




Applied Research Center
FLORIDA INTERNATIONAL UNIVERSITY

A collage of six images: top-left shows green foliage; top-middle shows a person in a blue lab coat working with equipment; top-right shows a yellow industrial structure; bottom-left shows a blue and green abstract pattern; bottom-middle shows a close-up of a person's face; bottom-right shows several blue pill containers with pills inside.

Project 3-Task 1: **An Integrated Flow and Mercury Transport** **Model for EFPC, Oak Ridge, Tennessee**

Presented: May 1, 2013
to USACE
by Lilian Marrero, E.I.
DOE Fellow

Worlds
Ahead

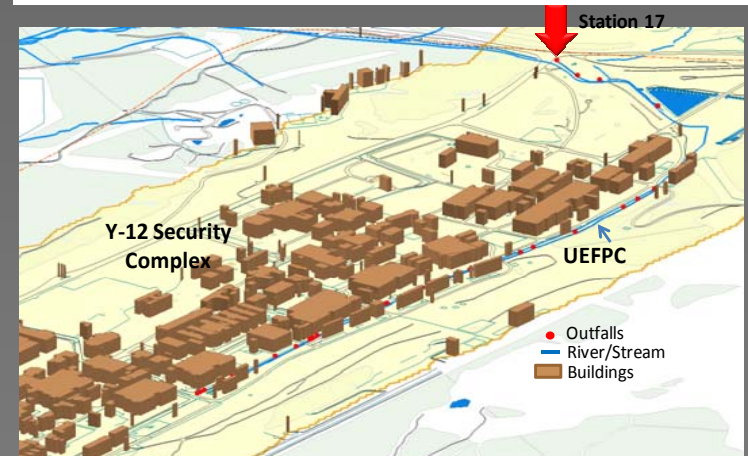
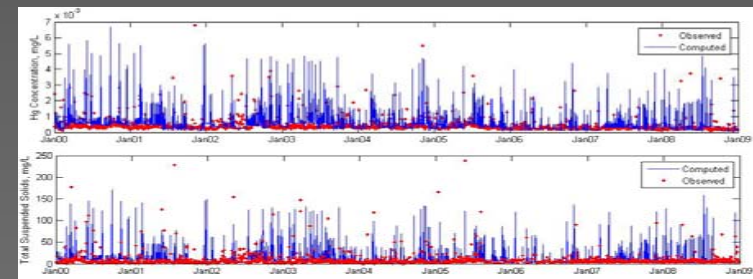
Advancing the research and academic mission of Florida International University.



Task 1

EFPC Model Update, Calibration, Uncertainty Analysis

- Developed and calibrated numerical model for hydrology, sediment and Hg transport in UEFPC (1996 to present).
- Reconfigured model to incorporate a sedimentation module and then extended it to include the entire EFPC watershed.
- Performed numerical simulations using a range of Manning's numbers, threshold run-off water depths, and drainage coefficients to calibrate flow from 2000 – 2008. MATLAB scripts were used for statistical analysis of observed and computed data.
- Provided U.S. DOE with assessment reports on the effectiveness of 8 different remedial scenarios.



Total suspended solids and Hg concentration compared with historical data at Station 17



Mercury (Hg) Contamination in Oak Ridge Reservation

> 2 mil. lbs Hg released to environment in soil, sediment, surface water, groundwater, buildings and other infrastructure during Li-isotope separation process to produce nuclear fusion weapons at Y-12 National Security Complex (NSC).



