Improvements of an Integrated Flow and Mercury Transport Model in East Fork Poplar Creek Watershed, Oak Ridge, Tennessee

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Introduction

The environment in the vicinity of Y-12 National Security Complex (Y-12 NSC), Oak Ridge, TN has been contaminated by mercury due to nuclear processing activities during the 1950s. The contamination exists within the soil, shallow groundwater beneath and adjacent to former process buildings, storm sewers, drains, stream sediment, and surface water. A significant reduction in mercury concentrations has been proposed in the area's natural waters. In order to achieve a more effective clean up effort the Environment and Water Resources Group at Florida International University's (FIU) Applied Research Center (ARC) has been tasked with developing a model for the site with the ultimate aim of assessing the impact of selected remediation scenarios.

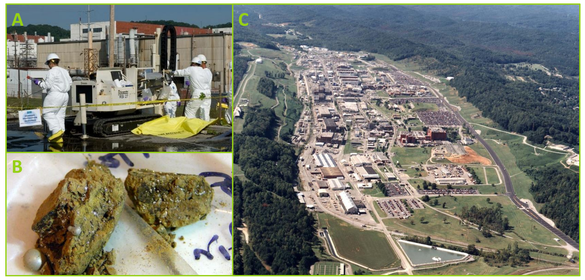

Figure 1: Soil sample collection at Y-12 (A), mercury contaminated soil (B), Y-12 NSC (C)

An integrated surface/subsurface model has been developed using the numerical model, MIKE, created by the Danish Hydraulic Institute (DHI). The purpose is to investigate the flow and transport of mercury in EFPC under the influence of a series of hydrologic events, to predict transport patterns within the watershed.

The conceptual model, summarized in Figure 2, was designed to consider the transport pathways of water-borne mercury from (i) stormwater and industrial wastewater outfalls, (ii) land surface and shallow groundwater, and (iii) streambed sediment to EFPC including outfalls, groundwater flow, and surface sheet flow.

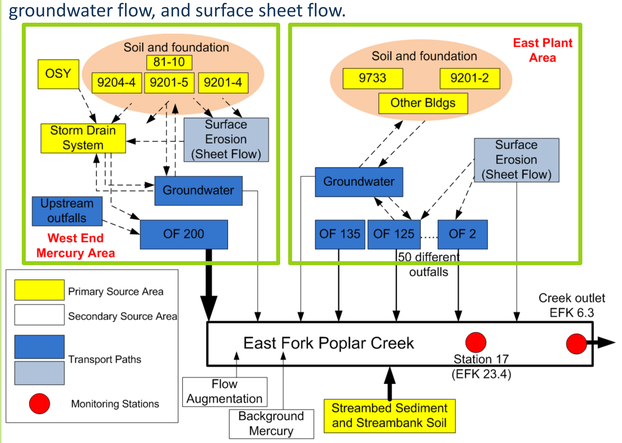

Figure 2: East Fork Poplar Creek Conceptual Model

Numerical Model

The model consists of MIKE 11, MIKESHE, and ECOLAB. These components are designed to couple the watershed hydrology with mercury transport. MIKESHE describes the hydrologic processes using physical laws (conservation of mass, energy, and momentum). It is 2-D in the overland phase, 1-D in the unsaturated, and 3-D in the saturated and vadose layers. MIKE 11 details the river flow and transport model through the hydrodynamic and advection modules. ECOLAB is an equations solver for the sedimentation and exchange of mercury within sediments, suspended particles, pore water, and dissolved mercury species.

