## QUARTERLY PROGRESS REPORT

January 1 to March 31, 2013

## Florida International University's Continued Research Support for the Department of Energy's Office of Environmental Management

Principal Investigators:

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Prepared for:

U.S. Department of Energy Office of Environmental Management Under Grant No. DE-EM0000598 The Applied Research Center (ARC) at Florida International University (FIU) executed work on five major projects that represent FIU-ARC's continued support to the Department of Energy's Office of Environmental Management (DOE-EM). The projects are important to EM's mission of accelerated risk reduction and cleanup of the environmental legacy of the nation's nuclear weapons program. The information in this document provides a summary of the FIU-ARC's activities under the DOE Cooperative Agreement (Contract # DE-EM0000598) for the period of January 1 to March 31, 2013.

Highlights during this reporting period include:

*Project 1*: Milestone 2012-P1-M16.1 was completed on time (1/31/13) and a summary document was provided to EM HQ and site POCs.

*Project 2*: The deliverable for task 1.1 was completed and a progress report was sent to DOE on 02/19/13.

*Project 3:* Milestone 2012-P3-M3.1 "Preliminary results summary of laboratory experiments" related to Task 3: Parameterization of Major Transport Processes of Mercury Species, was submitted to DOE on 1/18/2013.

Milestone 2012-P3-M4.1 "Sample Python scripts and ModelBuilder process workflow diagram" related to Task 4: Geodatabase Development for Hydrological Modeling Support, was submitted to DOE on 2/1/2013, and the technical report associated with Task 3 for the Parameterization of Major Transport Processes of Mercury Species was submitted on 2/18/2013.

Also, the Technical Report deliverables for Tasks 1 and 5 were submitted to DOE on 3/1/2013 and 3/19/2013, respectively.

*Project 4*: The development and deployment of the picture lite mobile application (Milestone 2012-P4-M3.6) and the technology lite mobile application (Milestone 2012-P4-M3.7) were completed on 1/18/13 and 2/15/13, respectively.

*Project 5*: No milestones or deliverables were due during this period.

### Project 1 Chemical Process Alternatives for Radioactive Waste

### Project Manager: Dr. Dwayne McDaniel

### **Task 2: Pipeline Unplugging and Plug Prevention**

<u>Peristaltic Crawler:</u> During this performance period, force tests were conducted with the peristaltic crawler having a thinner wall thickness to evaluate its response. These results were collected and compared with a previous crawler with thicker inner walls. Results showed that both provide similar force responses, indicating that the change in wall thickness has a minimal effect on the pull force. The thinner wall bellow was tested up to a pressure of 50 psi, developing a force of 108 lbs (Error! Reference source not found.).

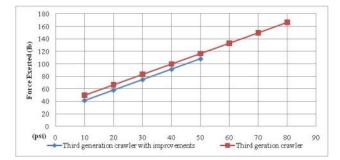


Figure 1-1 Crawler force test

Shrink sleeves were installed on the crawler unit to protect the pneumatic valves from exposure to the environment. This includes water from the flooded tests as well as material generated from the unplugging process. Final adjustments on the controller have also been made to optimize the crawler cycle times.

Additionally, tests to determine the pulling force required to run the tether assembly through one and two elbows were conducted using a bench scale testbed. The tests demonstrated that the stiffness of the tether does not pose a navigational impediment to the crawler unit. The average force required to run the tether through one and two elbows was approximately 13 lb and 22 lb, respectively. Navigational tests of the crawler were conducted using a bench scale testbed that included two elbows. The recorded time required to clear two elbows was 11 min and 45 sec.

During this period, FIU also continued with the development of the large scale experimental test loop as well as finalizing logistics for the testing. Space approval was requested and granted to assemble the testbed which includes three 90° elbows and has a total length of 500 ft. This loop (Error! Reference source not found.) configuration will allow for the evaluation of the crawler at significantly longer lengths then tested previously while navigating through three elbows. The pipeline layout shown defines the number of pipe sections, couplings, and elbows that will be required to assemble the testbed. The layout also ensures that the crawler testbed does not interfere with the asynchronous pulsing testbed currently being assembled in the same area.

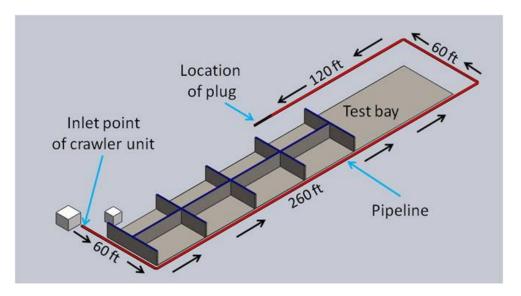


Figure 1-2 Layout of the 500 ft crawler testbed

<u>Asynchronous Pulsing System:</u> For the asynchronous pulsing system (APS), calibration curves have been developed for air quantities up to 5% (Error! Reference source not found.Error! Reference source not found.-3). The test results indicated that the effects of an air bubble entrained in the system on a transient pulse can be effectively mitigated by increasing the static pressure of the water above atmospheric pressure. As is visible in the figure, the effect of air being present in the pipeline caused very limited pressurization of the loop as the air is compressed. When that bubble is compressed to a certain density, the system begins to respond to a volume reduction in a similar manner to a no-air system. This behavior can be exploited to ensure larger pressure changes (i.e. more force loading) at the plug face. The observed relationship can now be used to determine the minimum static pressure value should be the minimum at which the compressibility of the system resembles the compressibility of water. These relationships will now be used to establish how much air can remain in longer pipe loops, and what will be the minimum static pressure required to cause significant dynamic loading of the plug during pulsing.