Y-12 Area



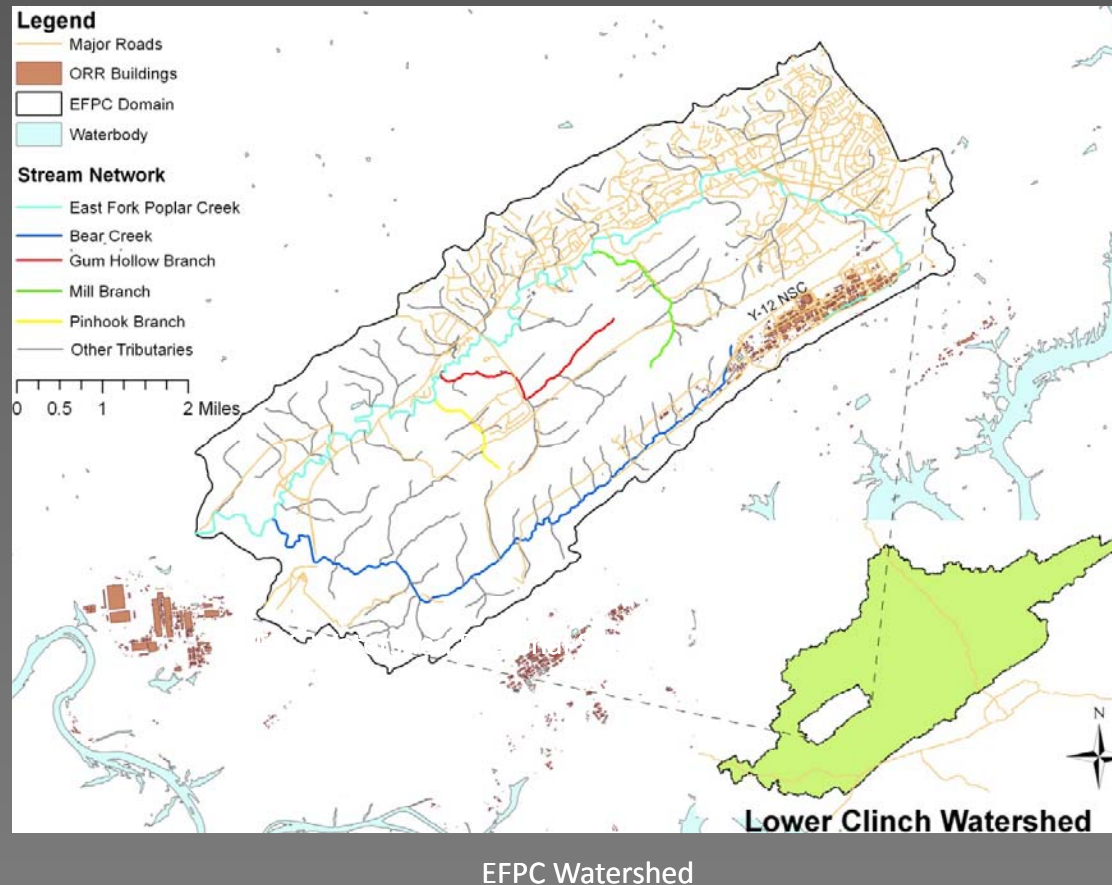
Soil Sample Extraction at Y-12



Soil Mercury Contamination



Introduction



- Streams:
 - EFPC – NE to SW
 - 24,610 m long
 - 287m – 226 m above SL
- General slope: 0.23%
- Domain Area: 29.7 sq. mi.
- Streams Length: 88 mi
- Knox Aquifer – solution conduits
- ORR - fractures



Research Objective

General Objective:

- Investigate the flow and transport of mercury (Hg) within EFPC.

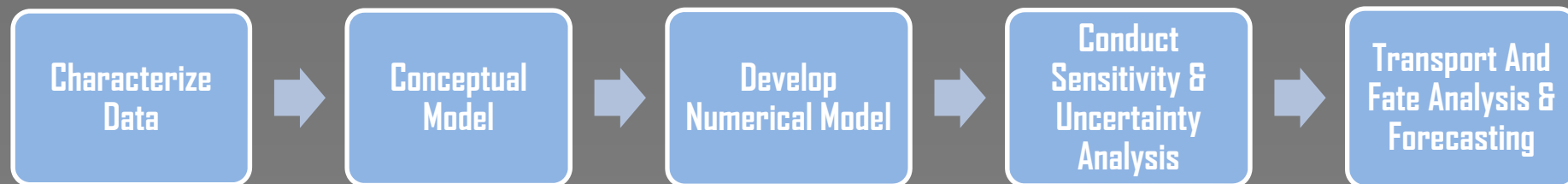
Detailed Objectives:

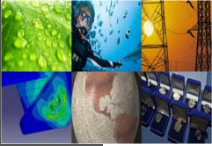
- Modify existing integrated surface and groundwater model for flow and Hg transport for EFPC (MIKE SHE and MIKE 11).
- Incorporate sedimentation module (ECO Lab).
- Analyze a range of hydrologic events and predict the transport patterns of mercury.
- Calibration.