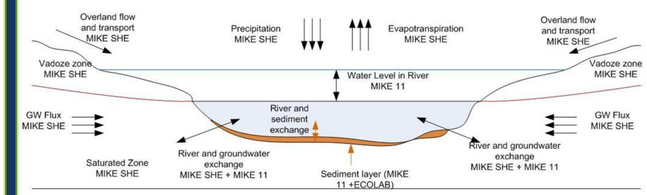

Figure 3: Numerical model diagram depicting MIKESHE, MIKE 11, ECOLAB, & their interaction phases

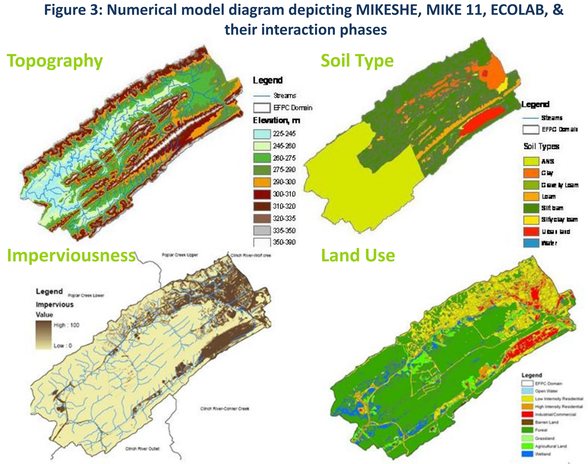

Figure 4: Typical Input Parameters

Layers	Sub-layers	Thickness, m	Lower level, m	Dispersivity, m
UZ1	2	0.1	-0.2	0.07[2]
UZ2	4	0.5	-2.2	0.07[2]
UZ3	8	5.0	-52.2	0.07[2]
Saturated moisture content = 0.35, Saturated hydraulic conductivity = 0.0086[1] m/d, Soil bulk density ρ_b = 1700[1] kg/m³ and Residual moisture content θ_r=0.15				
[1] UEFPC RI Report, 1998, Table E. 9.3 (DOE/OR/01-16411V 4&D2)				
[2] Tang et al., 2010				

Table 1: Unsaturated zone profile definition

Layers	Lower level, m	Thickness, m	Longitudinal Dispersivity, m	Transverse Dispersivity, m
SZ1	-3	3	0.07[2]	0.001
SZ2	-10	10	0.07	0.001
SZ3	-50	50	0.07	0.001
SZ4	-100	50	0.07	0.001
SZ5	-150	50	0.07	0.001
Primary effective porosity = 0.1[3&2], Secondary effective porosity = 0.05[3], Soil bulk density = 1700[1] Kg/m³, Specific yield = 0.2, Specific storage = 0.0001 1/m				
[1] UEFPC RI Report, 1998, Table E. 9.3 (DOE/OR/01-16411V 4&D2)			[3] Martin Marietta Systems, Inc., 1995	
[2] Tang et al., 2010			[4] Groundwater table contours are extracted from OREIS database	

Table 2: Saturated zone profile definition

Modifications

The following changes were made to the model:

- ❑ Van Genuchten's hydraulic conductivity and moisture content parameters for the upper and lower portions of the aquifer

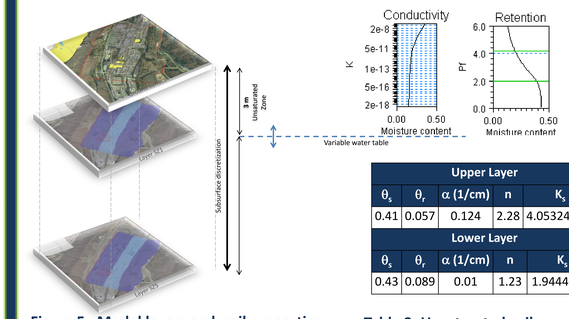

Figure 5: Model layers and soil properties

Upper Layer				
θ_s	θ_r	α (1/cm)	n	K_s
0.41	0.057	0.124	2.28	4.05324e-05
Lower Layer				
θ_s	θ_r	α (1/cm)	n	K_s
0.43	0.089	0.01	1.23	1.9444e-07

Table 3: Unsaturated soil properties

- ❑ Drainage system changed to routing based on gridded codes. A grid code map (level, time constant, drain code) is used to restrict the search area for the source-recipient reference system. Drain levels are used to calculate the amount and the code is used for routing.
- ❑ 25% of original Manning's number yield best fit.
- ❑ Hydraulic conductivity was changed from uniform to spatially distributed.
- ❑ Observation stations were added for water elevations, and discharge data (timeseries & shapefiles generated); existing stations were reviewed for quality assurance.
- ❑ Processed total mercury and methyl mercury data.