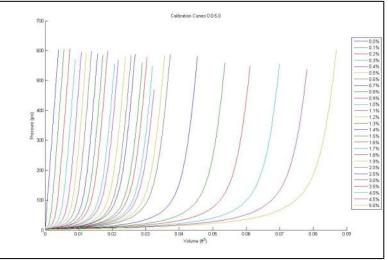


Figure 1-3 Calibration curves for various air quantities

Additionally, a large progressive cavity pump has been replumbed to be used as an alternative pressure source to perform asynchronous pulsing tests on the pipeline. A side-by-side comparative test was conducted on both the alternative pressure source (large progressive cavity pump) and the current asynchronous pulse unit. It was determined that they behave similarly; however, as can be seen by **Error! Reference source not found.**, the alternative pressure source was limited to only 150 psig. This can be overcome by utilizing a larger capacity pump. We investigated upgrading the current pump to increase its capacity and it was determined that it would cost the same as purchasing a new larger capacity pump.

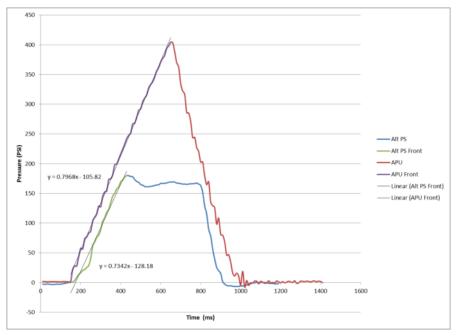


Figure 1-4 APU and alternative pressure source pulse test

A test loop was designed to test the APS and its functionality on a large scale, not previously tested. **Error! Reference source not found.** shows the loop which consists of two 135-foot runs on either side of a plug. Components to assemble the pipeline were ordered and received. The

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outdoor site was cleared and leveled and the pipeline supports were fabricated and anchored to the ground (**Error! Reference source not found.**). The elevations of the pipeline supports have been surveyed and adjusted to provide the proper pipeline slope. The next phase will include pressure testing the pipeline and installing pressure transducers.

To determine the best simulant material to manufacture plugs for the testing, engineers from FIU had a number of discussions with engineers for the AEM. It was decided that kaolin-plaster plugs could provide the necessary shear strength for testing and various compositions would be investigated. Several 1L samples were created in a laboratory setting by varying the combination of kaolin and plaster ratios and tested for shear strength. The samples were cured for 24-36 hours. A shear strength ranging from 5-26 kPa was obtained. The success of making high strength plugs is highly sensitive to variations in the preparation procedure and conditions. Hence, best practices relevant to the manufacturing of the plug were also discussed with AEM engineers and the recommendations were incorporated while developing the plug.

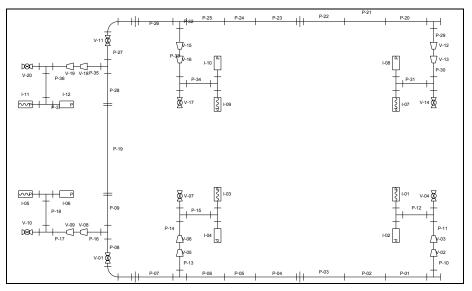


Figure 1-5 Large scale asynchronous pulsing test loop





Figure 1-6 Experimental testbed for asynchronous pulsing system

A number of posters were presented by DOE Fellows and Faculty at the 2013 Waste Management Symposium. This includes a professional poster entitled *Design Advances of Innovative Unplugging Technologies for High-Level Waste Pipelines* and 4 student posters related to this task shown below.

- *High-Level Waste Pipeline Unplugging Technologies: Asynchronous Pulsing System*, Jennifer Arniella (DOE Fellow), Amer Awwad. This poster showed the work and effort done on understanding how the air and the geometry of the pipeline affect the pressure waves.
- Development of Improved Bodies for a Peristaltic Crawler for Unplugging of Hanford Waste Transfer Pipelines, Jose Matos (DOE Fellow). The study described in this poster covers a new design of the crawler device which incorporates powerful, micro pneumatic cylinders in order to address these shortcomings.
- *Improved Third Generation Peristaltic Crawler for Removal of High-Level Waste Plugs in Hanford Site Pipelines*, Gabriela Vazquez (DOE Fellow), Tomas Pribanic. This poster showed the improved third generation pneumatic/hydraulic operated peristaltic crawler. The new design incorporates pneumatic valves to reduce cycle time, inspection camera for visual feedback, and a thin walled outer bellow for improved maneuverability.
- Acoustic Pulse Reflectometry for Identifying Pipeline Properties at Hanford Site, Lucas Nascimento (DOE Fellow). This poster showed studies related to Acoustic Pulse Reflectometry (APR), which is a technique that measures reflections from a volume to estimate plug formation and changes in pipeline geometry. This technique can be used to select unplugging technologies.

#### Task 12: Multiple-Relaxation-Time, Lattice Boltzmann Model for High-Density Ratio, Multiphase Flows

During this performance period for the lattice Boltzmann method (LBM) task, the contact–angledynamics problem was investigated using the 3D parallel LBM code. The forcing term added to the governing equations for the surface wetting was evaluated for accuracy. The value of the forcing term depended on the local density and the wetting coefficient and was applied in the normal direction to the surface. The normal were calculated on the last solid nodes which are designated as the surface nodes in the domain. The bounce-back routine that is implemented for the no-slip velocity boundary condition was also analyzed. A droplet placed initially at zero velocity next to a solid surface was simulated and it was observed that the solid surface was able to apply an attraction force on the droplet (Figure 1-7); however, it was found that the droplet volume reduced as the simulations were carried out which indicated that an error with the implementation of the forcing term may have caused the wetting boundary condition to act like a sink. Alternative approaches that use gradient functions to apply the force only at the interface will be investigated.

