YEAR END TECHNICAL REPORT

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Remediation and Treatment Technology Development and Support

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PROJECT 3 OVERVIEW

Approximately 75 to 150 metric tons of elemental mercury, which was used in a lithium-isotope separation process for production of nuclear fusion weapons, were released into East Fork Poplar Creek (EFPC) watershed from the Y-12 National Security Complex (Y-12 NSC) in eastern Tennessee, USA. Under typical environmental conditions, elemental mercury is oxidized to mercuric ion which has a greater solubility and mobility in groundwater and surface water. The increased mobility of the mercuric ion results in elevated concentrations of total mercury in soil, surface water and groundwater. The mercuric ion has high affinity to many organic ligands and in the water column the majority of the mercuric ions are bound to suspended and colloidal particles. Storm events increase the turbulence and velocity of river flow and may result in additional mobilization and transport of mercury downstream EFPC.

In order to analyze the mercury cycle in the environment and to provide forecasting capabilities for the fate and transport of contamination within the watershed, an integrated surface and subsurface flow and transport model for the Y-12 NSC was developed. The model couples the hydrology of the watershed with mercury transport and provides a tool for analysis of changes of mercury load as function of changes in hydrology, including remediation scenarios which modify the hydrological cycle. The model couples the overland and subsurface flow module with the river flow and transport module. The model includes the main components of the hydrological cycle: groundwater flow (3D saturated and unsaturated), 2D overland flow, 1D flow in rivers, precipitation, and evapotranspiration. Furthermore, the model includes 57 outfalls along Upper East Fork Poplar Creek (UEFPC) which have been listed in the National Pollutant Discharge Elimination System (NPDES) permit from 2005. A sedimentation module was included to simulate the interactions between sediment particles, water and mercury species within EFPC.

The numerical model was calibrated for the period of 1996-2009 using recorded stream flow and mercury concentrations measured in groundwater, surface water and soil. The model was subsequently applied to evaluate the effect of nine remediation strategies/scenarios in the UEFPC region on reducing the mercury concentrations. For each remediation scenario, flow duration curves and mercury load duration curves were compared at Station 17 for the computed and recorded data. The remediation efficiency was determined by comparing the percent daily reduction of mercury discharges downstream of Station 17. The results of numerical simulations showed that exchange of mercury species between sediment, pore water, aqueous media and suspended solids significantly affects the mercury load detected at Station 17.

A series of laboratory studies were conducted to analyze the effect of various environmental factors (pH, pE) on methylation and demethylation processes in the water column. Experimental work was used to obtain critical mercury exchange parameters between pore water, colloidal and suspended particles, and streambed sediment, which were applied in the numerical model to study the effect of sediment transport on mercury mobilization.

For year 2010-2011, the model, which was developed for the Y-12 NSC, was extended to include the EFPC watershed and the creek between Y-12 NSC and Station EFK 6.4. The research focused on conducting additional simulations using the EFPC watershed model which extend the studies for Y-12 NSC. In addition, flow and transport studies were conducted for the Bear Creek watershed (a sub-watershed of the larger EFPC watershed). A geodatabase was also

developed as a strategy for supporting hydrological model data input by creating a centralized data storage system to store model parameters instead of a collection of data layers, which provides a more stable foundation for building GIS-based water resources applications.

TECHNICAL PROGRESS SUMMARY FOR FY10-FY11

During FY2008-FY2011, FIU developed integrated flow and transport models of the East Fork Poplar Creek (EFPC) and White Oak Creek (WOC) watersheds. The models were used to conduct numerical simulations of 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). A geodatabase was developed as a tool for supporting hydrological model input and output data. A centralized data storage system was created to support building of GIS-based hydrological and transport models.

The main objectives of the research conducted during FY10-FY11 were to (i) Extend the existing EFPC model by including sedimentation and water quality modules for the entire EFPC watershed; (ii) Perform numerical simulation of the fate and transport of mercury and relevant organics, (including PCE, TCE, 1,2-DCE, *cis*-1,2-DCE, and vinyl chloride) in the upstream EFPC watershed to predict plume migration and to provide information about the exceedances of concentrations from the risk-based and hazard-based concentration values; (iii) Conduct numerical simulations for the analysis of planned remediation scenarios and utilizing data generated for TMDL calculations; (iv) Use the hydrological flow and transport data and numerical software for performance assessment analysis of planned mercury disposal activities to conduct probabilistic risk analysis of the paradigm design of a proposed disposal cell at upper Bear Creek; (v) Provide laboratory data for critical mercury transformation and exchange processes for use in the existing hydrological models (i.e., methylation/demethylation, exchange of mercury species between soil, porewater and sediment); and (vi) Develop a geodatabase to support hydrological model development.

TASK 1: EFPC MODEL UPDATE, CALIBRATION AND UNCERTAINTY ANALYSIS

The 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. Details are provided in APPENDIX T1-001. 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 will be 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.

TASK 2: SIMULATION OF TMDL FOR THE ENTIRE EFPC

A report entitled "Mercury Interactions with Suspended Solids at the Upper East Fork Poplar Creek, Oak Ridge, TN" (APPENDIX T2-001) has been 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" (APPENDIX T2-002) and a poster entitled "Numerical Simulation of Mercury Fate and Transport in Upper East Fork Poplar Creek, Oak Ridge, TN" (APPENDIX T2-003), were presented in the poster session of the Waste Management Symposium 2011 in Phoenix, AZ and awarded best professional poster presentation and paper by the American Nuclear Society (ANS), as well as best poster in the environmental remediation track.

TASK 3: LABORATORY EXPERIMENTS FOR METHYLATION/DEMETHYLATION AND TRANSPORT PARAMETERS OF MERCURY

Experimental work was conducted 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) ,sea water). 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 doublespiked isotope $(^{199}Hg^{2+}$, Me²⁰¹Hg) 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 $(9.45 \times 10^{-3}$ E^{-1} m²) and low photomethylation rate $(3.90\times10^{-6} \text{ E}^{-1} \text{ m}^2)$ 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) 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.

TASK 4: GEODATABASE DEVELOPMENT FOR HYDROLOGICAL MODELING SUPPORT

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 stored in the geodatabase directly supports hydrological model 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; 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).

TASK 5: MODELING SUPPORT FOR NEW CERCLA DISPOSAL CELL AT ORR

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, ARC-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", which is included in (APPENDIX T5-001). 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, ARC-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" (See APPENDIX T5-002). 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.

TASK 6: STUDENT SUPPORT FOR MODELING OF GROUNDWATER FLOW AND TRANSPORT AT THE DOE SITE IN MOAB, UTAH

ARC-FIU has 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, the City of Moab and Arches National Park. (APPENDIX T6-001) 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 µg/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.