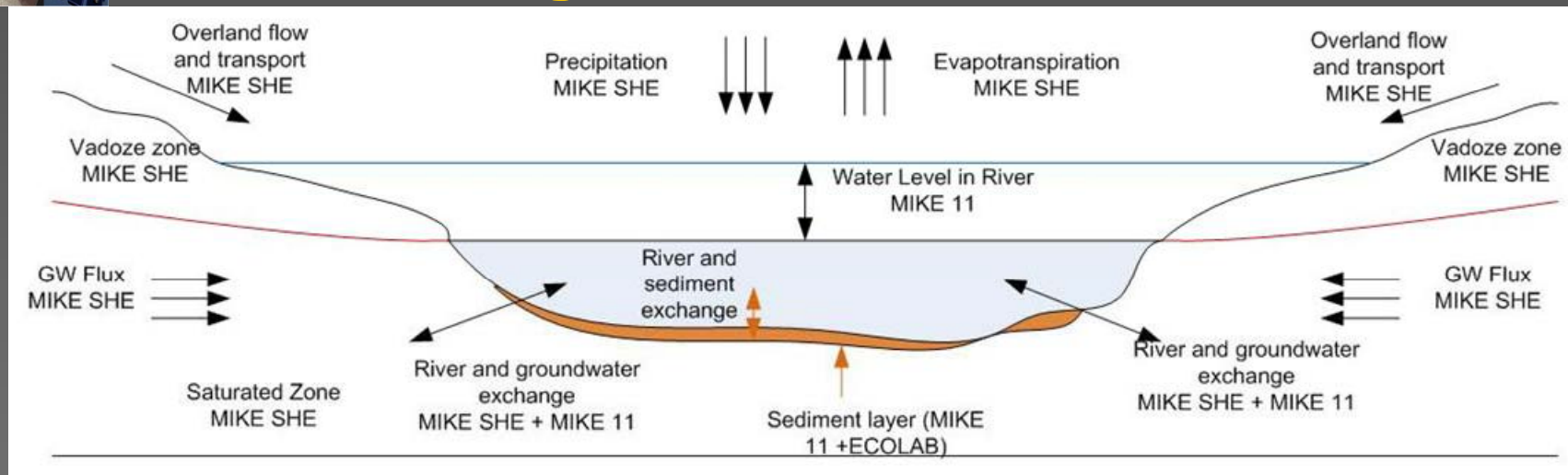
Methodology

- Model simulations using observed total suspended solids and total mercury concentration timeseries.
 1. Time series plots of observed and simulated values for fluxes or state variables (e.g., stage, sediment concentration, and biomass concentration).
 2. Observed versus simulated scatter plots, with a best-fit linear regression line displayed, for fluxes or state variables.
 3. Cumulative frequency distributions of observed and simulated fluxes or state variables (e.g., flow duration curves).





Modeling Approach



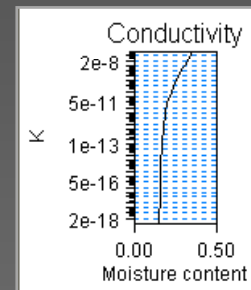
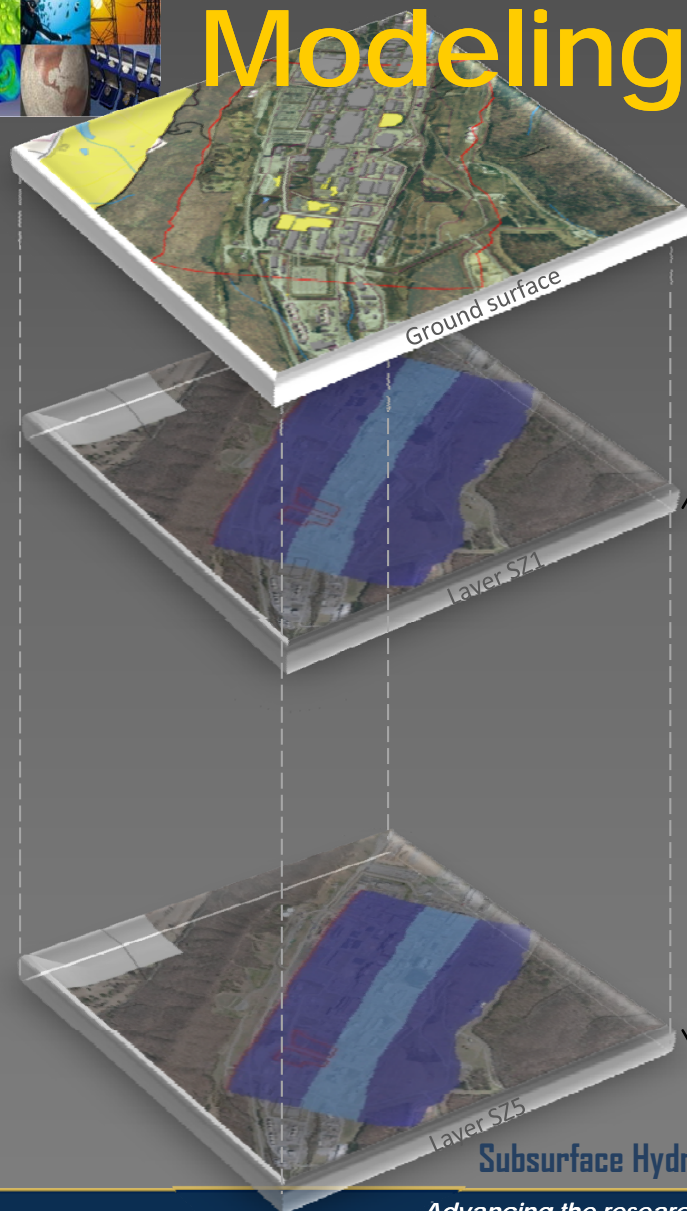
Model Modules Conceptual Interaction

MIKE SHE: 3-D saturated and unsaturated groundwater flow, 2-D overland flow model deterministic, physically based & fully distributed hydrological modeling system. It consists of the Water Movement and Water Quality modules.

MIKE 11: 1-D river flow model. Solves vertically integrated equations for the conservation of continuity and momentum. Hydrodynamic (HD) & advection (AD) modules.

ECOLAB: Numerical ecological model used to simulate the fate and transport of mercury at the water and sediment interface.

Modeling Approach



- The unsaturated zone uses Van Genuchten's Model.
- Hydraulic conductivity is a function of moisture content.
- Flow/transport is predominantly in a vertical direction.
- Flow and transport in the saturated zone is 3-D and predominantly in a horizontal direction.

