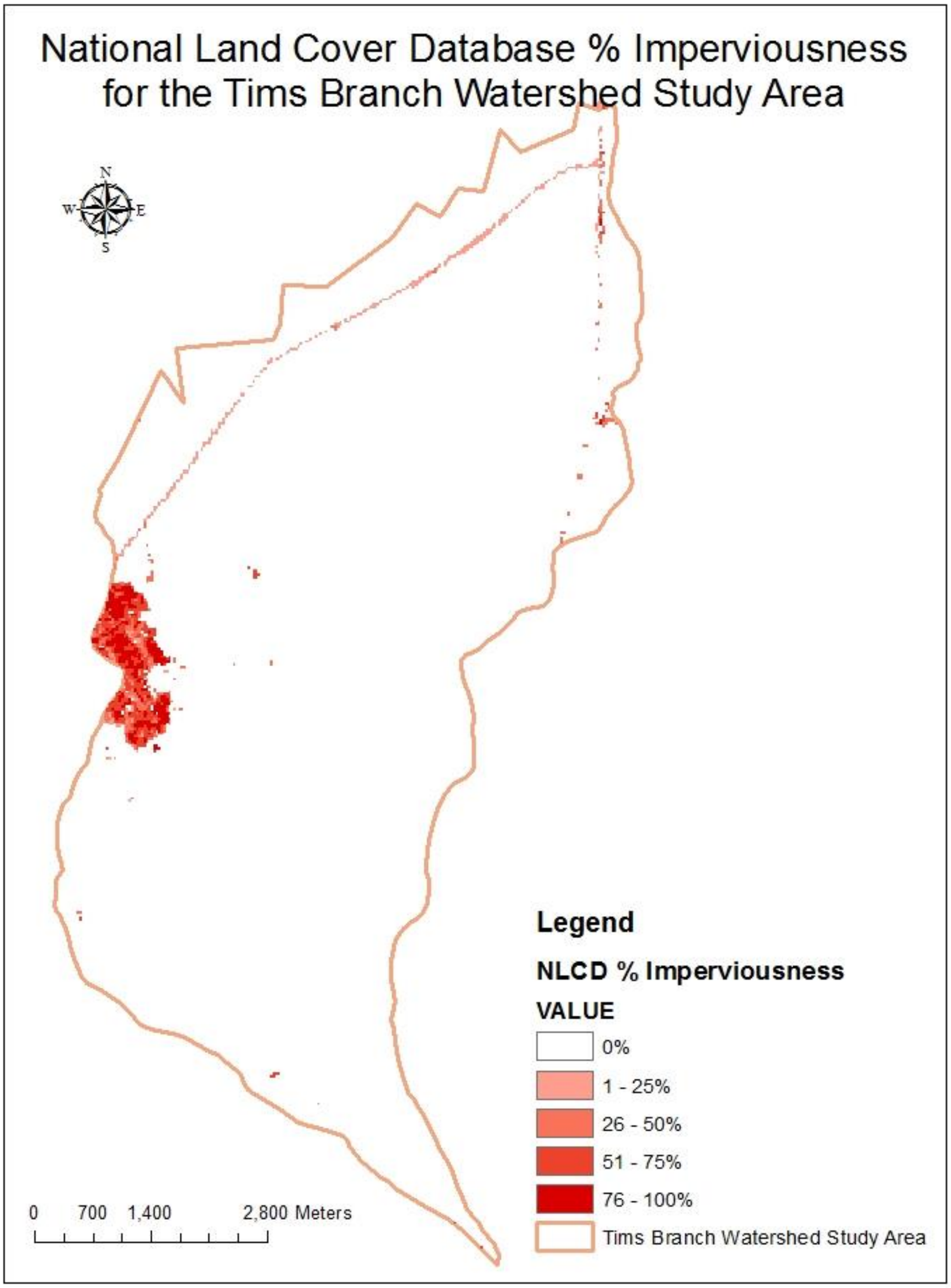