TASK 1: EFPC MODEL UPDATE, CALIBRATION AND UNCERTAINTY ANALYSIS - HYDROLOGICAL MODELING OF CONTAMINANT FATE AND TRANSPORT IN THE Y-12 NATIONAL SECURITY COMPLEX UPSTREAM OF EAST FORK POPLAR CREEK

INTRODUCTION

An integrated surface/subsurface numerical model has been developed by ARC-FIU in conjunction with P2S using DHI's MIKE suite of modeling products to simulate the groundwater flow, and 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 originated upstream of UEFPC in the Old Salvage Yard (OSY) and Building 81-10, which are both located in the West End Mercury Area (WEMA) of the Y-12 NSC. Details are summarized in APPENDIX T1-001. The model has been calibrated using subsurface flow and concentration records extracted from the OREIS database. The simulation results were used to calculate the revised risk levels (RLs) for the chemicals of concern (COCs) and serve as benchmarks 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.

RESULTS AND DISCUSSION

[Figure 1](#page-13-0) shows the sorbed point sources and PCE plume source in the OSY that were used in the model. The source dimensions were 50x50x10 feet for all cases except for mercury which was 50x50x2 feet. Separate sets of simulations were performed for half mass for all COCs (33x33x5 feet). Simulation results were then compared with risk-based and hazard based target concentration values (see [Table 1\)](#page-14-0).

Figure 1. Sorbed point sources and PCE plume source in Y-12 OSY.

Variations of dissolved PCE concentration in groundwater at points 1 and 2 (as shown in [Figure](#page-15-0) [2\)](#page-15-0) in the first $(0 - 3$ m depth) and second $(3 - 10$ m depth) layers of the saturated zone, were compared with the risk-based target concentrations.

Table 1. Simulation and Results Summary

Figure 2. Computed PCE concentrations downstream PCE sources and upstream EFPC

The figure (top left) at point 1 of the first layer of saturated zone $(SZ1, 0-3$ m depth), (top right) at point 2 of the first layer of saturated zone $(SZ1, 0-3$ m depth), (bottom left) at point 1 of the second layer of saturated zone $(SZ2, 3 - 10 \text{ m depth})$, (bottom right) at point 2 of the second layer of saturated zone $(SZ2, 3 - 10 \text{ m depth})$. Points which were used to for calculating PCE concentrations are shown in [Figure 1.](#page-13-0)

CONCLUSIONS AND PROPOSED WORK

Mercury in soil is not a potential groundwater contaminant exceeding industrial hazard levels. This is mainly due to the high soil-water partitioning coefficient associated with mercury species which are mostly adsorbed to soil particles.

PCE, 1,2 DCE, Cis-1,2 DCE, and VC are sources in soil within the RAB with potential to equal or exceed industrial groundwater hazard and risk concentration levels. [Table 1](#page-14-0) summarizes the maximum concentration values adjacent to the source area. Only VC concentration shows an exceedance from the risk-based target concentration value while the others are either below or equal to the risk or hazard levels.

VOC contaminants in soil and groundwater do not migrate to surface water and decay below industrial groundwater risk and hazard levels within approximately 20 years. Currently, the OREIS database and literature is being reviewed to define the VOC source characteristics and transport parameters more accurately.

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TASK 2: SIMULATION OF TMDL FOR THE ENTIRE EFPC - SEDIMENT TRANSPORT AND WATER QUALITY MODULE

INTRODUCTION

Recent field surveys have demonstrated that more than 85% of the mercury currently released to UEFPC is derived from stream sediments, bedrock, and floodplain soils through colloidal transport and/or diffusion from highly contaminated pore water. To address the impact of sediment transport on the water quality and transport of mercury in the UEFPC watershed, a water quality and sediment transport module was included in the MIKE hydrological model previously developed by ARC. The model was recalibrated using data from the OREIS database and field survey results. Uncertainty and sensitivity analyses were performed using the critical velocity, settling velocity, particle production rate, resuspension rate, and sediment-water carbon partitioning coefficient.

A report entitled "Mercury Interactions with Suspended Solids at the Upper East Fork Poplar Creek, Oak Ridge, TN" details the water quality modeling, calibration, and uncertainty analysis, and sensitivity analysis (APPENDIX T2-001). A scientific article entitled "Simulation of Flow and Mercury Transport in UEFPC, Oak Ridge, TN" (APPENDIX T2-002) and a poster entitled "Numerical Simulation of Mercury Fate and Transport in Upper East Fork Poplar Creek, Oak Ridge, TN" (APPENDIX T2-003) based on the extended watershed model, were submitted to the Waste Management Symposium 2011 in Phoenix, AZ. The article was awarded best professional poster presentation and paper by the American Nuclear Society (ANS) and best poster in the environmental remediation track.

RESULTS AND DISCUSSION

Numerical simulations have been performed for two cases: with and without sediment-mercury interactions. Computed mercury load duration curves at the integration point of the creek (Sta. 17) for the period of 2000-2009 were compared with the corresponding historical records for both cases in [Figure 3.](#page-17-0)

Figure 3. Mercury load duration curves at Sta. 17. (•) compared to simulations including mercurysediment interactions (—) and simulations without mercury-sediment interactions, (- - -) computed without considering mercury-sediment interactions

As shown in [Figure 3,](#page-17-0) sediment-mercury interactions significantly affect the concentration of mercury recorded at Sta. 17. Higher current velocity during wet seasons increases the shear stress on the highly contaminated streambed sediments, and resuspends more mercury-laden fine particulates (colloidal transport). The colloidal transport is determined by comparing the total suspended solids (TSS) and mercury loads to the flow probability exceedance curve at different flow conditions as shown in [Figure 4.](#page-18-0) The streambed pore water within the reach contains very high concentrations of dissolved mercury often exceeding 20 μ g/L (approximately 30 to 50 times of the concentration in overlying surface water); thus, dissolved mercury in sediment pore water contributes to the high mercury concentration in the creek water. As shown in [Figure 5,](#page-18-1) 75% of mercury concentration is in the form of suspended particulates, almost 10% is adsorbed from water to sediment particles and only 3% is diffused from pore water

Figure 4. Load duration curves at Sta. 17 based on flow probability exceedance.

Figure 5. Contribution of sediment transport processes in the concentration of aqueous mercury in water.

CONCLUSIONS AND PROPOSED WORK

The water quality simulations on UEFPC correlate with the observed mercury concentrations downstream of Sta. 17 [\(Figure 3\)](#page-17-0). Colloidal transport contributes to more than 85% of the total mercury flux leaving the UEFPC watershed [\(Figure 5\)](#page-18-1)

High flow conditions in the river increase the current velocity and bed shear stress, thus, intensifying the resuspension of mercury particulates which increases the concentration of mercury in the creek [\(Figure 4\)](#page-18-0).

Sensitivity analysis showed that colloidal transport is highly affected by the critical current velocity in the creek. The resuspension rate is the most influential parameter in generating local resuspension along the creek (peaks). In general, the TSS load increases when the resuspension rate and/or particle production rate increases, and when the settling velocity and/or the critical velocity decreases. Importance of sedimentation parameters in terms of colloidal transport sensitivity are as follows: critical current velocity > resuspension rate > particle production rate > settling velocity.