Subsurface Hydrology



Modeling Approach

MIKE SHE

Evapotranspiration & Precipitation

- SVAT
- Kristensen and Jensen
- 2-Layer Water Balance
- Net recharge

OZF

- 2D Finite Difference- Diffusive Wave
- Semi Distributed

Overland Zone Flow (OZF)

UZF

- 1D Finite Difference
 - Richards Equation
 - Gravity Flow
- 2-Layer Water Balance
- Net Recharge

Unsaturated Zone Flow (UZF)

SZF

- 3D Finite Difference - Darcy Flow
- Lumped Conceptual - Linear Reservoir

Saturated Zone Flow (SZF)

MIKE 11

Hydrodynamic (HD) Module

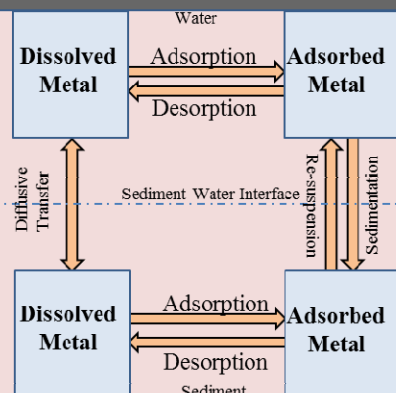
- 1D St Venant Equations:
 - Kinematic wave
 - Diffusive wave
 - Fully Dynamic
- Flow Routing:
 - No-Routing
 - Muskingum (M)
 - M-Cunge

Advection (AD) Module

- 1D St Venant Equations:
 - Kinematic wave
 - Diffusive wave
 - Fully Dynamic
- Flow Routing:
 - No-Routing
 - Muskingum (M)
 - M-Cunge