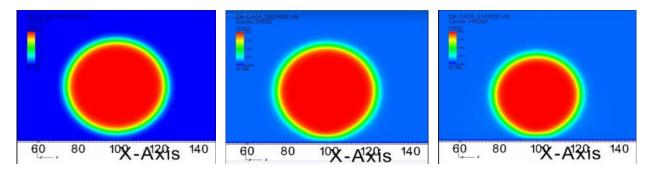
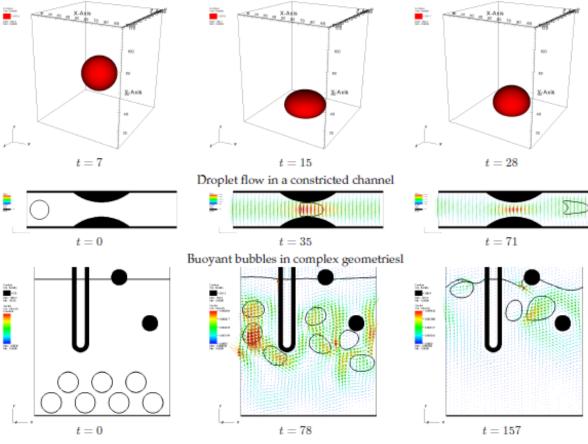


Figure 1-7 LBM simulation of 3D droplet placed next to a solid surface at different time instances

Additionally, the 3D LBM code was utilized to investigate the motion of buoyant bubbles and droplets in various configurations. The case studies included collision of a droplet with a solid surface, motion of a droplet in a constricted channel under inertial flow and buoyant gas release event in a simplified waste tank (Figure 1-8). The cases studied allowed us to observe the effect of structures on the two phases. In the case of the constricted channel problem, the circular droplet retained an elongated shape after it passed through the constriction while, for the buoyant gas bubble release event simulation, some bubbles were found to be held by the horizontal pipe structures, represented in the domain as circular objects, which delayed the increase of the gas phase in the headspace.



#### Collision of a droplet at a sollid surface

Figure 1-8 Case studies of various bubble configurations

Finally, a literature review has been initiated in order to investigate the possible turbulence models available for multiphase flow simulations using the lattice Boltzmann method. Focus will be given to the Large Eddy Simulation (LES) implementations in the lattice Boltzmann method; however, other models will also be reviewed. The LES implemented in LBM is a Smagorisky sub-grid-model which uses the strain-rate tensor for the subgrid stress. This will be obtained from the non-equilibrium moments of the MRT-LBM. In addition, the applicability of the LBM to model fluids of Bingham plastic type will be examined. Bingham model is used to describe the viscoplastic characteristics of the sludge material found at DOE nuclear waste tanks. For this, non-Newtonian flow applications of LBM are being reviewed. For non-Newtonian fluids, the viscosity is a function of the local strain-rate, which makes LBM very suitable for incorporating non-Newtonian effects since it allows direct computation of the strain-rate. The outcome of this literature review will aid in developing the technical tasks for the next fiscal year.

This research was also presented at the 2013 Waste Management Symposium including a professional poster entitled *Implementation of Surface Wetting Effects in Computational Fluid Dynamics Simulations Using the Lattice Boltzmann Method*, which was presented during session 100. In addition, two student posters were presented by DOE Fellows within this task:

• A Lattice Boltzmann Method for the Analysis of Gas Behavior in Hanford Tanks and Computer Simulations of Multiphase Flow Systems Applied to Transfer of High-Level Waste was presented by DOE Fellow Jaime Mudrich in the Student Poster Competition.

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In this poster, computer simulations were presented based on the 3D multiphase lattice Boltzmann method for high density ratio systems. The method is capable of incorporating complex geometries generated in CAD software. The geometries are voxelized and then imported for use in multiphase flow simulations. Surface wetting features enable accurate simulation of contact angles.

• Computer Simulations of Multiphase Flow Systems Applied to Transfer of High-Level Waste, Francisco Bolanos (DOE Fellow), Seckin Gokaltun. This work presented computer simulations dealing with 2D and 3D multiphase Lattice Boltzmann Method for high density ratio systems. The method is intended to accurately represent and predict fluid fluids in high level waste storage tanks. Simulations of computer model are presented and compared to benchmark case.

### Task 15: Evaluation of Advanced Instrumentation Needs for HLW Retrieval

FIU discussed with WTP engineers on the possibility of using the solid-liquid interface monitor (SLIM) developed at FIU to determine the amount of solids remaining on the bottom of a staging tank after a pulse jet mixing cycle which is intended to remove the waste. FIU held preliminary discussions with WTP engineers at the Hanford meeting on slurry simulants, tank profile, and logistical aspects of this task. Also, FIU discussed the sonar timing aspects with the manufacturer of the 3D profiling sonar, to determine possible improvements to the scan time. FIU will incorporate several recommendations provided by the manufacturer into the proposed test strategy.