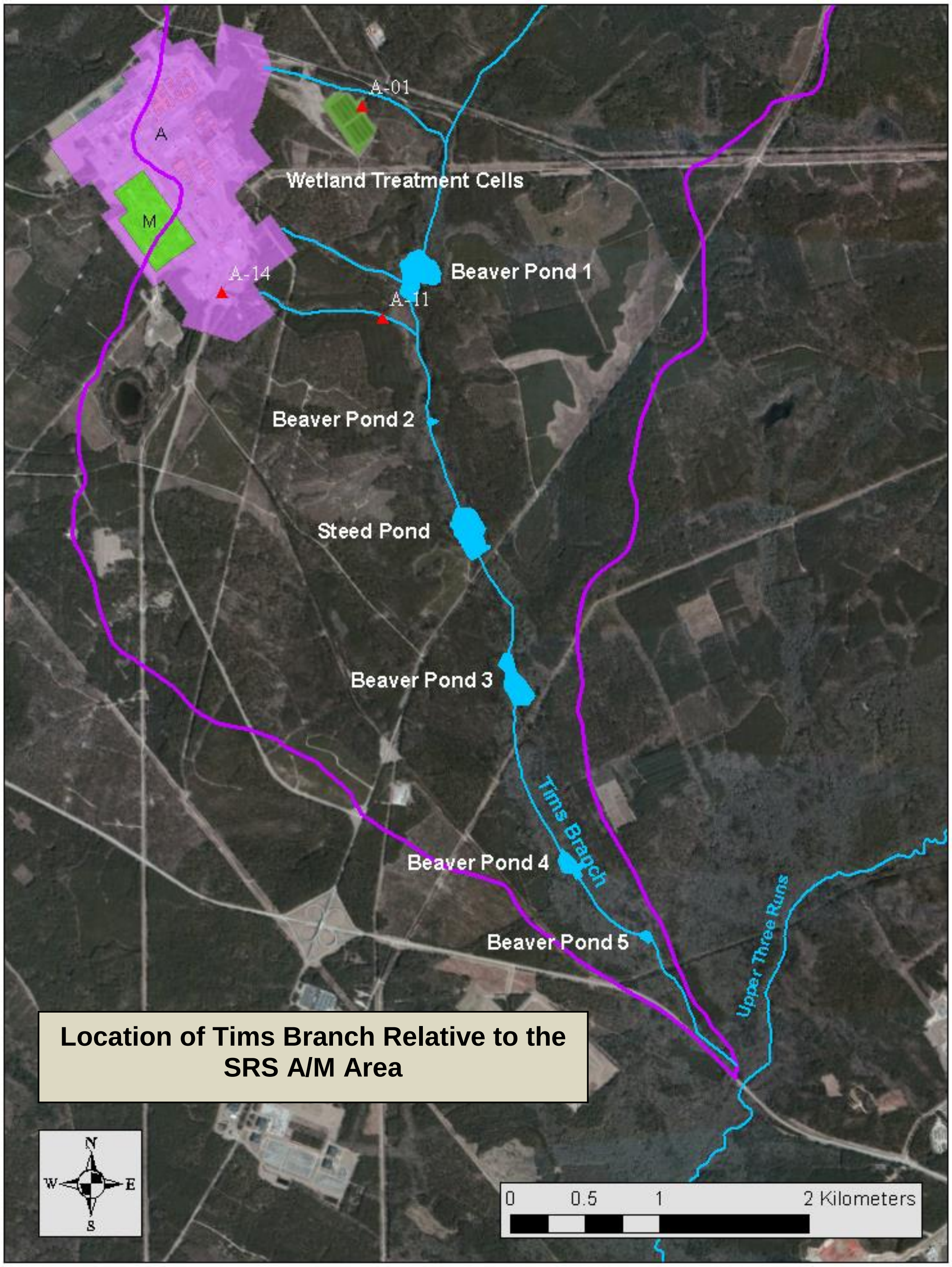