Currently, the water quality and sediment transport is being extended for the entire EFPC watershed. Methylation/demethylation and photosynthesis processes will be incorporated into the water quality module for better prediction of fate and transport of mercury along EFPC

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TASK 3: LABORATORY EXPERIMENTS FOR METHYLATION/DEMETHYLATION AND TRANSPORT PARAMETERS OF MERCURY -

COMPARISON OF MEHG PHOTODEMETHYLATION IN EAST FORK POPLAR CREEK WITH TROPICAL AQUATIC ECOSYSTEMS

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) ,sea water). 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.

HG METHYLATION AND DEMETHYLATION IN VARIOUS MATRICES (WATER, SEDIMENT, FLOC, AND PERIPHYTON) IN EAST FORK POPLAR CREEK AND SELECTEDAQUATIC ECOSYSTEMS

Laboratory double-spiked isotope (199Hg^{2+}) , Me²⁰¹Hg) 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 $(9.45 \times 10^{-3} \text{ E}^{-1} \text{ m}^2)$ and low photomethylation rate $(3.90 \times 10^{-6} \text{ E}^{-1} \text{ m}^2)$ were observed in natural water, indicating the importance of photodemethylation in decreasing the concentration of MeHg in water. Significant methylation of spiked 199 Hg²⁺ (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) 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.

TASK 4: GEODATABASE DEVELOPMENT FOR HYDROLOGICAL MODELING SUPPORT

INTRODUCTION

During fiscal years 2007-2010, FIU-ARC developed an integrated watershed model for Y-12 NSC, White Oak Creek (WOC), and East Fork Poplar Creek (EFPC). Each model was used to model hydrology and contaminant fate and transport within each watershed. These models include overland, stream and groundwater flows in the variable and fully saturated zones, and the complex biological and chemical dynamics of mercury species. They provide insight into the fluxes of water and concentration of mercury to offer a better understanding mercury fate and transport. More than a hundred simulations were completed to calibrate the models, to derive model uncertainties, and to provide analysis of remediation scenarios. The work resulted in hundreds of gigabytes of model input data and simulation results. An advanced spatial data structure was needed to address the management, processing, and analysis of the numerical and visual inputs and results.

A geographic information system (GIS) database (or geodatabase) was developed to support the hydrological model development by creating a centralized data storage system to for model parameters instead of a collection of data layers, which provides a more stable foundation for building GIS-based water resources applications.

The ORR Geodatabase [\(Figure 6\)](#page-23-0) developed by FIU-ARC is a multiuser relational database management system (RDBMS) built upon a Microsoft SQL Server platform using Environmental Systems Research Institute (ESRI) ArcSDE technology. The system was deployed on an advanced Windows server with the latest technology and hardware. ARC-FIU put together a custom server that far exceeds ESRI's ArcGIS Server 10 minimum requirements with respect to memory, CPU speed, security and backup capabilities. The Microsoft Windows 2008 R2 Server Standard, Enterprise (64-bit) operating system was paired with MS Advanced SQL Server 2008, and the Microsoft .NET framework was installed with ArcGIS Server, which provides a user interface that facilitates data access, database connectivity, cryptography, web application development, numeric algorithms, and network communications. ArcSDE and/or ArcGIS Server provide a gateway between GIS clients and the RDBMS, which in this case, is SQL Server. User accounts which facilitate the direct SQL connection from FIU-ARC's ArcGIS Desktop 10 clients to the ArcGIS Server and the ORR Geodatabase.

Figure 6. The Oak Ridge Reservation Geodatabase system architecture.

The integrated database makes data more accessible to project team members for editing and data management. The hydrological models developed at ARC use standard Geographic Information systems (GIS) data derived from readily available sources such as the Oak Ridge Environmental Information System (OREIS), USGS, NRCS STATSGO or SSURGO soil database, and the U.S. EPA MRLC or NALC land cover database.

The multiuser functionality of database system is its most significant feature as it facilitates simultaneous editing of the geographic data utilized and generated during hydrological model development and model simulation. A mechanism referred to as "versioning" records all the database changes so GIS transactions can be stored in the database and the metadata for each "version" can be used to isolate multiple edit sessions, share replicas, synchronize contents across multiple databases, perform automatic archiving, and support historical queries.

The ORR Geodatabase is based on the ArcHydro and ArcGIS Base Map data models. Arc Hydro is a geodatabase and a set of accompanying tools designed to support water resources applications within the ArcGIS environment. These models were used as templates as there were many input data types in common with the ORR Geodatabase. Modifications were made for

project specific input parameters. The information stored in the ORR Geodatabase directly supports model development and calibration.

Development of an ArcSDE-based hydrogeological GIS database facilitates centralized storage, backup, accessibility, organization and management of observed model data inputs, and computed simulation data into a structured, coherent and logical computer-supported system. The hydrologic geodatabase model used in this project possesses a structure that enables linkage with scalable hydrologic modeling tools and applications to model hydrologic systems and in this case, test the potential impacts of various D&D scenarios on the ORR watersheds. The ArcSDE geodatabase can be used to automate and simplify the process of calling stored GIS and timeseries data required to populate the hydrologic modeling tools with required parameters. This serves as a powerful tool for contaminant flow and transport analyses that require large amounts of high-quality spatial and temporal data.

RESULTS AND DISCUSSION

The following describes the methodology employed in development of the ORR Geodatabase.

Subtask 1: Identification and compilation of the data required to be managed with a GIS

This included compilation of vector and raster map products as well as timeseries tabular data either downloaded or generated during model simulation. Associated metadata was also collected to be stored in the geodatabase. All data files were archived within system folders organized according to the various data inputs required for model development.

Subtask 2: Representation of data into one or more geographic datasets based on model requirements

Feature and raster datasets were defined based on some of the key aspects of each data theme. Map use (i.e. how each dataset will be used—for editing, GIS and hydrological modeling and analysis, mapping and 3D display), data sources, need for integration with other key layers, spatial relationships and data integrity rules were also specified. Discrete features were generally represented as feature classes of points, lines, and polygons, however, advanced data types such as topologies, networks, and terrains were also represented in the geodatabase. Specifications such as whether the data is an original downloaded file, a file modified for model development or a file generated from running model simulations were also defined. File modification was necessary for example when modeling an entire watershed vs. modeling a small subdomain of the watershed which required generalization of feature representations for use at smaller scales.

Subtask 3: Geodatabase design

The geodatabase elements desired for each data theme were defined and the geodatabase designed based on existing designs from the ArcGIS data models which were studied for ideas, patterns and best practices.

Subtask 4: Assignment of responsibilities for building and maintaining each data layer

This determined who was assigned the data maintenance work, as well as how data import, conversion, transformation, and export to all project team members and stakeholders was to be carried out. Editing workflows which defined editing procedures and integrity rules were also specified.