FIU commenced the installation and configuration of the 3D profiling sonar into a small-scale mock-up tank. This setup will be used to evaluate the sonar's ability to scan a volume of interest within a 15-20 second window of time. Several areas of interest are being designed to test its ability to detect the structures and their profiles. One configuration consists of concentric cylinders of varying thickness and heights to determine resolution ranges for objects with oblique geometries. Another configuration consists of a sloped surface with steps that allow a measure of area and resolution to detect within the timeframe. These objects will be finalized within the coming months and will be assembled and/or manufactured using FIU's 3D printer. In addition to this work, FIU is discussing with the sonar vendor possible improvements to the system software to expedite the scanning and processing time.

### Task 16: Computational Simulation and Evolution of HLW Pipeline Plugs (New Task)

A summary document was completed as the deliverable to milestone 2012-P1-M16.1. The document summarized the literature review efforts initiated to advance the plug formation knowledge base and was provided to DOE EM HQ and site engineers. The review focused on four areas: (i) Overview of Waste Transfer System, (ii) Plugging Mechanisms and Waste Transfer Dynamics (iii) Current Analysis Tools-Capabilities and Limitations and (iv) Use of CFD modeling to predict the plug formation process. Technical gaps were identified and a multiphysics computational model that accounts for waste chemistry coupled with fluid dynamics has been suggested to improve on existing studies.

A 2-D model simulating steady state laminar flow of a fluid in a horizontal pipe was developed. A series of simulations were carried out in a 28-m long pipe with a diameter of 0.04 m. The

working fluid used was water and it has a uniform inlet velocity of 0.075 m/s. The results showed a uniform velocity profile that transitioned into fully developed flow. The modeling results were compared with the experimental results and the comparison showed excellent fit between observed and computed velocity profiles. As a second step, the transport model was implemented and simulations were conducted to determine the effect of various transport parameters (diffusivity) on the advection-dispersion patterns and results. The theory of the chemical reaction model is under review and testing as the third step of model development. Efforts are underway to do a mesh optimization study to improve the accuracy of modeling results.

Also, a 2-D model was developed investigating selected chemical parameters of three dissolved species in a pipe simulating laminar flow conditions using COMSOL Multiphysics software. Two modules were used to simulate the reacting flow conditions: (a) Laminar flow module and (b) Transport of diluted species module. The modules were coupled to distribute the chemical species throughout the model under laminar flow conditions, and then simulate the synthesis chemical reaction between the species. The concentration profiles of the chemical species were analyzed and the results demonstrated the ability of the software to accurately solve for reacting flow conditions.

A student poster entitled *Computational Simulation and Evolution of High-Level Waste Pipeline Plugs at Hanford* was presented by Dania Castillo (DOE Fellow) at the 2013 Waste Management Symposium Student Poster Competition. This poster showed the multi-physics module that is being developed to efficiently simulate and predict the formation of a plug in a high level waste pipeline. The simulations will demonstrate the relationship between plug formation and critical flow velocity, pipeline geometry and the physical properties of the waste stream during the transfer process.

### Milestones and Deliverables

The milestones and deliverables for Project 1 for FIU Year 3 are shown on the following table. Milestone 2012-P1-M16.1 was completed on time (1/31/13) and a summary document was provided to EM HQ and site POCs. This document will be submitted to OSTI.

Task	Milestone/ Deliverable	Description	Due Date	Status	OSTI
	2012-P1-M2.1	Complete engineering scale pipeline unplugging using the asynchronous pulsing system	5/10/2013	On Target	
	Deliverable	Summary Document for 2012-P1- M2.1	5/10/2013	On Target	
Task 2: Pipeline Unplugging and Plug Prevention	2012-P1-M2.2	Complete experimental validation of improvements to peristaltic crawler	11/09/2012	Complete	
	Deliverable	Summary Document for 2012-P1- M2.2	11/09/2012	Complete	
	2012-P1-M2.3	Complete engineering scale pipeline unplugging testing using the modified peristaltic crawler	5/03/2013	On Target	

FIU Year 3 Milestones and Deliverables for Project 1

	Deliverable	Summary Document for 2012-P1- M2.3	5/03/2013	On Target	
Task 12: Multiple- Relaxation-Time,	2012-P1-M12.1	Integration of mesh generation with appropriate boundary conditions in the 3D MRT LBM for simulation in complex geometries	5/16/2013	On Target	
Lattice Boltzmann	Deliverable	Summary Document for 2012-P1- M12.1	5/16/2013	On Target	
Model for High- Density Ratio, Multiphase	2012-P1-M12.2	Investigation of multiphase LBM models for Non-Newtonian fluids and turbulence modeling	5/16/2013	On Target	
Flows	Deliverable	Summary Document for 2012-P1- M12.2	5/16/2013	On Target	
Task 15:	2012-P1-M15.1	Complete Phase II candidate technology testing at Vendor facility	8/15/2012	Complete	
Evaluation of Advanced	Deliverable	Summary Document for 2012-P1- M15.1	8/15/2012	Complete	
Instrumentation Needs for HLW Retrieval	2012-P1-M15.2	Complete USS analysis and recommendations for Hanford	10/15/2012	Complete	
Keuleval	Deliverable	Summary Document for 2012-P1- M15.2	10/15/2012	Complete	
Task 16: Computational	2012-P1-M16.1	Complete literature review on plug prevention methods	1/31/2013	Complete	
Simulation and Evolution of HLW Pipeline Plugs	Deliverable	Summary Document for 2012-P1- M16.1	1/31/2013	Complete	
	2012-P1-M1.0	Waste Management Symposium 2013abstract submitted	8/17/2012	Complete	OSTI <sup>1</sup>
Draigat wide	Deliverable	Draft Project Technical Plan	06/18/2012	Complete	
Project-wide	Deliverable	Quarterly Progress Reports (all tasks and projects combined)	Quarterly	On Target	
	Deliverable	Draft Year End Report	06/28/2013	On Target	OSTI

### Work Plan for Next Quarter

- All Tasks: Draft the Year End Report for DOE.
- Task 2: FIU will complete additional calibration curves for the APS to extrapolate the relationship between entrained air and pressure degradation. In addition, several transient tests will be performed to determine the pressure overshoot caused by the drive phase, and how that compares to the static pressure readings found during the calibration curves experiment. The pressure overshoot, and its effects in the presence of air, will allow FIU to develop an additional parametric relationship for system control and monitoring. Finally, the alternative pressure source will be tested on a larger scale loop.