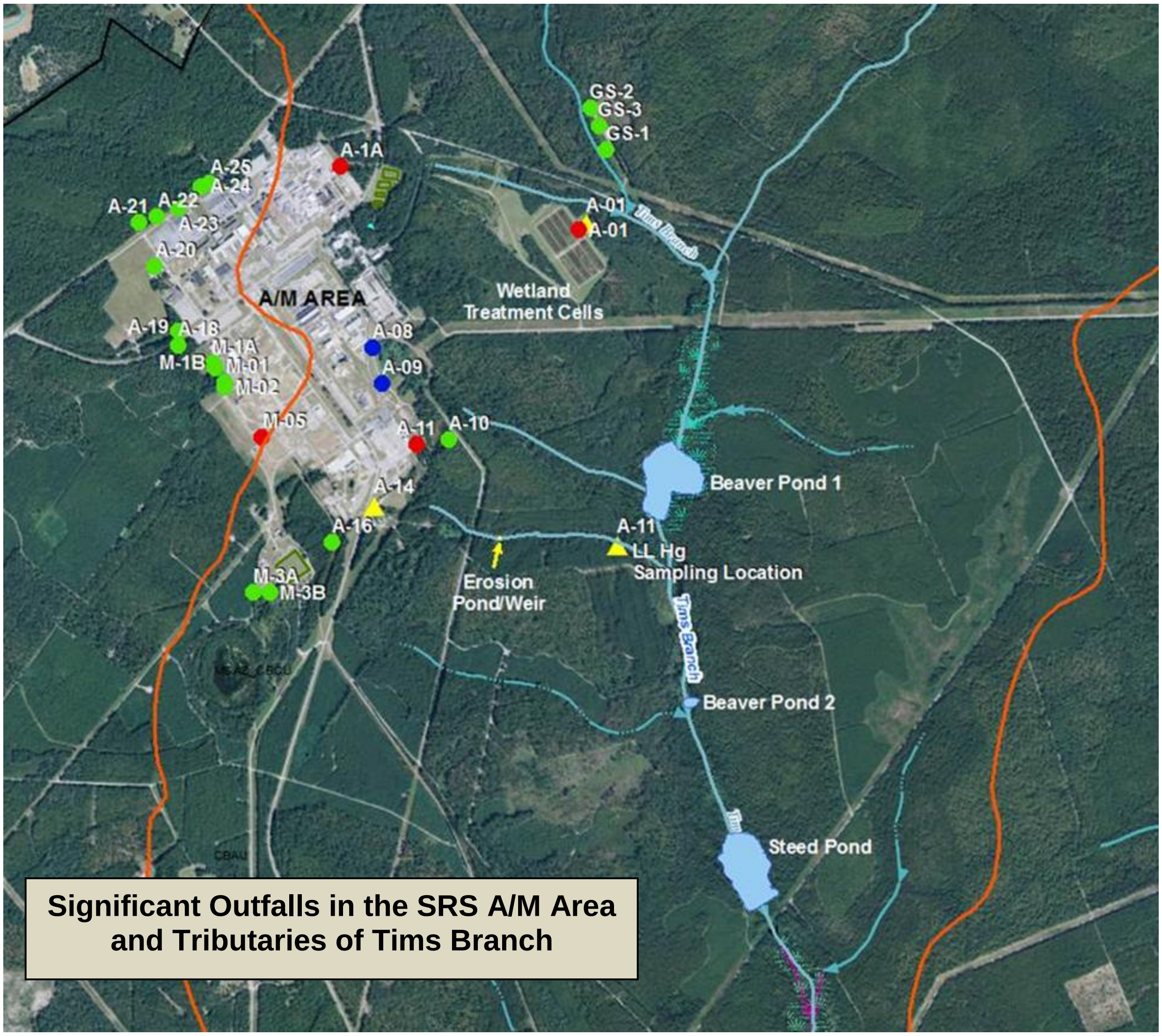