Subtask 5: Building a working prototype

This involved testing, review and refinement of the geodatabase design. A sample geodatabase was first generated using a personal geodatabase, and samples of each data type required for model development or generated from the numerical simulations were uploaded to ensure that there were no data incompatibility issues before populating the final geodatabase. Once a working schema was established, data was loaded into the ArcSDE geodatabase.

Subtask 6: Documentation of geodatabase design

The Geodatabase Diagrammer tool for ArcGIS 10 was used to generate a schema diagram in MS Visio of the ORR geodatabase as seen in [Figure 7](#page-27-0) below. The ArcGIS geodatabase is an XMLbased GIS data exchange system which facilitates the export and import of preconfigured data as XML files which contains both the data definition and the data itself. The data definition is what provides the basic information for creating the 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.

CONCLUSIONS AND PROPOSED WORK

As FIU-ARC continues to conduct model simulations to support the remediation activity at ORR, there will be an ongoing need for update of the geodatabase and utilization of the integrated GIS-hydrological modeling system developed. During FY2011, the database will continue to be populated with simulation data derived from Tasks 1, 2, 3 and 6. Work scope will involve (1) Importing simulation input files into the database along with versioning; (2) Population of the database with simulation outputs from the Y-12 NSC, WOC and EFPC models; and (3) Set-up of the database to provide remote access to input and output files.

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TASK 5: MODELING SUPPORT FOR NEW CERCLA DISPOSAL CELL AT ORR

SUBTASK 1: IDENTIFICATION AND SCREENING OF DISPOSAL CELL CANDIDATE SITES AT ORR , OAK RIDGE, TN

Introduction

Oak Ridge Reservation (ORR) located in the city of Oak Ridge, Tennessee, is a nuclear materials management facility, built during World War II, as part of the Manhattan Project for the largescale production of fissionable material to be used in the production of nuclear weapons. The three main ORR facilities, Y-12 National Security Complex (Y-12 NSC), the East Tennessee Technology Park (ETTP, which is called K-25), and Oak Ridge National Laboratory (ORNL, which is called X-10) were constructed in 1943. The Y-12 NSC, an 811-acre facility located in Bear Creek Valley (BCV), is the world's first large-scale uranium enrichment operation, separating fissionable isotopes of uranium through an electromagnetic process. The 1,500-acre K-25 was built in the northwest part of ORR as the production and development facility for uranium enrichment using the gaseous diffusion process. X-10, a 2,900-acre facility located in Bethel Valley, housed the world's second large-scale nuclear reactor and served as a research and development center to develop nuclear weapon production technologies. ORR facilities and the related watersheds are shown in [Figure 8.](#page-28-0)

Figure 8. Oak Ridge Reservation facilities (OREIS database) with watersheds outlined in purple.

During and after the operation of the Y-12 NSC and K-25 facilities spills and leaks from process buildings contaminated soil and rock, subsurface drainage pathways, shallow groundwater, and surface water with approximately 2000 metric tons of mercury. Furthermore, waste from ORR operations has been temporarily disposed of in various types of trenches, pits, and settling ponds

contributing to the release of contaminants in Melton Valley, Bethel Valley, Bear Creek Valley, Chestnut Ridge, the White Wing Scrap Yard, and ETTP for several decades.

ORR's storage and disposal facilities were not capable of accommodating the expected cleanup waste volumes. In 1999, following a feasibility study and evaluation of disposal options ([**Error! eference source not found.**] and [**Error! Reference source not found.**]) DOE decided to consolidate the waste into an "on-site" centralized disposal facility in accordance with the CERCLA 40 Code of Federal Regulations 300.5 [**Error! Reference source not found.**]. It is ssumed that a CERCLA on-site action would also be supported under CERCLA Section 104(d)4, which allows the U.S. Environmental Protection Agency (EPA) to consider multiple facilities as one when "the facilities are reasonably related on the basis of geography or on the basis of the threat or potential threat to the public health or welfare or the environment." DOE predicted that site cleanup activities would generate between 223,000 yd^3 (170,500 m³) and 1.1 million yd^3 $(850,000 \text{ m}^3)$ of CERCLA waste including low-level radioactive waste (LLW), hazardous waste as defined under the Resource Conservation and Recovery Act of 1976 (RCRA), polychlorinated biphenyls (PCBs) as defined under the Toxic Substances Control Act of 1976 (TSCA), and mixed waste consisting of combinations of these waste types [**Error! Reference source not found.**].

East Bear Creek Valley was selected for the new disposal facility following the 1998 feasibility and evaluation study of 1998 [**Error! Reference source not found.**] and Record of Decision ROD) of 1999 [**Error! Reference source not found.**]. The ROD called for the design, construction, operation, and closure of an on-site earthen disposal cell and its supporting facilities in 1999. The new Environmental Management Waste Management Facility (EMWMF) has been actively accepting ORR CERCLA waste in compliance with the approved EMWMF waste acceptance criteria (WAC) since May 2002. Typical waste placed in the facility originates from contaminated soils, dismantled buildings, and scrap piles. The EMWMF is a 120-acre site and currently contains four cells totaling the size of almost 20 football fields. Cells 1 and 2, as shown in [Figure 9,](#page-30-0) were initially constructed and went into operation in 2002 with a disposal capacity of $400,000$ yd³. Cells 3 and 4 [\(Figure 9\)](#page-30-0) were completed in 2005, increasing the total disposal capacity to 1,200,000 yd^3 . Cell 5 is currently under construction and will bring the disposal capacity to $1,650,000$ yd³. Current waste generation forecasts indicate that the capacity of cells 1-5 may be exhausted by approximately 2014-2015. While the ROD does not explicitly limit the maximum volume of waste to be disposed of at the EMWMF, the evaluation of alternatives in the feasibility study considered a range of waste volume estimates that could require a total disposal capacity up to approximately 1.7 million yd^3 . The proposed action under the Environmental Science Division (ESD) is the expansion of the EMWMF to a design capacity of approximately 2.2 million yd^3 through the construction of an additional disposal cell, designated Cell 6. [Figure 9](#page-30-0) includes the proposed Cell 6.

Additional CERCLA waste disposal capacity will be needed sooner than originally planned due to acceleration of the schedule and increase in the scope of cleanup activities at ORR facilities from the previous baseline. In addition, the Integrated Facility Disposition Program (IFDP) currently undergoing conceptual design will generate significant additional waste volume. The total volume of wastes generated from the CERCLA program at the ORR, including the IFDP, is estimated to exceed the capacity of the EMWMF, even with the additional capacity provided by

this ESD. However, the proposed expansion of EMWMF will allow adequate time for the evaluation of additional disposal capacity to meet longer-term requirements for future waste 1999 ROD [**Error! Reference source not found.**].

Figure 9. Aerial photo of EMWMF and disposal cells.