<sup>&</sup>lt;sup>1</sup>Announcement of published journal or conference paper will be submitted to OSTI

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- FIU will initiate the design of the test bed to perform the experimental testing of the Peristaltic Crawler System on an engineering scale pipeline (500 ft approximately). Improvements on the manifolds that hold the bullet pneumatic valves will be investigated to eliminate potential air leaks. The programmable logic controller software will also be optimized to provide faster navigational speed, this includes a secondary sequence specifically programmed to increase the speed of the unit when turning through 90° elbows. A second crawler unit will be fabricated and additional bellows will be procured to perform experimental pressurization/depressurization fatigue tests. Lastly, the system will be integrated into a skid for ease of transportation and deployment.
- Task 12: FIU will complete the verification of the wall boundary conditions in the 3D MRT LBM code in order to generate simulations with complex geometry from voxelated data and wetting of droplets on solid surfaces with various hydrophobicity properties. For this purpose, the dynamic simulations of bubbles and droplets in domains with solid boundaries will be simulated. The results will be presented in a poster at the Waste Management Symposium. The literature review for turbulence modeling for multiphase LBM will also be initiated.
- Task 15: FIU will continue to work with Hanford and SRS engineers on defining the initial testing of SLIM. This will include determining various simulant material and concentrations.
- Task 16: FIU will review the Particle Tracing Module of COMSOL which will include particle tracing, particle growth kinetics and particle-particle interactions. This information will assist in incorporating particle deposition in the model. Efforts will also focus on simulating a spherical particle falling in water in a 3" horizontal pipe and determining its terminal velocity.

### Project 2 Rapid Deployment of Engineered Solutions to Environmental Problems

### Project Manager: Dr. Leonel E. Lagos

# Task 1.1: Sequestering Uranium at the Hanford 200 Area by *In Situ* Subsurface pH Manipulation using Ammonia (NH<sub>3</sub>) Gas Injection

A progress report for the evaluation of morphological changes of uranium-bearing precipitates over time was completed. The scanning electron microscopy and energy dispersive spectroscopy (SEM/EDS) analysis provided primarily qualitative insight into the morphological changes that occurred on the surface of the precipitate with increased time in solution. It was noted that the evolution of sample morphology with increased time in solution for the high bicarbonate precipitates is similar for samples prepared with and without calcium. Conclusions regarding the best methods for sample preparation were drawn based on comparisons of samples prepared under varying conditions. Supplementary SEM/EDS analysis is ongoing to further support the data described in the report.

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The data from the recently completed progress report on SEM/EDS analysis for evaluation of morphological changes of precipitate samples with time was presented in poster form at the Waste Management Symposia, Phoenix, AZ. The presentation offered the opportunity to receive input from professionals in the industry, some of whom were equipped with extensive backgrounds in similar or related research.

A new sample holder for powder XRD analysis was fashioned from plastic. The choice of plastic was made to avoid the interference caused by the aluminum in the sample holder made for past attempts at sample analysis.

Complementary analytical techniques are being researched to further validate the speciation predictions about the uranium form. Dialogue with research labs, both inside and outside of Florida International University that are equipped with capable instrumentation, has been opened. Sample evaluation by Raman Spectroscopic Microscopy has begun in hopes of targeting the fine uranium-bearing crystal structures of interest. Should the structures be indistinguishable with the technique, mapping the crystal locations via SEM on a grid pattern will be researched to facilitate point targeting for Raman analysis.

In order to continue with Raman Microscopy, a method for mounting the sample that will assure that there is no contamination in the instrument was researched. Though this analysis can be done without mounting to the glass slide, extra care is being taken considering the uranium content in the sample. In addition, Transmission Electron Microscopy (TEM) has been proposed and investigated as a potential technique for phase characterizations. Research into TEM diffraction patterns is ongoing.

FIU continued experiments with a new batch of samples that contains 10 mM of calcium (Ca) to study its effect on the removal of U(VI) after ammonia gas pH manipulation in the synthetic solutions mimicking pore water composition found in the vadose zone at the Hanford Site 200 Area. After completing of pH adjustments, the samples were injected with ammonia gas until a pH of 11 was reached. Two (2) ppm of U(VI) were then added to each sample and duplicates of each sample were made. The KPA instrument was used to measure the U(VI) concentrations. An inductively coupled plasma optimal emission spectrometer (ICP-OES) was used to measure the silica (Si), aluminum (Al), and calcium (Ca) concentrations. Inorganic carbon (IC) of the supernatant solutions was analyzed via a Shimadzu TOC analyzer with an autosampler (TOC-V CSH).