Manning's Roughness Coefficient within Model Domain
Tims Branch Watershed, Savannah River Site
N
W
E
S
0 0.5 1 2 3
Kilometers
Legend
Manning's M (1/n)
21
23
25
41
81
90


National Land Cover Database % Imperviousness
for the Tims Branch Watershed Study Area
N
W
E
S
Legend
NLCD % Imperviousness
VALUE
0%
1 - 25%
26 - 50%
51 - 75%
76 - 100%
Tims Branch Watershed Study Area
0 700 1,400 2,800 Meters


A-01
A
Wetland Treatment Cells
M
A-14
Beaver Pond 1
A-11
Beaver Pond 2
Steed Pond
Beaver Pond 3
Tims Branch
Beaver Pond 4
Beaver Pond 5
Upper Three Runs
Location of Tims Branch Relative to the SRS A/M Area
N
W
E
S
0 0.5 1 2 Kilometers



Significant Outfalls in the SRS A/M Area and Tributaries of Tims Branch

APPENDIX C: SUB-PROJECT REPORT FROM DR. OMAR ABDUL-AZIZ

Project 3: Environmental Remediation Technologies (EM-12)

Sub-Project Report from Dr. Omar Abdul-Aziz

May 17, 2015

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

Background

This research includes the modeling of migration and distribution of humate injected into the subsurface systems during deployment for the in-situ treatment of radionuclides, metals and organics. The task will provide coupling between flow and transport of contaminants in the subsurface and will investigate the spatial and temporal changes within the subsurface to simulate the response of the system after injection of humate. The task will develop an analytical tool for optimization of the coupling of injection rates, concentration of humate and location of the injection wells.

Needed Support from Dr. Abdul-Aziz

- Subsurface model development: Development of a subsurface flow and transport model with injection wells (using ASCEM or other available numerical model). The model will be capable of simulating flow, transport and chemical reactions.
- Calibration, Verification and Simulations: Conduct a series of simulations to verify model response, including simulations of groundwater levels, concentrations and transport of conservative tracers and reactive substance.

Accomplishments

Subject to stringent deadline of May 17, 2015 and limited time, the ARC modeling team mainly focused on the development of surface water model for the Tims Banch Watershed in this reporting period. Tims Branch is a small braided, marshy, second-order stream that starts at the northern portion of the Savannah River Site (SRS) and passes through Beaver Ponds 1-5 and Steed Pond, eventually discharging into the Upper Three Runs (Fig. 1). Its drainage area is around 16 km^2. The length of this stream from outfall A-014 to Upper Three Runs is approximately 8 km. The average width of the stream varies between 2-3 m. Subject to the complex drainage and watershed processes, a coupled surface water and groundwater transport model has been developed for the Tims Branch Watershed using the MIKE11-MIKESHE-ECOLAB platform. The modeling tool, upon calibrations and validations, should provide predictions of subsurface flow, transport and chemical reactions under different climate, environment and management scenarios. Please refer to the accomplishments in Task 2 for further details.