A preferred site for the near-future extra CERCLA waste has not been selected. Development and analysis of the on-site disposal options requires evaluation of four final candidate sites - East Bear Creek Valley (EMWMF expansion), West Bear Creek, White Wing Scrap Yard, and Chestnut Ridge. A comparative analysis of four alternative sites in terms of geologic and hydrologic characteristics and differences was completed with the results shown in [Table 2](#page-31-0) (more detailed view in APPENDIX T5-001). The subjective risks from candidate disposal sites were compared to the EMWMF and assigned a risk rating with respect to their hydrologic characteristics. The parameters were subdivided into saturated zone, unsaturated zone, surface water and siting criteria. As a result, the Chestnut Ridge Paradigm was selected from the three candidate sites

Table 2. Parametric analysis of relative risk from new candidate sites compared to that from EMWMF

1 is equivale
2 is better
3 is superior N/A is not available
TBD is to be determin

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SUBTASK 2: PERFORMANCE CHARACTERISTICS OF SELECTED WASTE IMMOBILIZATION TECHNOLOGIES

Introduction

According to the Remedial Investigation/Feasibility Study (RI/FS) for the Disposal of Oak Ridge Reservation Waste (DOE, 1998), the existing storage and disposal facilities at Oak Ridge Reservation (ORR) up to the late 1990's would be incapable of accommodating the cleanup waste volumes expected to be generated as a result of the 1980 CERCLA mandate. As such, the U.S. DOE identified several locations on-site ORR to serve as disposal facilities. Several issues have arisen, however, surrounding the potential impact of consolidation of various waste types into centralized locations and has sparked the need for further research into effective long-term and low-cost waste disposal methods. ARC-FIU has therefore 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 (See APPENDIX T5-002). 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 could be applied. The best available technologies for hazardous debris treatment including extraction, destruction and immobilization methods were therefore also provided in the report.

The Environmental Management Waste Management Facility (EMWMF) is a disposal facility located in East Bear Creek Valley designed for cleanup of waste from the nuclear material management facility of ORR in Tennessee. Typical waste at EMWMF includes contaminated soils, dismantled buildings, and scrap piles. The site contains four cells, Cells 1 and 2 having a disposal capacity of 400,000 yd³, and Cells 3 and 4 a total disposal capacity of 1,200,000 yd³. A fifth cell is under construction and will add to the current disposal capacity, bringing it to a total of 1,650,000 yd^3 , which according to waste generation forecasts, may potentially be exhausted by 2014-2015.

Figure 10. Aerial photo of EMWMF and the disposal cells.

Chemical tests of the leachate collection system of EMWMF have reported uranium and other metals that are a potential risk for groundwater contamination. Additionally, DOE has banned recycling of radioactive metals; therefore, large amounts of debris-containing steel and copper are being thrown into the waste disposal cell. 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.

In accordance with the EPA and RCRA requirements, all contaminant concentrations must be reduced to acceptable levels (i.e. below maximum contaminant levels or MCLs) by using the most effective technologies. The U.S. DOE has therefore proposed a long-term project to immobilize radioactive and other heavy metals from the collection system, by converting them to chemically stable forms which will reduce or eliminate their concentration in the leachate.

Results and Discussion

Chemical Composition of EMWMF Disposal Cell Leachate

Leachate can contain both dissolved and suspended material, and its composition varies widely depending on the age of the landfill and the type of waste. The main mechanism by which a leachate is generated is precipitation which percolates through waste deposited in a landfill. Once in contact with decomposing solid waste, the percolating water becomes contaminated and flows out of the waste material as leachate. Additional leachate volume is produced during the decomposition of carbonaceous material producing a wide range of other materials including methane, carbon dioxide and a complex mixture of organic acids, aldehydes, alcohols and simple sugars. The leachate and run-off from EMWMF contains a diverse range of chemicals (e.g. uranium, iron, copper, potassium, boron, and others) that might interact among them modifying the chemistry of the site. [Table 3](#page-35-0) summarizes the concentration of selected radioactive contaminants.

	Contaminant Concentration in Runoff (pCi/L)	Concentration in Leachate (pCi/L)*
^{137}Cs	$0.9 - 1.2$	$0.5 - 3.0$
99Tc	$1.0 - 2.2 \times 10^3$	$0.23 - 1.23 \times 10^3$
$\rm{^3H}$	$0.87 - 1.8 \times 10^3$	$0.56 - 2.57 \times 10^3$
^{90}Sr	$3.8 - 6.1 \times 10^{1}$	$0.3 - 2.4 \times 10^{1}$
36 _{Cl}	$1.36 - 3.0x10^2$	$0.9 - 7.6x101$
233 U and 234 U	$2.5 - 5.3 \times 10^2$	$0.08 - 1.64 \times 10^{2}$
235 U and 236 U	$1.2 - 4.4 \times 10^{1}$	$1 - 2 \times 10^{0}$
238 U	$3.5 - 7.5 \times 10^{2}$	$0.09 - 1.65 \times 10^{2}$
^{14}C	$0.33 - 1.0x10^2$	$7.7 - 10$

Table 3. Concentration of Major Contaminants in EMWMF Leachate and Run-Off

The concentration of the contaminants present in the EMWMF leachate shall meet the maximum contaminant levels (MCLs) specified for those chemicals. Some of these values are listed below in [Table 4.](#page-35-1)

Mercury (inorganic) 2 Chromium (total) 100

Uranium Immobilization Technologies

Uranium immobilization technologies include various chemical and physical processes including: (i) uranium precipitation using zero-valent iron, compounds of divalent iron, limestone, lime (CaO), or other calcium carbonates, (ii) surface complexation using permeable reactive barriers (PRBs) including hydroxyapatite (HAP) and Apatite II™, and barriers of iron and other zero-valent metals, (iii) conversion to insoluble minerals such as carnotite [a potassium uranium vanadate mineral, $K_2(UO_2)_2(VO_4)_2$ which is immobile, (iv) pulverized concrete barriers, (v) prevention of high alkalinity wastes being placed over uranium-bearing organic-rich soils (e.g., cement-stabilized wastes), (vi) bioremediation of uranium which includes direct or indirect reduction of U(VI) to U(IV), biofilms-sulfate-reducing bacteria (SRB), and dissimilatory iron-reducing bacteria (DIRB)[.Figure 11](#page-36-0) illustrates some of the most effective and available technologies to immobilize uranium.

Figure 11. Uranium immobilization technologies.

Chemical precipitation is a technique that induces the formation of a separable solid substance from a solution, either by converting the substance into an insoluble form or by changing the composition of the solvent to diminish the solubility of the substance in it. Theprocess depends greatly upon pH. Surface complexation involves the formation of a complex metal by a coordinate bond between a metal ion and an anion. The product, being more soluble, decreases the opportunity for adsorption or precipitation. This term is also used for describing inorganic contaminant adsorption in aqueous environments. Impermeable barriers are used to prevent the flow of contaminants from a system.