The results of the ICP-OES analysis were as follows: silica reported a high average removal ranging from 70% to 100% in all Si/Al ratios tested. Aluminum showed high average removal ranging from 84% to 100% in all ratios except for Si/ Al ratios of 1:1 for the 25 mM HCO<sub>3</sub>, 50 mM HCO<sub>3</sub> and 75 mM HCO<sub>3</sub> samples, where the removal rate ranged from 23% to 50%. Finally, calcium showed average removal of 80%-100% in all ratios except the Si/Al ratio of 1:10 for the 0 mM HCO<sub>3</sub> sample in which the average removal was 30%. As stated before, no magnesium was added to this batch of samples. A new run of ICP will be made to rerun samples for calcium (Ca) and aluminum (Al) with a higher dilution factor; the results will be stated in the next monthly report.

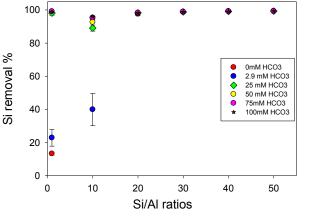
The results for the KPA analysis showed that the percent removal of U(IV) for all Si/Al ratios is ranging from 96% to 99.9%.

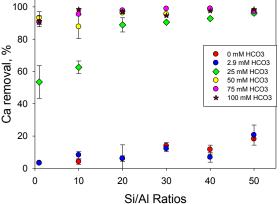
The experimental results showed that the removal of inorganic carbon (IC) was in the 65-87% range for 25, 50, 75, and 100 mM of bicarbonate and Si/Al ratios between 1 and 50; the IC removal for the 2.9 mM HCO3 set was found between 21% and 57%. The results for the removal of IC in this set are higher than was previously observed for 5 mM of calcium, which averaged between 10-25%. Perhaps, the presence of a greater concentration of calcium, 10 mM, initiates the formation of CaCO<sub>3</sub> species, which might be co-precipitated with Si gel.

FIU initiated retesting of samples containing 10 mM of Ca for calcium (Ca) and silica (Si) using a higher dilution factor for ICP-OES analysis and the results were as follows: silica again showed a high average removal, ranging from 70% to 100%, except for the sample containing 0 mM HCO<sub>3</sub> of Si/Al ratio of 1:1, which showed no removal. The removal of calcium was in the 80% to 100% range in all ratios including the Si/Al ratio of 1:10 for the 0 mM HCO<sub>3</sub> sample that had previously showed a low average removal of 30%.

Due to some inconsistency in results from the previous run of samples containing 5 mM of Ca, a new batch of samples was started. Samples preparation procedures followed experiments using 10 mM Ca. The samples were prepared from the stock solutions of Al, Si, and HCO<sub>3</sub><sup>--</sup> made in deionized water from Al(NO<sub>3</sub>)<sub>3</sub>•9H<sub>2</sub>O, Na<sub>2</sub>SiO<sub>3</sub>•9H<sub>2</sub>O, and KHCO<sub>3</sub>, respectively. 36 samples were made in total containing 0 mM, 2.9 mM, 25 mM, 50 mM, 75 mM and 100 mM of HCO<sub>3</sub> with Si/Al ratios of 1, 10, 20, 30, 40, and 50 each. The volume of each sample was adjusted to 50 mL with deionized water and the pH was adjusted to 8 via titration of nitric acid

After completing pH adjustments, ammonia gas was injected until pH reached 11. These solutions were used for preparation of duplicate U-bearing samples. Each sample was prepared using 20  $\mu$ L of 5 mM of Ca, 100  $\mu$ L of 2 ppm of U(VI), and 4,880  $\mu$ L of solution with pH adjusted to 11.. All control and experimental tubes were kept in an incubator/shaker at 100 rpm and at a temperature of 25 °C. After two days, the solutions were centrifuged for 15 minutes at 4000 rpm. The inductively coupled plasma-optical emission spectroscopy (ICP-OES) (PerkinElmer) and Shimadzu TOC analyzer (TOC-V CSH) were calibrated and samples of the supernatant from each vial were analyzed to determine the remaining Al, Si, and Ca concentrations in each solution. Samples were diluted with 1% nitric acid in the range of 20- 50 times. To conduct inorganic carbon (IC) analysis, the supernatant of each test sample was diluted 100 times with previously boiled DIW.





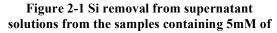


Figure 2-2 Ca removal from supernatant solutions from the samples augmented with 5mM of Ca

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Silica had a high average removal percent ranging from 89% to 99%, except for the samples containing 0 mM and 2.9 mM of HCO3 of Si/Al ratio 1:1 and 1:10 where the removal averaged from 10-40% (Figure 2-1). As previously determined, the results for Si removal were correlated with the removal of U(VI) from the solutions. Aluminum removal followed the Si pattern with the average removal noted between 95 and 100% except for the sample containing Si/Al ratio 1:1 at 0 mM of HCO<sub>3</sub> where there was no removal observed and ratio 1:10 at 0 mM of HCO<sub>3</sub> and 2.9 mM HCO3 where Al removal deviated between 20-80%. Figure 2-2 shows the removal of Ca, which is assumed to be due to the precipitation of calcium carbonate; the results showed a greater percent of Ca removed at higher bicarbonate concentrations. The results for removal of inorganic carbon were in the range of 20-60% with higher values correlated to higher IC concentrations.

Continued review of uranium solubility literature for the preparation of isopiestic method laboratory set up. 15-mL nickel crucibles with lids were ordered and received and the appropriate dimensions were obtained for manufacturing. A preliminary assessment of the isopiestic chamber layout was verified. In order to fit within the layout, it would require some remanufacturing of the crucible lids. Initiated research on the necessary piece of aluminum to be used for having a uniform temperature distribution inside the chamber; the final height of the chamber is contingent upon head space requirements to be finalized.