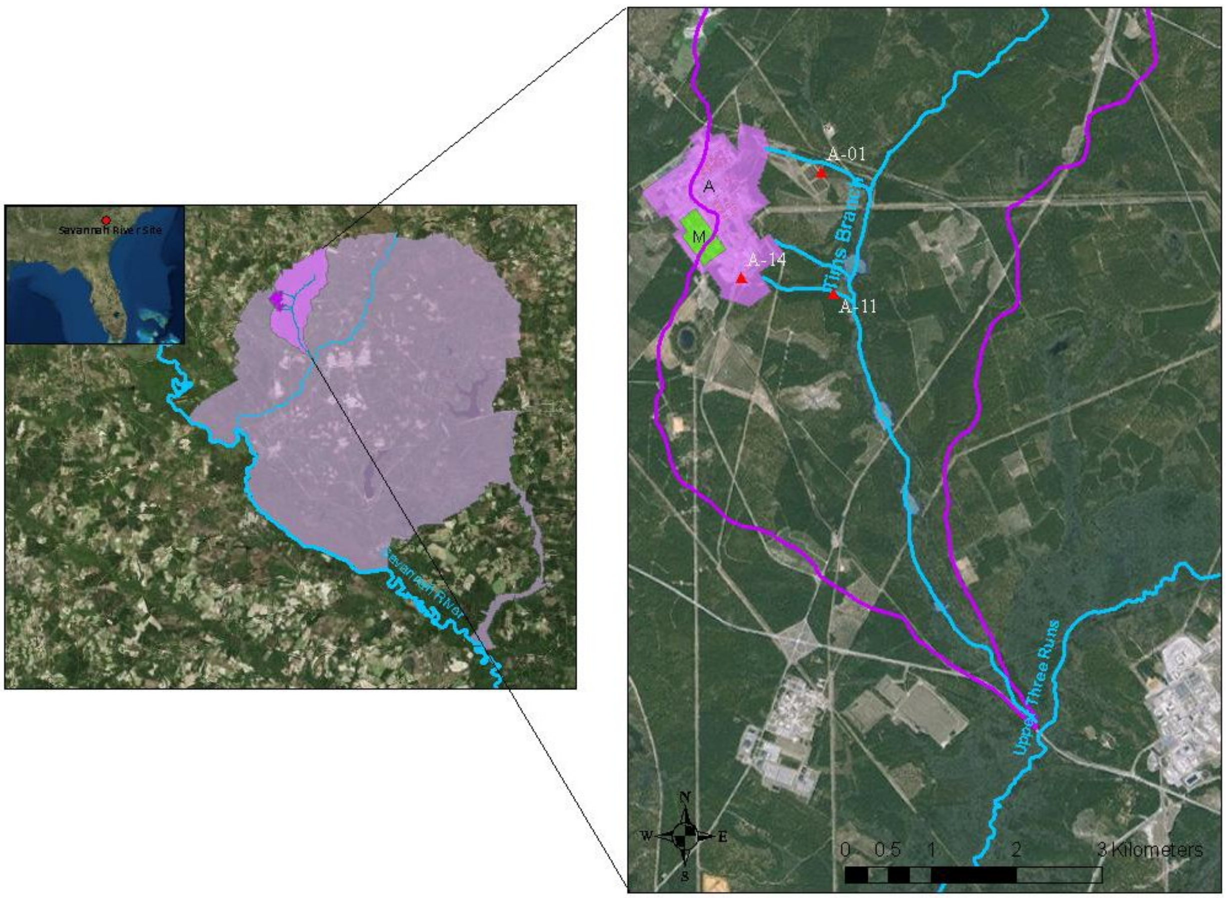


Fig. 1. The Tims Branch Watershed study area within the Savannah River Site, U.S.A.

Task 2: Surface Water Modeling of Tims Branch

Background

The task will perform modeling related to water, sediment, mercury and tin in Tims Branch at Savannah River Site (SRS). This site is 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 experienced controlled step changes in boundary conditions. The task will develop and test 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.

The developed surface water and sediment transport models will be applied to the Tims Branch system at the SRS to simulate and predict the behavior of mercury, tin and other reactive pollutants (e.g., uranium). An evaluation of the available literature and models related to mercury and tin transformations (e.g., methylation) in stream ecosystems such as Tims Branch will also be done. A literature review will also be conducted to collect SRS site characterization data required for model development. Spatial and temporal data collected will be stored and managed in a GIS database (geodatabase). SRS data will include (1) river discharges and stages, (2) water quality parameters relevant to flow and transport of contaminants (pH, total suspended solids, contaminant concentrations), (3) time-series of boundary conditions (rainfall, evapotranspiration, outfalls, river stages and discharge).

Needed Support from Dr. Abdul-Aziz

- Review of available data: A review of available data (temporal and spatial) will be conducted to determine model data requirements for the corresponding numerical model (ASCEM or other available models)
- Development of a preliminary conceptual model for Tims Branch

- Development of analytical, numerical and statistical models for Tims Branch

Accomplishments

A detailed review of the previous studies and available data has already been done and reported to the DOE on May 31, 2015. Dr. Abdul-Aziz supervised Dr. Merhnoosh Mahmoudi (post-doc) in performing and preparing the review. As a summary, more than 30 SRS-DOE reports and 100 published journals were reviewed. In total 10 reports and 40 journal articles were relevant to this project. Particular emphasis was given to identify studies exclusively focusing on hydrological modeling efforts for the Tims Branch.

Dr. Abdul-Aziz provided a crucial guidance on the data requirement and approximation (e.g., channel geometry and bathymetry in case of unavailability) for developing a surface water model for the Tims Branch Watershed. Most of the available data on climatic, hydrologic and hydraulic, land use/cover, and pollutant variables have already been gathered and organized using a ArcGIS platform (see Fig. 2 as an example). The remaining data on streamflow and ground water level are currently being gathered for the model calibration and validation.