Selection of the appropriate technology is dependent on the uranium geochemistry as well as site-specific environmental conditions. Levels of dissolved uranium in groundwater systems depend on: (a)Content and leachability of uranium in sediments, (b) proximity of water to the uranium source, (c) hydraulic isolation of the water, (d) climatic effects and seasonal variability, (e) pH and Eh of the water as uranium is immobilized under reducing conditions and mobilized under oxidizing conditions, (f) concentration of substances that may form complexes or precipitate insoluble uranium minerals such as carbonate, phosphate, vanadate, fluoride, sulfate, silicate, calcium and potassium, and (g) presence of highly sorptive materials (e.g., organic matter, or Fe/Mn/Ti oxyhydroxides)

Interaction of Iron with Uranium and Other Metals Present In the Disposal Cell

Uranium (IV) is predominant under reducing conditions and has a very low solubility, while uranium (VI) is predominant under oxidizing conditions and has moderate solubility. Under oxidizing conditions in an aqueous environment, uranium (VI) exists as the linear uranyl dioxide ion (UO_2^{2+2}) as well as a multitude of mononuclear (UO_2OH^+) and polynuclear $(UO_2(OH)_2)$ hydrolysis species. Redox conditions in the environment have a very substantial effect on the mobility of uranium. [Figure 12](#page-37-0) illustrates the pe-pH diagram for the $U-O_2-CO_2-H_2O$ system. The migration of uranium is increased in the presence of mobile colloids and in aqueous phase. Uranium becomes immobile during the formation of uranium precipitates and adsorption to stationary solids.

Figure 12. pe-pH diagram for the U-O2-CO2-H20 system.

Elemental iron (Fe^0) , which is commonly used in permeable reactive barriers, can immobilize uranium by the reduction of uranium (VI) to insoluble uranium (IV)(Fiedor, J. N.; Bostick, W. D.; Jarabek, R. F.; Farrel, J., 1998). Zero-valent iron serves as a reducing agent, resulting in reductive precipitation of uranium to its tetra valent state. The corrosion products that are formed on the surface of Fe^0 serve as adsorption agents for uranium (VI) complexes (Wang, et al., 2005). The dominant removal mechanism of uranium by $Fe⁰$ is dependent on environmental conditions. Under oxygenated conditions, the dominant removal mechanism of uranium is adsorption of U (VI) complexes to the $Fe⁰$ corrosion products, while under deoxygenated conditions, the dominant removal mechanism is reductive precipitation. However, even under deoxygenated conditions the adsorption can take place and account for partial removal of uranium (Fiedor et al., 1998).

Apatite II™ Permeable Reactive Barrier

Apatite II™ is the patented name (PIMS NW, Inc.) for a series of reactive minerals to stabilize metals, such as Pb, U, Cd, Zn, Cu and Al, by binding them into new phosphate minerals (metalapatitephases such as autunite) with very low solubility that are stable over geologic time(Wright, et al., 2004). Its nominal composition is $Ca_{10-x}Na_x(PO_4)_{6-x}(CO_3)_x(OH)_2$ where $x < 1$. Most metals in solution will be immobilized on the apatite mineral by precipitation (U, Pb, Pu, Lanthanides), co-precipitation (transition metals) or by surface sorption (most metals).

Stabilizing mechanisms of Apatite II™ include precipitation, pH buffering, chemisorption, and biological reduction. Apatite II™ reacts in acid media releasing phosphate and increasing pH up to 6.5 to 7. The low but sufficient concentration of $PO₄³$ in solution (about 100 ppb $PO₄³$ or less resulting in no phosphate loading or eutrophication, particularly important in ecosystem restoration and maintenance) exceeds the solubility of the metal-apatite phase allowing the rapid precipitation of phases such as Pb-pyromorphite or U-autunite. The excellent long-term stability comes from the extremely low solubility products (K_{sp}) of the resultant metal-apatites $(K_{sp} = 10^{-7})$ ⁴⁹ for autunite). Along with its thermodynamic stability, high adsorption capacity and the rapid kinetics of the metal-phosphate precipitation, it ensures immobilization of metals in the face of most transport mechanisms.

Uranium Precipitation Using Carnotite

Uranium (VI) can be reduced and converted to carnotite by adding potassium metavanadate $(KVO₃)$ to an aqueous medium and forming dissoluble carnotite $[K_2(UO_2)_2(VO_4)_2]$. Under oxidizing conditions and pH 6, small quantities of V^{5+} (<2 μ M) and \overrightarrow{K} (<2 mM) precipitate U(VI) and decrease dissolved uranium concentrations below maximum contaminant level (0.13 μ M).

Pulverized Concrete Barrier

Typical waste placed in the EMWMF originates from contaminated soils, dismantled buildings, and scrap piles. Large voids or spaces often result from the disposal of contaminated building debris in the landfill. Instead of using clean soil as filler, the use of pulverized demolished concrete has been proposed to reduce the empty volume. In evaluating this alternative, however, it is important to consider the possible interactions between the pulverized debris and the rest of the waste. The pulverized material is mainly composed by steel-reinforced concrete, thus a considerable amount of iron would be incorporated into the landfill. Cured concrete could contain up to 2% of unreached calcium oxide (quick lime). Once the debris has been pulverized, the potential exists for the calcium oxide to be released and interact with other hazardous waste in the landfill, modifying the conditions within the system and potentially disrupting the chemical equilibrium. One of the major concerns in the disposal cell is the possibility of chemical reactions causing the mobilization of uranium and other hazardous wastes. Introduction of any contaminated materials may alter the landfill conditions such as pH, conductivity,

toxicity, reactivity, corrosivity, or mobility in a manner that can be either detrimental or beneficial. According to Coleman et al. 2005, pulverized concrete (made up primarily of hydrated Portland cement) may be effective in the immobilization of heavy metals from aqueous solutions due to its high pH and ion exchange/sorption capacity. In their study, crushed concrete fractions of approximately 1–2 mm in diameter [made up of mature (i.e., \geq 95% hydrated) Portland cement paste] were effective in removal of Cu^{2+} (35 mg g⁻¹), Zn²⁺ (33 mg g⁻¹) and Pb²⁺ (37 mg g^{-1}) from metal nitrate solutions. Pulverization of concrete-based demolition waste produces a large volume of irregularly sized aggregate fractions which can potentially increase the availability of reactive surface area of any unhydrated CaO (lime) that may have been "trapped" within aggregate sand grains or disconnected pores. The extent of reactivity, however, is dependent on the final particle size distribution of the pulverized concrete.

COD Impact of Disposing Iron and Copper

DOE has banned recycling of radioactive metals significantly increasing the amount of steel and copper being thrown into the waste disposal cell. Zero-valent iron is oxidized to Fe₂O₃ (Fe⁺³) which is very insoluble even in high pH conditions. In the acidic environment of disposed wastes, Fe⁺³ is reduced to Fe⁺² and its solubility increases. The reduced iron (Fe⁺²) is more likely to mobilize through the landfill to the creek and become oxidized. This puts a COD load in a stream and creates iron deposition $[Fe(OH)₃]$ and a high likelihood of anaerobic fungus generation on the stream bed.