Channel Flow

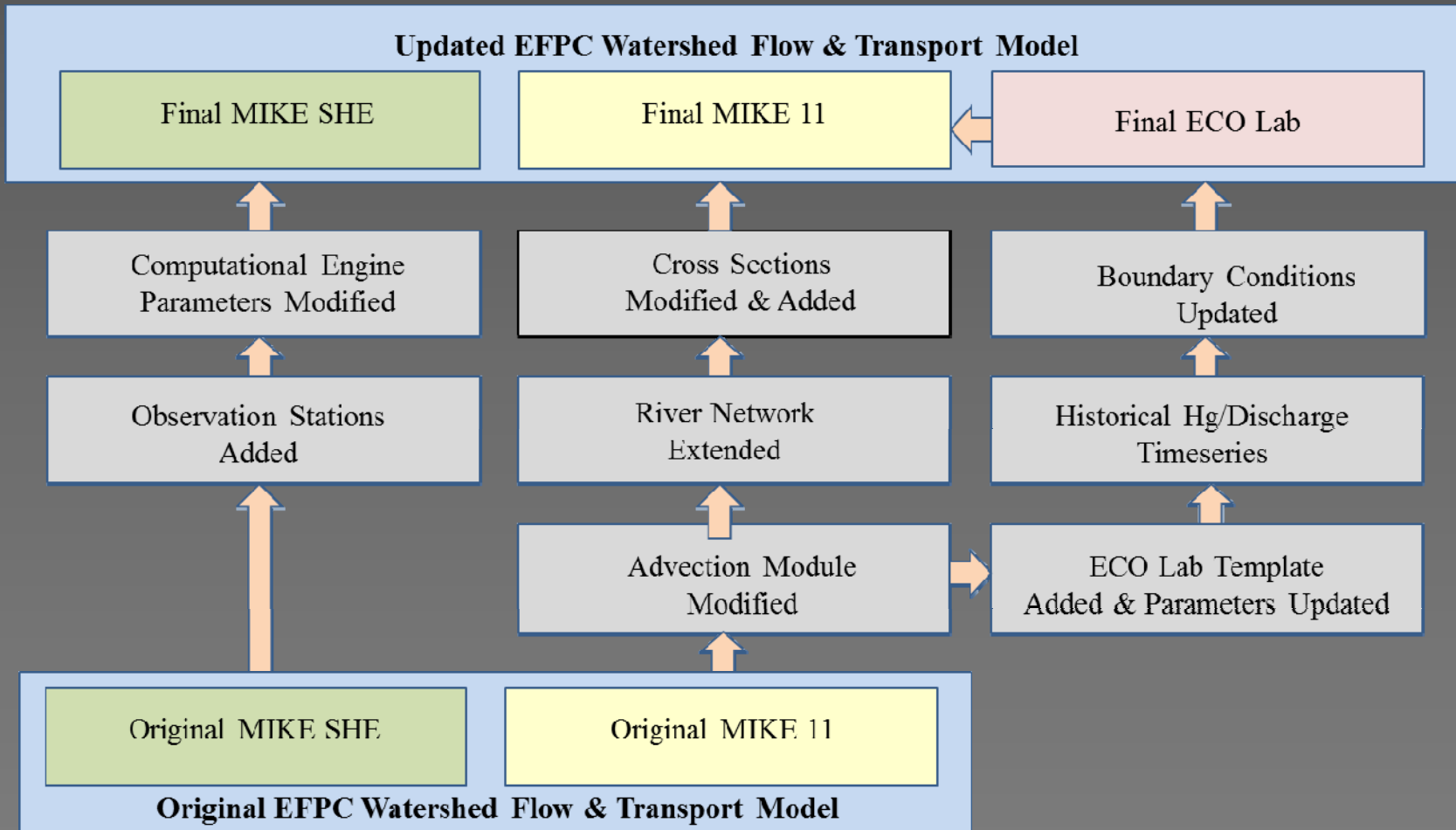
ECO Lab



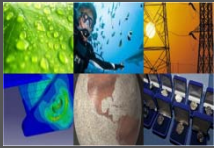
Schematic of the modular set-up and processes of MIKE SHE, MIKE 11, and ECO Lab arranged in accordance to the EFPC model structure.



Modeling Approach



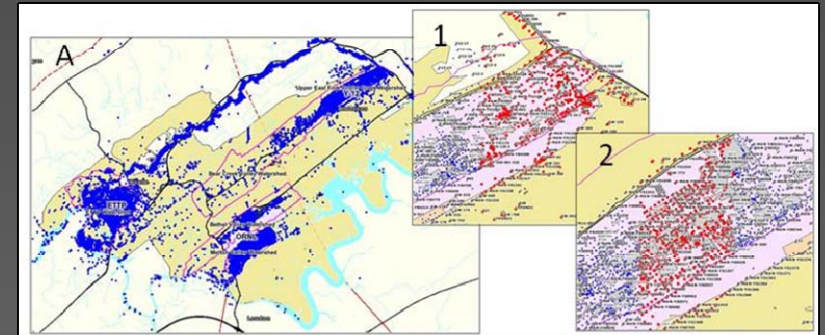
Overview of EFPC Model Updates



Model Updates

Data extracted, categorized, GIS, timeseries (dfs2) :

- Groundwater levels
- Surface water levels
- Mercury Concentrations
- EFK 13.8, 18.2, Sta. 3538250



OREIS spatial query tool (A), and sample segments extracted (1) - (2).

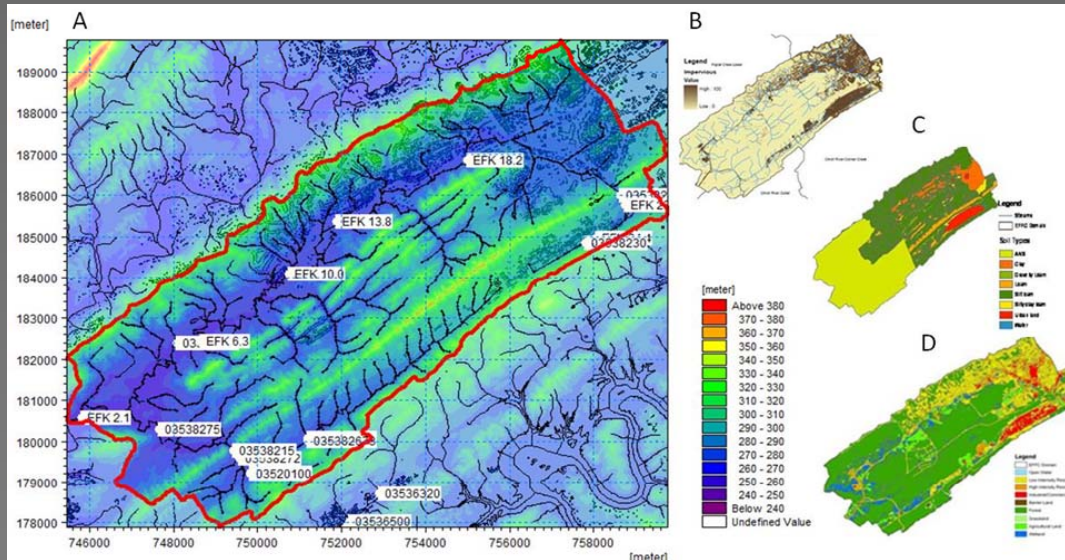
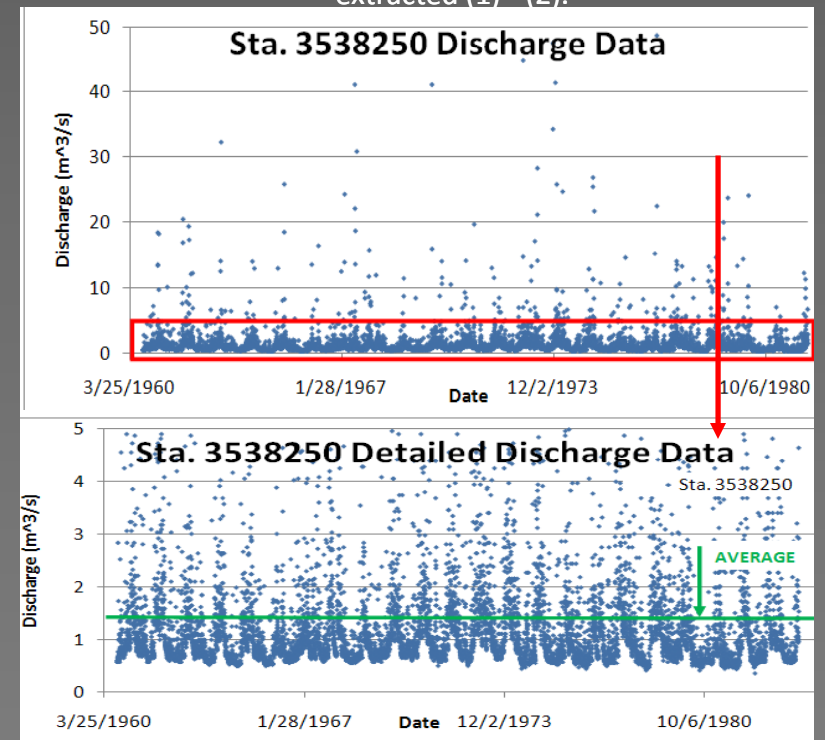
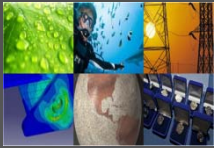