Finalized the design of the aluminum containment block to hold 15-mL nickel crucibles with lids inside the isopiestic chamber. Researched, purchased and received materials and tooling for the manufacturing of the isopiestic chamber.



## Figure 2-3 Aluminum containment block for having an uniform temperature distribution inside the isopiestic chamber

FIU continued the revision of the manuscript entitled, "Effect of bicarbonate on the dissolution of sodium meta-autunite" for submission to the Chemical Geology Journal. This manuscript presents results on the single-pass flow-through (SPTF) experiments that were conducted to estimate the rate of uranium release from Na meta-autunite,  $Na_2[(UO_2)_2(PO_4)_2].3H_2O$ , as a function of bicarbonate (0.0005-0.003 M) in the pH range of 6-11 and a temperature range of 5-60°C. The effect of bicarbonate ions on the uranium release from autunite minerals has not been

reported before. The manuscript was updated with more details on the SPFT reactors design and discussions on the effect of bicarbonate on dissolution rates at higher pH.

FIU continued the revision of the manuscript entitled, "Comparison of the kinetic rate law parameters for the dissolution of natural and synthetic autunite in the presence of bicarbonate solutions" after peer-review in the Chemical Geology Journal. This manuscript presents results on the single-pass flow-through (SPTF) experiments that were conducted to estimate the rate of uranium release from Ca meta-autunite, as a function of bicarbonate (0.0005-0.003 M) in the pH range of 6-11 and a temperature range of 5-60°C. The manuscript was updated with new speciation modeling results for the becquerelite phase, provided more details and explanations on Transition State Theory and a discussion on the mechanisms of Ca-autunite dissolution.

A scope of work was developed for FIU Year 4. A new task 2 was incorporated in the project, "Remediation Research and Technical Support for Savannah River Site." This task will include two (2) technical subtasks entitled "FIU's support for groundwater remediation at SRS F/H – Area (subtask 2.1)" and "Monitoring of U(VI) bioreduction after ARCADIS demonstration at F-Area (subtask 2.2)". Both subtasks will be carried out in collaboration with scientists at the Savannah River Site.

Two students presented the posters shown in Figures 2-4 and 2-5 based on the results from this task in the student poster competition section of Waste Management 2013 Symposium. DOE Fellow, Robert Lapierre, presented a poster entitled, *Analysis of morphological changes of uranium-bearing precipitates over time by SEM/EDS* (Figure 2-4).

This poster showed the effects of variables on the morphology and composition of U-bearing precipitates created as a result of ammonia gas pH manipulation in the Hanford 200 Area vadose zone conditions. The analysis of samples by scanning electron microscopy and energy dispersive spectrometry gauged the impact of variables such as time, bicarbonate concentration, and calcium concentration.

DOE Fellow, Claudia Cardona, presented a poster entitled U(VI) sequestration in the presence of bicarbonate and calcium ions via subsurface pH manipulation using ammonia gas injection (Figure 2-5). This poster presented studies conducted on the Injection of NH<sub>3</sub> to target uranium contamination in the vadose zone to reduce radionuclides mobility in subsurface. The effect of porewater constituents such as Si, Al, Ca, HCO<sub>3</sub> on the U(VI) co-precipitation process is unknown. The research investigates the effect of porewater constituents on the removal of U(VI).

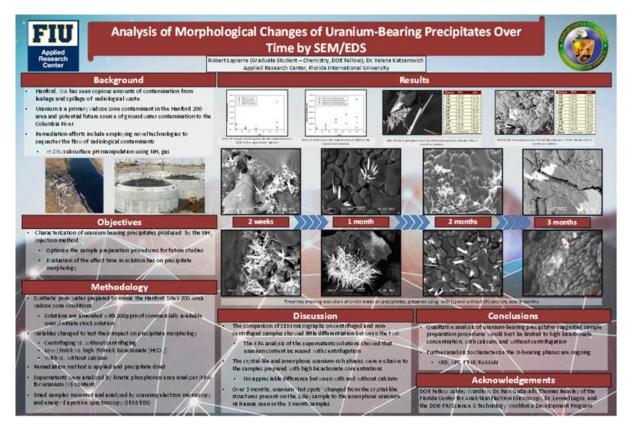


Figure 2-4 DOE Fellow Robert Lapierre Poster presented at the 2013 Waste Management Symposium

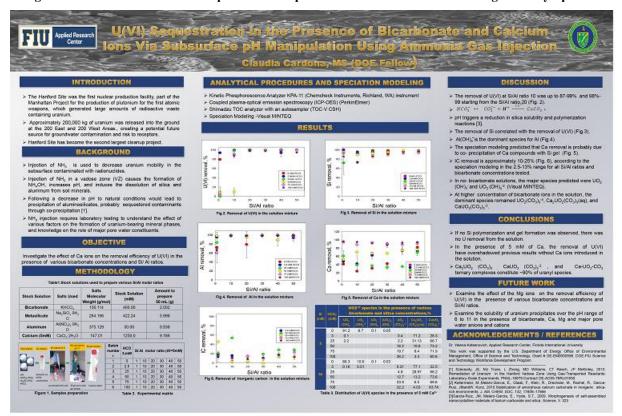


Figure 2-5 DOE Fellow Claudia Cardona Poster presented at the 2013 Waste Management Symposium

Training for the DOE Fellow Robert Lapierre for independent access and use of the facility X-Ray Diffractometer was undergone and completed. The training provided new insights into the technique and potential approaches to get the best possible results of FIU samples XRD analysis. Access to the instrument signup website was provided after completing training. Samples have been selected for grinding and an appointment is imminent.