Debris Treatment Technologies

The land disposal restriction (LDR) program for hazardous wastes was established to reduce the toxicity and/or mobility of the hazardous constituents of the waste in the environment. These hazardous contaminants can leach into groundwater and/or surface water affecting human health and the environment. Specific constituent levels must be achieved before the hazardous waste can be land disposed (i.e. by using treatment standards). The [Code of Federal Regulations -Title](http://cfr.vlex.com/source/code-federal-regulations-protection-environment-1089) [40: Protection of Environment](http://cfr.vlex.com/source/code-federal-regulations-protection-environment-1089) (40 CFR Ch.1 § 268.45) establishes that hazardous debris must be treated prior to land disposal and before any immobilization technology could be applied. [Figure](#page-40-0) [13](#page-40-0) shows the best available alternative treatment standards for hazardous debris. Each contaminant must be pretreated, unless EPA determines under $\S 261.3(f)(2)$ that the debris is no longer contaminated or has already been treated to the required waste-specific treatment standards. Selection of the appropriate technology must be based on the characteristics of the debris (i.e., ignitability, corrosivity or reactivity). Hazardous constituents subject to treatment are listed in §§ 268.40 (applicability of treatment standards). The treatment selected should provide the level required.

Figure 13. Alternative treatment standards for hazardous debris.

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TASK 6: STUDENT SUPPORT FOR MODELING OF GROUNDWATER FLOW AND TRANSPORT AT THE DOE SITE IN MOAB, UTAH

INTRODUCTION

The Moab Uranium Mill Tailings Remediation Action (UMTRA) Project is managed by the U.S. Department of Energy (DOE) Office of Environmental Management located in Grand Junction, Colorado. The site is a former uranium-ore processing facility located about 3 miles northwest of the City of Moab, Utah, and lies on the west bank of the Colorado River at the confluence with Moab Wash. One of the interim remedial actions for reducing groundwater contamination is to evaporate the groundwater which is withdrawn from the wells located between the mill tailings and Colorado River. Presently, a Landshark evaporating system (manufactured by Resources West, Inc) is utilized to atomize and disperse in the air up to 125 gpm of groundwater withdrawn from the aquifer. The system uses a large flow rate ratio of air to water (1500/1 by volume).

An estimate of the air pollution potential when the Landshark evaporating system is used to disperse contaminated groundwater in the air was provided by ARC-FIU (See APPENDIX T6- 001). The operation of an alternative ammonia treatment using an ammonia stripping tower also was analyzed to determine the maximum concentrations of emissions at the source and the ammonia mass flow rate emitted from the tower at 700 gpm treatment capacity. The calculations use the Gaussian dispersion model to determine the peak concentrations at selected sites in the vicinity of the tailings, the City of Moab and the Arches National Park.

The water and air flow rates of the Landshark equipment and air stripper are used to determine the bulk concentration and the mass flow rate of point source dispersal of each contaminant in the air. Ammonia and metals are the primary contaminants addressed by the Landshark analysis and ammonia is the only contaminant addressed by the air stripper analysis. The average wind velocity and direction measured at the site were applied in the Gaussian air dispersion model to determine the steady state concentration 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. By assuming steady state emissions and a fully developed plume, the methodology provides a conservative estimate of the maximum concentrations in the vicinity of the tailings and at the adjacent sites.

Calculated downwind ammonia concentrations at all major receptor points (Tailings, Offices, Matheson Wetland Preserve, City of Moab, and Arches National Park) are below 8-hr OSHA's exposure limits of 25 ppm (0.018 µg/m^3) and the odor threshold is 5 pm. In addition, the Landshark evaporator provides significant dilution (1500 times) at the point source.

The operation of two concurrently operating Landshark evaporators will not result in concentration increase at the specified locations, however, the contaminants will likely travel further. However, the Landshark evaporators should not be used to evaporate tailings fluids or evaporation pond water that is significantly higher in ammonia concentrations. This water should be discharged to an irrigation system on the berm of the tailings to prevent aerosol transport and inhalation. The ammonia concentrations from the stripping tower are below the 8-hr OSHA's exposure limit and odor threshold.

RESULTS AND DISCUSSION

A Landshark evaporating system manufactured by Resources West, Inc is utilized to temporarily reduce the groundwater contamination at the Moab site. The system uses a large air to water flow rate ratio (1500/1 by volume) to atomize and disperse groundwater extracted from wells in the air. The groundwater contains a range of inorganic contaminants that can impair water quality in the vicinity of the evaporator. The Gaussian dispersion model was applied to assess the distribution of contaminants as function of average wind speed. The calculated concentrations were compared to ATSDR's toxicological profiles of the contaminants and the 8-hour exposure limit. Following assumptions were used for the air dispersion model:

- 1. A steady state fully developed plume, with constant wind speed and mass emission rates. This approach provides a conservative estimate of the pollutant concentrations (therefore the greatest risk) downwind;
- 2. Completely suspended aerosol particles that are carried with the plume and have a zero deposition rate. This assumption results in a conservative estimate of the concentrations downwind, since the bulk concentration of the fluid decays only as a function of diffusion and dispersion.

The atmospheric conditions at the Moab site have been accounted for by considering the prevailing stability regimes. During summer the atmosphere is "unstable" and during winter it is "stable", therefore simulations have been performed for three different atmosphere stability classes; B, being moderately unstable, D, being neutral, and F, being moderately stable. The calculations were performed for distances from 100 m to 12 km and for five selected locations the concentrations were compared to the current 8-hour OSHA inhalation limits of exposure:

- i) A point located 700 ft from the Landshark on Tailings with a south-north wind direction;
- ii) A point located near the offices, 0.5 miles from the Landshark with a wind direction of west-southwest to east-northeast;
- iii) The Matheson Wetlands Preserve approximately a mile southeast of the site with a westnorthwest to east-southeast wind direction;
- iv) The City of Moab approximately 3 miles south west of the site with a northwestsoutheast wind direction;
- v) Arches National Park which has a common boundary with the site from the north. The center of the park is located about 7.5 miles from the Tailings with a southwest-northeast wind direction.