ArcGIS ArcMap GUI showing (1) A/M Area, Tims Branch and several major tributaries with flow direction arrows, significant hydrologic and man-made features (e.g. ponds, weir, outfalls, etc.); (2) table of contents on the left serves as a legend for some of the features; (3) on the right, the SRS geodatabase structure can be viewed.

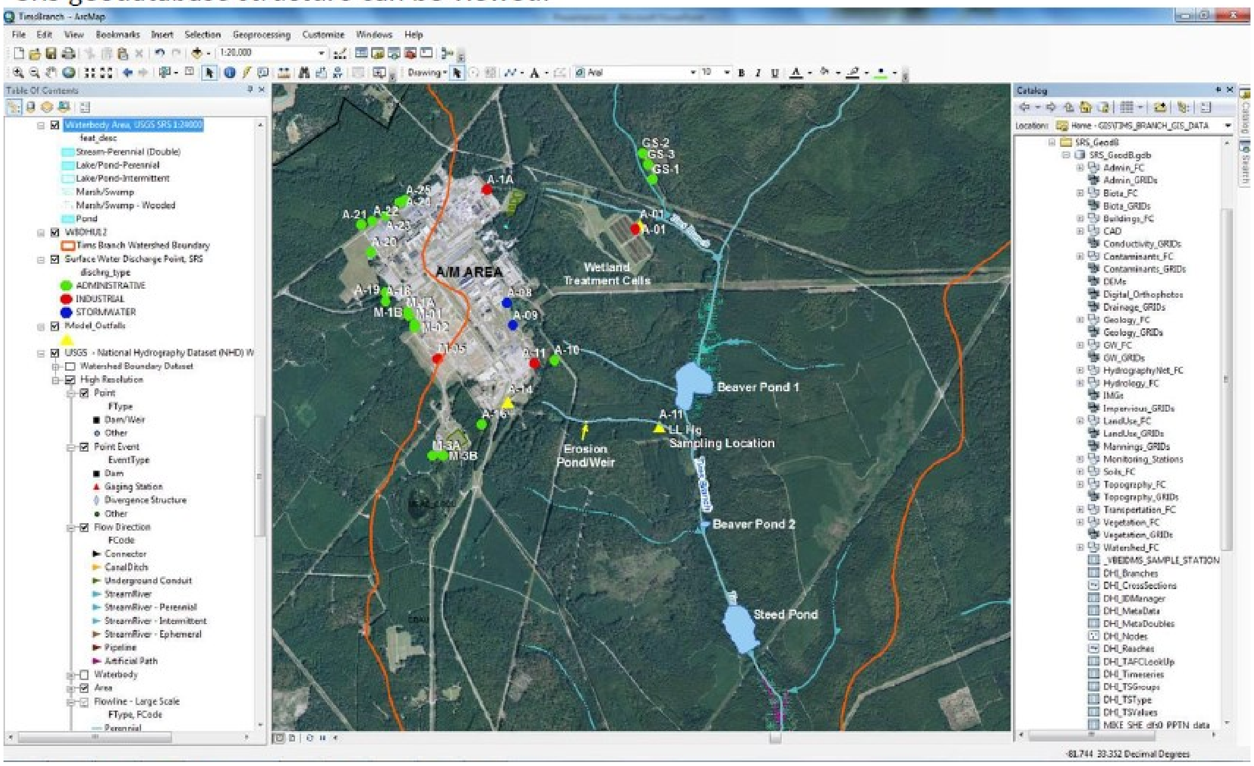


Fig. 2: Organization of available data on a ArcGIS platform.

Modeling hydrological processes and sediment transport mechanisms require a detailed understanding of soil and sediment characteristics, geologic formation, topography, climate, and hydraulic properties. Mechanistic understanding from the literature review was leveraged to develop a conceptual model (see Fig. 3) of water and pollutant transport for the Tims Branch Watershed. The conceptual model will also incorporate processes and features such as discharge points, groundwater/surface water interaction, geological formation, atmospheric characterization, infiltration, sediment erosion /deposition, etc.