Image overlay of observation stations, streams, water bodies, and topography (A), imperviousness (B), soil type (C), and land use (D).



Data Extracted for Observation Sta. 3538250



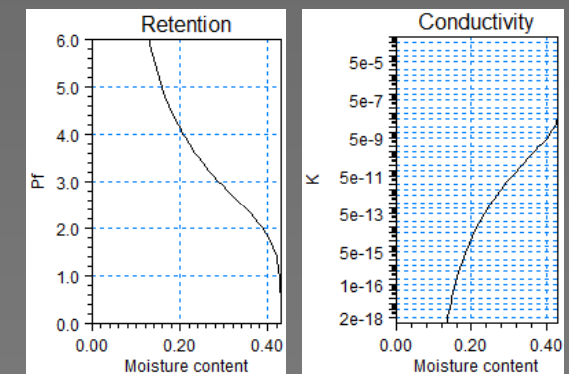
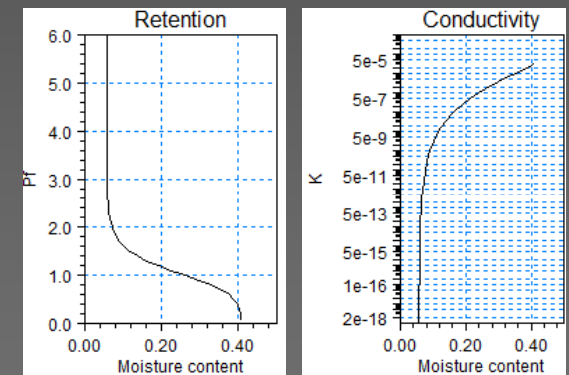
Model Updates

Hydraulic Conductivity Curve Parameters

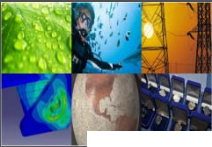
Upper Layer					Lower Layer				
K_s	α	n	Shape factor	m	K_s	α	n	Shape factor	m
4.05e-5	0.124	2.28	0.5	0.5614	1.95e-7	0.01	1.23	0.5	0.1869

Upper and lower aquifer retention curve parameters

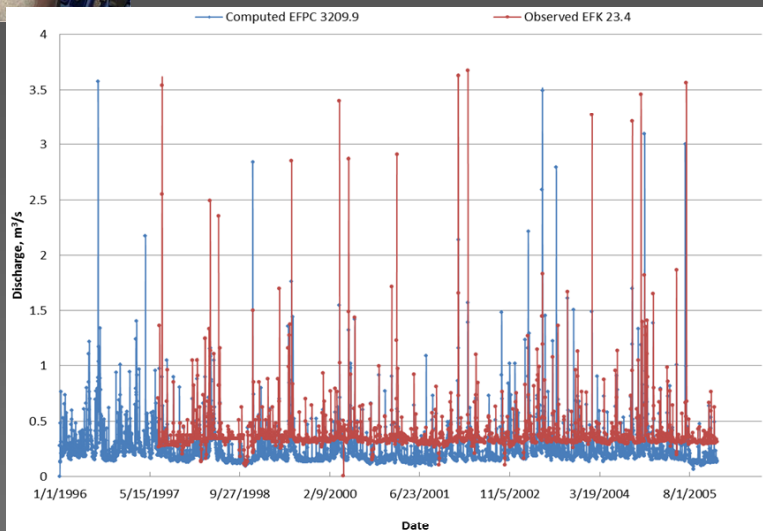
State Variables	Value	Constants	Value
Mercury	0.01 mg/l	Organic-carbon partitioning coefficient	50000 l/kg
Adsorbed mercury	0.1 mg/l	Desorption rate in water	1 day ⁻¹
Dissolved mercury in sediment pore water	0.1 g/m ²	Desorption rate in sediment	0.1 day ⁻¹
Adsorbed mercury in sediment	10 g/m ²	Fraction of organic carbon in SS	0.1
Suspended solids	50 mg/l	Fraction of organic carbon in sediment	0.2
Mass of sediment	10000 g/m ²	Thickness of water film	0.1 mm
Forcing		Mole weight of heavy metal	92 g/mole
Thickness computational grid layer	2 m	Density of dry sediment	250 kg/m ³ bulk
Total water depth	8 m	Porosity of sediment	0.8 m ³ H ₂ O / m ³ Bulk
Current speed	0.2 m/s	Settling velocity of SS	0.1 m/day