Class Units	Exposure Limits	C_{GW}	C_{Tailings} Class B	C_{Office} Class D	C_{MWP} Class F	C_{Moab} Class F	C_{ANP} Class F	
Analyte	μ g/m ³	μ g/L	$\mu g/m^3$	$\mu g/m^3$	μ g/m ³	$\mu g/m^3$	$\mu g/m^3$	
Aluminum	15,000	$0.150(\pm 0.000)$	3.6E-03	3.4E-03	2.4E-03	1.5E-03	2.5E-03	
Ammonia	25	$400.0(\pm 129.9)$	0.148	0.146	0.103	0.092	0.026	
	ppm		ppm	ppm	ppm	ppm	ppm	
Antimony	500	$0.034(\pm 0.006)$	7.1E-04	6.8E-04	4.8E-04	2.9E-04	5.0E-04	
Arsenic	10	$0.039(\pm 0.000)$	9.2E-04	8.9E-04	6.3E-04	3.8E-04	6.5E-04	
Barium	15,000	$0.008(\pm 0.003)$	2.2E-04	2.1E-04	1.5E-04	8.8E-05	1.5E-04	
Beryllium	$\overline{2}$	$0.002(\pm 0.000)$	4.3E-05	4.1E-05	2.9E-05	1.7E-05	3.0E-05	
Cadmium	5	$0.003(\pm 0.000)$	7.8E-05	7.5E-05	5.3E-05	3.2E-05	5.5E-05	
Calcium		$473.7(\pm 55.8)$	$1.1E + 01$	$1.1E + 01$	$7.7E + 00$	$4.7E + 00$	$8.0E + 00$	
Chromium	0.5	$0.007(\pm 0.002)$	1.3E-04	1.2E-04	8.7E-05	5.2E-05	9.0E-05	
Cobalt	100	$0.005(\pm 0.001)$	1.1E-04	1.0E-04	7.2E-05	4.4E-05	7.5E-05	
Copper	100	$0.010(\pm 0.000)$	2.3E-04	2.2E-04	1.6E-04	9.4E-05	1.6E-04	
Fluoride	2,500	$2.038(\pm 0.106)$	4.7E-02	4.6E-02	3.2E-02	1.9E-02	3.3E-02	
Iron		$0.776(\pm 0.063)$	1.8E-02	1.7E-02	1.2E-02	7.2E-03	1.2E-02	
Lead	50	$0.013(\pm 0.000)$	3.1E-04	3.0E-04	2.1E-04	1.3E-04	2.2E-04	
Magnesium		$672.5(\pm 161.7)$	$1.7E + 01$	$1.6E + 01$	$1.1E + 01$	$6.8E + 00$	$1.2E + 01$	
Manganese	5,000	$4.113(\pm 1.109)$	9.7E-02	9.3E-02	6.6E-02	4.0E-02	6.8E-02	
Nickel	1,000	$0.023(\pm 0.011)$	4.3E-04	4.1E-04	2.9E-04	1.7E-04	3.0E-04	
Potassium		$214.4(\pm 82.9)$	$5.0E + 00$	$4.8E + 00$	$3.4E + 00$	$2.0E + 00$	$3.5E + 00$	
Selenium	200	$0.053(\pm 0.012)$	1.3E-03	1.2E-03	8.7E-04	5.2E-04	9.0E-04	
Silver	10	$0.011(\pm 0.000)$	2.6E-04	2.5E-04	1.8E-04	1.1E-04	1.8E-04	
Sodium		4212.5(±1578.9)	$1.0E + 02$	$9.8E + 01$	$6.9E + 01$	$4.2E + 01$	$7.2E + 01$	
Thallium	100	$0.035(\pm 0.000)$	8.3E-04	8.0E-04	5.6E-04	3.4E-04	5.8E-04	
Uranium	50	$2.605(\pm 0.808)$	6.4E-02	6.1E-02	4.3E-02	2.6E-02	4.5E-02	
Vanadium	100	$0.007(\pm 0.004)$	1.3E-04	1.2E-04	8.5E-05	5.1E-05	8.8E-05	
Zinc	1,000	$0.007(\pm 0.000)$	1.7E-04	1.6E-04	1.2E-04	7.0E-05	1.2E-04	
Concentration in groundwater, standard deviations are shown in parentheses $C_{\rm GW}$ Concentrations in vicinity of offices C_{Office} Concentrations at the Matheson Wetland Preserve C_{MWP} C_{Moab} Concentrations at the City of Moab Concentrations at the Arches National Park $C_{\rm AMP}$								

Table 5. Estimated Maximum Concentrations at Each Sample Point

Variation with Distance

[Figure 14](#page-45-0) illustrates the computed spread pattern of four contaminants from the source assuming a constant wind speed of 2.5 m/s. This figure represents the worst case scenario in which there is a possibility that ammonia concentration reaches the OSHA's inhalation exposure limit at the first receptor point. As demonstrated by the modeling results, the most important factor affecting the dispersion of contaminants is the stability in the atmosphere, and then, the wind velocity.

Figure 14. An example of concentration decay with distance at 2.5 m/s average wind speed.

Comparison of OSHA's 8-hr Limit and Calculated Concentrations

In all stability classes as demonstrated in [Figure 14,](#page-45-0) after a distance of 3 km, concentrations decrease until a point where they become negligible. For the farthest points, the stability class B undergoes an inversion of places, meaning that for distances more than 1 km, concentrations associated with the unstable stability decrease exponentially. [Figure 15](#page-46-0) compares the calculated concentrations and the exposure limits at the first 2 and the last 2 receptor points.

As shown in [Figure 15\(](#page-46-0)a) for the first receptor point on the Tailings, the calculated concentrations for stability class B are the highest, and ammonia produces a concentration of 0.148 ppm which is the closest to the exposure limit. At point 2 (Offices), concentration values predicted by all stability classes are very close as shown in [Figure 15\(](#page-46-0)b). However, stability class D has the highest values with ammonia being the closest to the exposure limit with the concentration of 0.146 ppm. Under neutral atmospheric conditions the air movement is very low, and therefore, it will take longer distance for contaminants to disperse compared to stability class B, and thus, the maximum concentration happens at the farther point.

Figure 15. Comparison between exposure limits and computed concentrations at the (a) Tailings (b) Offices (c) City of Moab and (d) Arches National Park.

In the City of Moab (point 4) and Arches National Park (point 5), the concentration of all the 25 contaminants present in the produced mist is very low compared to the exposure limit of each.

Comparison of Landshark and Ammonia Air Stripping Tower

In the present study, using of an induced-draft stripping tower has been considered as an alternative for Landshark evaporators to remove the ammonia from the contaminated groundwater using well configuration 5 and dilute it in the air. Computed concentrations downwind are compared with OSHA exposure limits for both Landshark operations and ammonia stripping tower in [Table 6](#page-47-0) and [Table 7](#page-47-1) respectively.

Table 6. Computed Concentration of Ammonia for Different Atmospheric Stability Classes at Different Receptor Points Downwind Using Landshark Operation

Table 7. Computed Concentration of Ammonia for Different Atmospheric Stability Classes at Different Receptor Points Downwind Using Ammonia Stripping Tower

CONCLUSIONS AND PROPOSED WORK

A transport model developed by DOE contractors will be utilized to simulate density dependent flow and nitrogen and uranium reactive transport. SEAWAT will be used to solve groundwater flow, transport of contaminants, and brine migration in the ground water simulations.

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