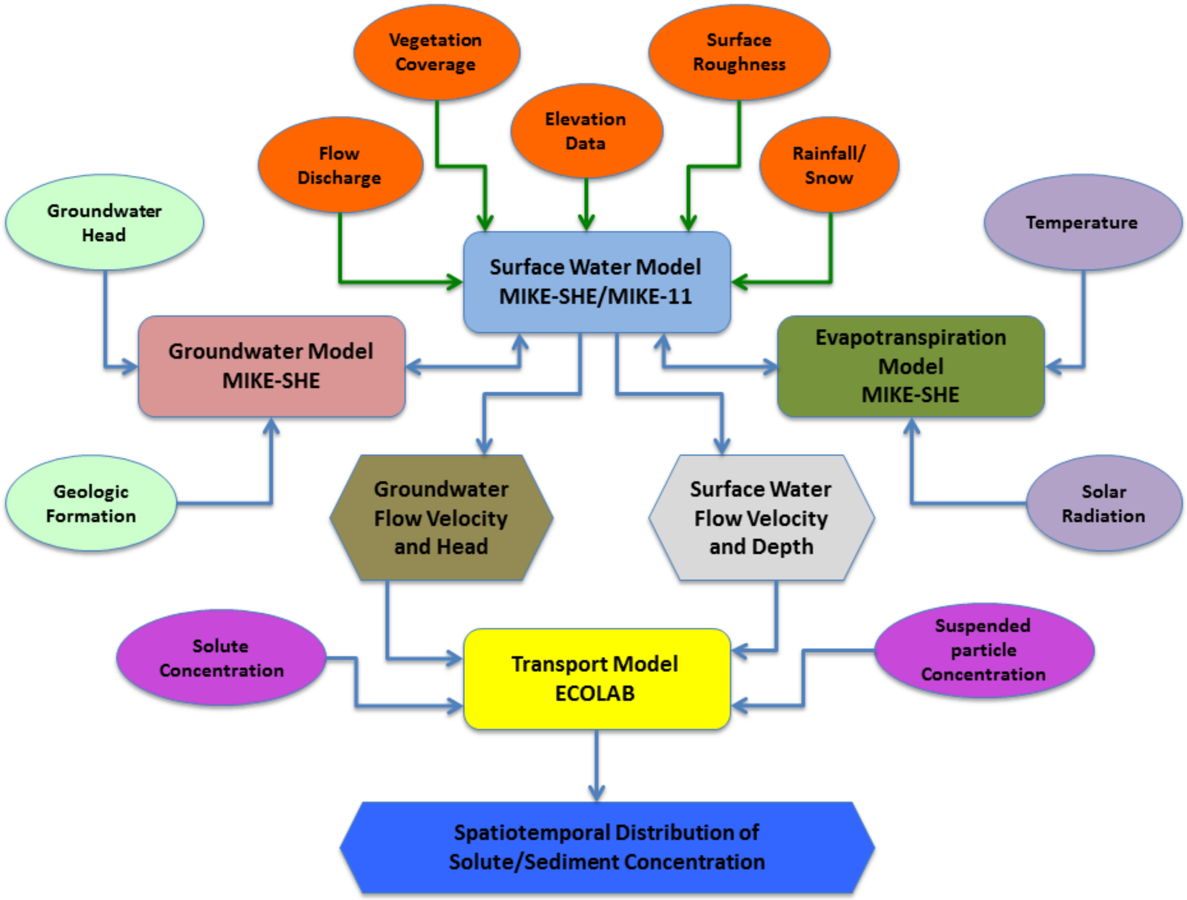


Fig. 3: A conceptual model of water and pollutant transport for the Tims Branch Watershed.

The conceptual model is used to develop a detailed water (both surface and subsurface) and pollutant transport model for the study area using a MIKE package that included the MIKE-SHE, MIKE-11 and ECOLAB. An advantage of the MIKE package is that its built-in GIS interface facilitates an efficient incorporation of input data and presentation of model results. Dr. Abdul-Aziz and his research team provided important guidance and mentoring to Dr. Mehrnoosh Mahmoudi in parameterizing the Tims Branch Watershed (which has a very complex drainage network) with an appropriate number of links and nodes, as well as for developing the MIKE-SHE/MIKE-11 watershed model for this area. In particular, upon examining the photographs from the recent site visit of Dr. Mahmoudi and Ms. Angelique Lawrence and leveraging the shared field knowledge, Dr. Abdul-Aziz guided the plan and process of the Tims Branch Watershed model development and evaluations.