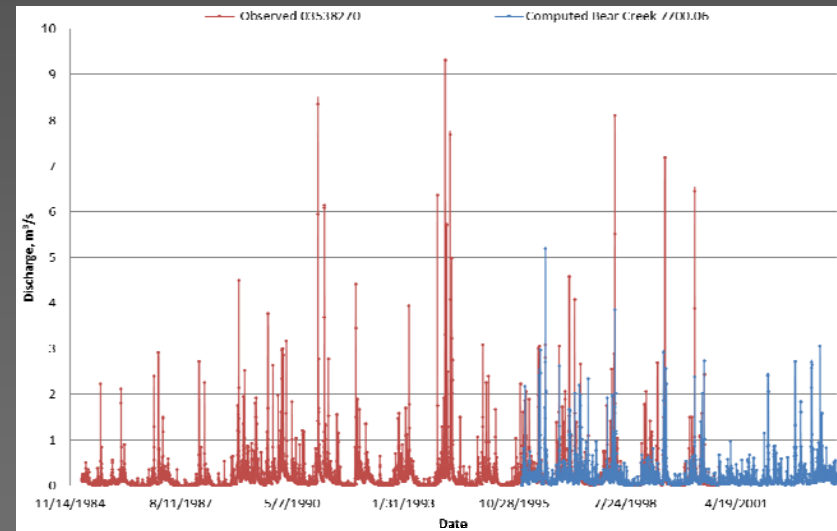
Retention & Hydraulic Conductivity Curves for Upper & Lower Aquifer layers



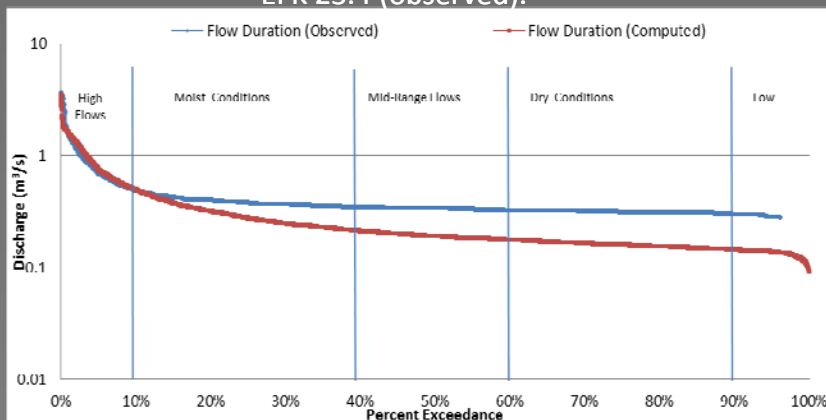
Results, Calibration, Sensitivity



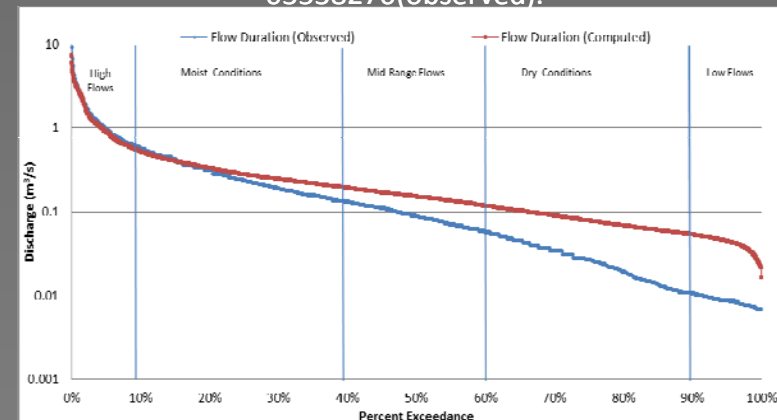
Comparison of discharges timeseries at EFPC 3209.9 (computed) and EFK 23.4 (observed).



Comparison of discharges timeseries at BC 7700.06 (computed) and 03538270 (observed).