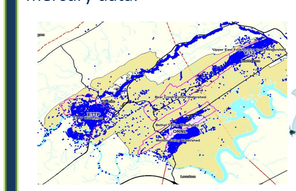

Figure 6: OREIS database used for data extraction

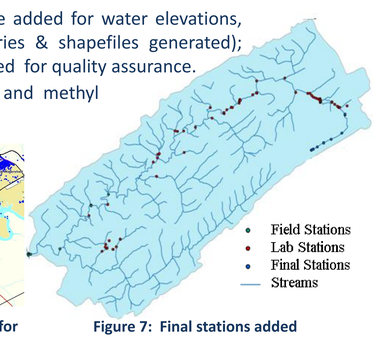

Figure 7: Final stations added

- ❑ ECOLAB incorporated as a MIKE 11 water quality module

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/m²	Desorption rate in sediment	0.1 day^{-1}
Adsorbed Mercury in sediment	10 g/m²	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/m²	Thickness of water film	0.1 mm
Forcing		Moleweight of heavy metal	92 g/mole
Thickness computational grid layer	2 m	Density of dry sediment	250 kg/m³ bulk
Total water depth	8 m	Porosity of sediment	0.8 m³ H_2O / m³ Bulk
Current Speed	0.2 m/s	Settling velocity of SS	0.1 m/day

Table 3: ECOLAB state variables, constants, and forcing

Simulations

Figure 8: Simulations summary diagram

Simulations were executed for a series of scenarios to assess the impact of the hydraulic parameters (i.e. horizontal and vertical hydraulic conductivity, and Manning's number were varied within accepted ranges) and determine the best fit with observed data. Drainage routing alternatives were also incorporated.

Results

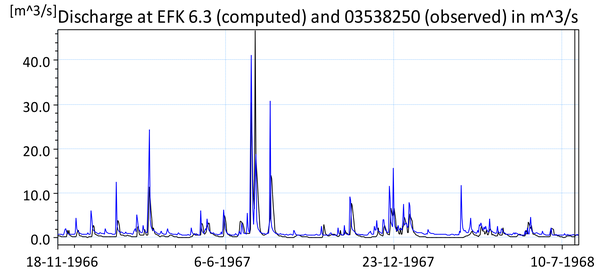

Figure 9: Simulations summary diagram

Computed results for station EFK 6.3 are within 2% of observed for station 0358250 as shown in Figure 9 above.

Conclusions

- ❑ Rainfall facilitates the exchange of mercury through hydrologic zones
- ❑ Mercury attenuates downstream of EFPC
- ❑ Sediment-mercury interactions significantly affect Hg transport
- ❑ High flow conditions re-suspend mercury particulates increasing concentration in the creek

Future Research

- ❑ Statistically determine hydraulic conductivity spatial distribution, porosity, and storage coefficients.
- ❑ Calibrate EFPC model using total suspended solids (TSS) and total mercury (TM) concentration timeseries at key stations.
- ❑ Incorporate sedimentation module
- ❑ Perform an uncertainty analysis and statistical tests

References

1. DOE, 2010. Remediation Effectiveness Report for the U.S. DOE ORR, DOE/OR/01-2437&D1.
2. Elsa Cabrejo, 2010, Mercury Interaction with Suspended Solids at the Upper East Fork Poplar Creek, Oak Ridge, TN, Florida International University, Environmental Eng. Dept., Master Thesis
3. FIU, 2010, Integrated Surface and Subsurface Mercury Transport Model of Y-12 National Security Complex, oak ridge, Tennessee
4. Stephanie Long, 2009, An Integrated Flow and Transport Model to Study the Impact of Mercury Remediation Strategies for East Fork Poplar Creek Watershed, Oak Ridge, Tennessee, Florida International University, Environmental Eng. Dept., Master Thesis

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