The MIKE software package was developed by the Danish Hydraulic Institute (DHI). The integrated flow and transport model (MIKE-SHE/MIKE-11/ECOLAB) will analyze the effect of hydrological events and point sources on the erosion, resuspension, and transport of pollutants (e.g., tin, mercury) in the Tims Branch Watershed. The model includes all important components of the hydrological cycle such as precipitation, evapotranspiration, infiltration, overland flow, and groundwater flow (saturated and unsaturated), as well as the fate and transport of sediment and pollutants. The relevant processes for flow and transport simulation for the Tims Branch MIKE models is presented in Fig. 4.

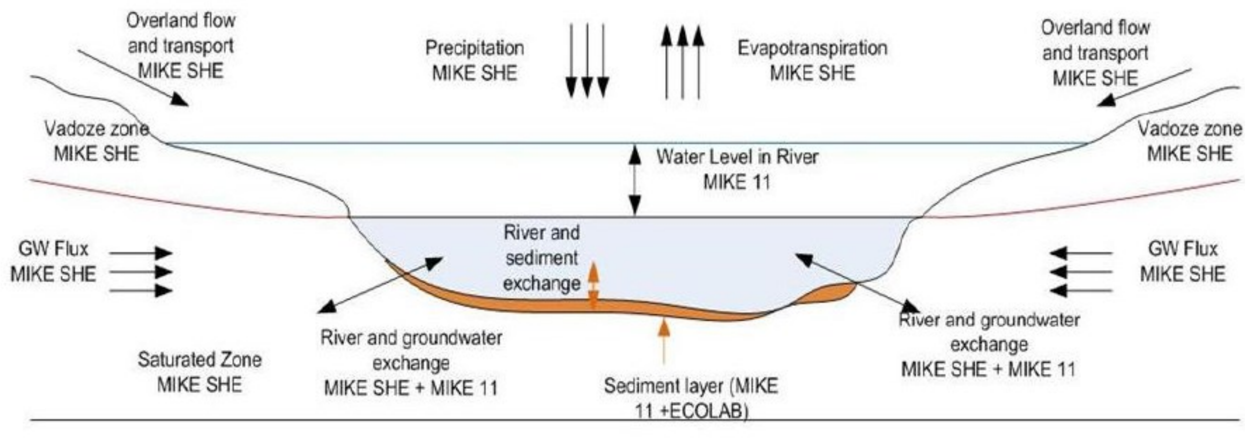


Fig. 3: Flow and transport components included in the model

Fig. 4: The detailed process layout of the Tims Branch MIKE modeling tool.

The MIKE-11 is a 1-D river modeling system. It is one of the most advanced and comprehensive watershed hydrology models available in current literature. MIKE-11 is routinely used by regulators for analysis of flows in streams, rivers and canals under complex water management scenarios. It has also been used to study, design and manage floodplains, dam breaks, and operation of control structures. MIKE-11 uses an implicit, finite difference scheme to solve the nonlinear equations (e.g., Saint-Venant, diffusion wave, kinematic wave) of open channel flow numerically. MIKE-SHE is a fully integrated model for a 3D simulation of overland, subsurface, and river flows. It has been successfully applied at multiple scales, using spatially distributed and continuous climate data, to predict a broad range of integrated hydrologic, hydraulic, and transport variables. ECOLAB is an ecological solver provided by DHI. ECOLAB is coupled with MIKE-11 for ecological modeling. An ECOLAB template can be developed by the user to model the ecological processes of heavy metal transport, eutrophication, xenobiotics, etc.

Upon calibrations and validations with observed data (streamflow, groundwater level), the model will predict the concentrations, fate and transport of tin (and its possible methylation) and other targeted pollutants (e.g., mercury) in the Tims Branch watershed. The watershed-scale model will be capable of providing predictions in the relevant streams under different climate, environment and management scenarios.

Conclusions and Next Steps

Dr. Abdul-Aziz provided the requested support as needed by the ARC modeling team. Overall, the project accomplishments and progress are in line with the proposed objectives and goal for the reporting period. The ARC team has made a good plan to successfully accomplish the proposed modeling tasks as below.