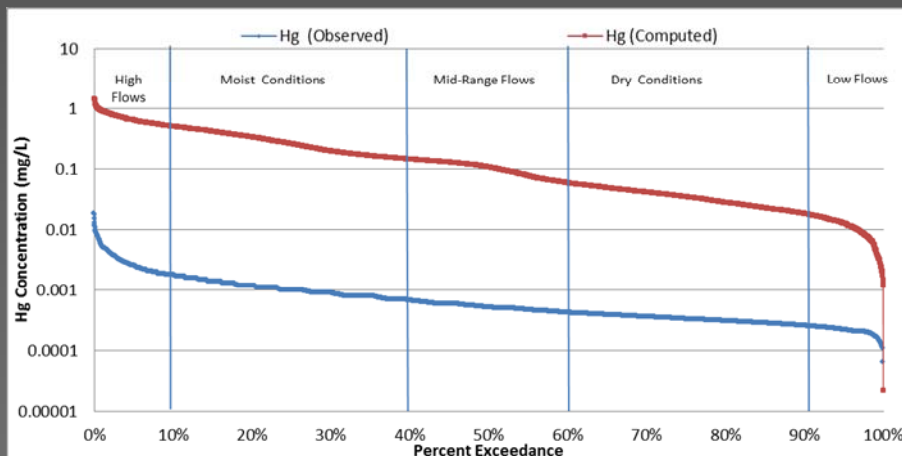
Comparison of flow duration curves for EFPC 3209.9 (computed) and EFK 23.4 (observed).



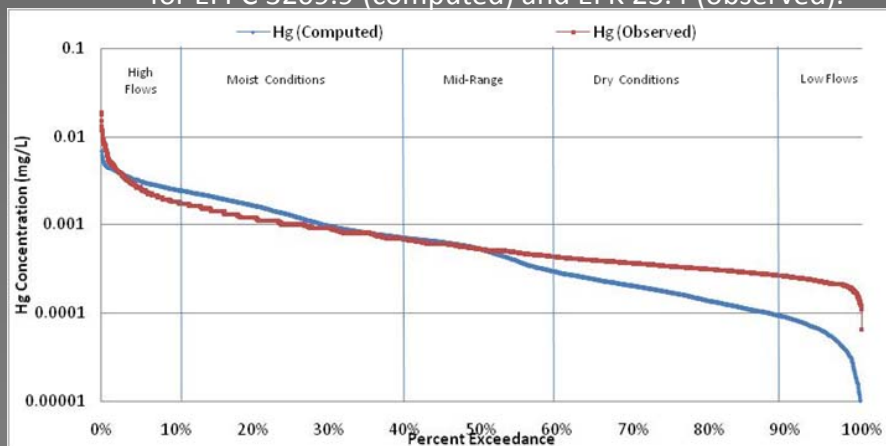
Comparison of flow duration curves for BC8728.87 (computed) and 03538273 (observed).



Results, Calibration, Sensitivity



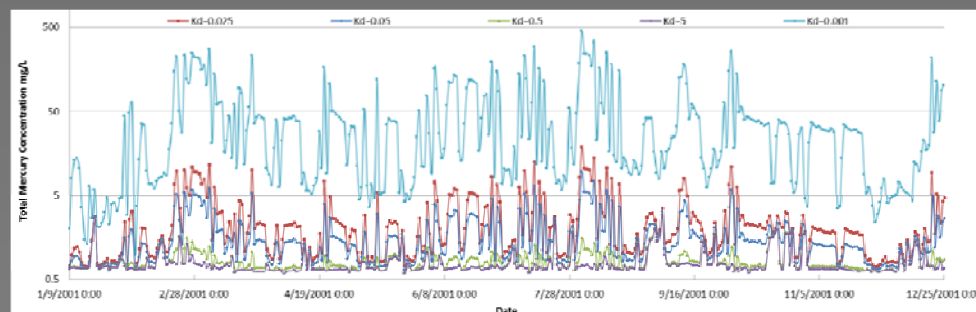
Comparison of pre-calibration Hg concentration probability exceedances for EFPC 3209.9 (computed) and EFK 23.4 (observed).



Comparison of post-calibration Hg concentration probability exceedances for EFPC 3209.9 (computed) and EFK 23.4 (observed).



Observed and computed TSS load and Hg concentration load for observed and computed Station 17.



Total Hg timeseries depicting sensitivity to organic partition coefficient (K_d) for various simulations.



Conferences

Waste Management Symposia (WMS) International Symposium on Persistent Toxic Substances

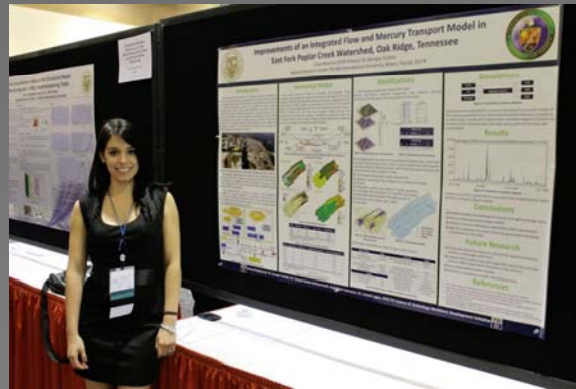
- Location: Phoenix, AZ
 - Time:
 - Spring of 2012
 - Spring of 2013
 - Outcome
 - 2 Student Poster
 - 1 Professional Presentation
 - 1 Published Paper
- Location: Miami, FL
 - Time:
 - Fall 2012
 - Outcome
 - 1 Professional Presentation
 - 1 Published Paper



Internship at Sullivan International, Inc.



DOE Fellows Class of 2011



WMS Poster Exhibition 2012



WMS 2013



Acknowledgements

THANK YOU!

DOE-EM

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