The undergraduate student, DOE Fellow Valentina Padilla, had been working on the presentation on her research for the DOE Fellow weekly meeting. Also, she began the investigation into environmental conditions of Savanna River Site F-Area, where she will be performing her summer internship in the upcoming months.

### Task 1.2: Investigation on Microbial Meta-Autunite Interactions – Effect of Bicarbonate

FIU completed the bioleaching experiment with inserts. Sterile 6-well cell culture plates with inserts were used in the non-contact bioleaching experiments where natural Ca meta-autunite and bacteria cells were kept separately. A 3.2 ml aliquot of sterile media was dispensed in the appropriate well and 2.5 ml inside the insert receptacle. The total volume inside each well added up to 5.7 ml. The culture ware inserts have 0.4  $\mu$ m cylindrical pores that transverse the membrane and only allow the diffusion of soluble uranium. Ten mg (10 mg) of sterilized autunite powder was added to the bottom of the well:

0 mM HCO3: well 2, 3, 4 3 mM HCO3: well 6, 7, 8 5 mM HCO3: well 10, 11, 12 10 mM HCO3: well 14, 15, 16

Periodically, 20 µl samples aliquots were taken according to the sampling schedule and ashed on a hot plate in the presence of concentrated plasma grade nitric acid and hydrogen peroxide solutions. Wet digestion in seven-ml scintillation glass vials was continued until a dry white precipitate was obtained, then vials were dry ashed in a furnace at 450°C for 15 min. The samples were inoculated on the fifth day of experimentation with 55,000,000 cells/mL of G968 strain. KPA analysis was performed; a minimization of temperature was completed to prevent evaporation of the samples; however, it seems that the results did not illustrate bacterial leaching, just dissolution due to bicarbonate. Prepared 5% PTYG hard media for future use.

DOE Fellow Paola Sepulveda prepared and gave an oral presentation entitled, *Investigation on Microbial Dissolution of Uranium (VI) from Autunite Mineral*, to the Waste Management 2013 Symposium, Session 97. The results from this task will be published in the Symposium's proceedings.

FIU reviewed procedures for poor images obtained in the AFM analysis in its search for a solution on how to fix them. A new batch of synthetic ground water (SGW) was made to prepare samples for AFM imaging. This media was composed of 88.21 mg/L of CaCl<sub>2</sub>.2H<sub>2</sub>O, 19.99 mg/L of MgCl<sub>2</sub>, 5.22 mg/L of KCl, and 520.58 mg/L of HEPES. Media was prepared in deionized water (DIW), autoclaved at 121°C, 15 psi for 15 minutes, and allowed to cool down to about 30°C. Then the media solution was equally distributed between four 250-ml bottles and separately amended to contain 0, 3, 5 and 10 mM of KHCO<sub>3</sub>. Media pH in each bottle was

adjusted to pH 7.3. Each bicarbonate media solution was filter-sterilized (0.2  $\mu$ m) and kept refrigerated until the time of imaging. Future analysis of the samples will supplement data obtained in AFM with SEM-EDS data.

FIU prepared bacteria for AFM imaging; log7.5 bacterial cells was added to 4 mL of solution to make 1 ppm U(VI) amended with 10 mM bicarbonate. Unfortunately, AFM images did not come out good; there were high precipitates and high roughness analysis. This could be caused by secondary minerals; so, FIU had to re-prepare SGW without calcium or magnesium. This media was composed of 5.22 mg/L of KCl, and 520.58 mg/L of HEPES. The media was prepared in deionized water (DIW), autoclaved at 121°C, 15 psi for 15 minutes, and allowed to cool to about 30°C. Then the media solution was equally distributed between four 250-ml bottles and separately amended to contain 0, 3, 5 and 10 mM of KHCO<sub>3</sub>. The media pH in each bottle was adjusted to pH 7.3. Each bicarbonate media solution was filter-sterilized (0.2 µm) and kept refrigerated until the time of imaging. To obtain better results, SEM analysis will be performed for better quality images; while AFM analysis will be performed to obtain quantitative data such as roughness analysis and adhesion forces. In preparation for biodissolution experiment with synthetic autunite, HEPES buffer media was made from 5% minimal PTG media consisting of 5 g/L peptone, 5 g/L tryptone, 10 g/L glucose, 0.6 g/L MgSO<sub>4</sub>.7H<sub>2</sub>O, and 0.07 g/L CaCl<sub>2</sub>.2H<sub>2</sub>O. Yeast extract, due to the high phosphorus content, was not included in the media. The media was prepared in deionized water (DIW), autoclaved at 121°C, 15 psi for 15 minutes, and allowed to cool to about 30°C. Then media solution was equally distributed between four 250-ml bottles and separately amended to contain 0, 3, 5 and 10 mM of KHCO<sub>3</sub>. The media pH in each bottle was adjusted to pH 7.5 with 0.1 mol/L HCl or NaOH and buffered with 20 mM 2-(2-hydroxyethyl)-1-piperazine ethanesulfonic acid sodium salt hydrate (HEPES-Na). Each bicarbonate media solution was filter-sterilized (0.2 µm) and kept refrigerated until the time of the experiment. FIU then began the bioleaching experiment with synthetic Na-autunite. Autunite microbial bioleaching experiments were conducted with 100 mL foam stoppered glass serum bottles containing 50 mL of sterile media buffered with 20 mM HEPES-Na and 91 mg of meta- autunite to provide an U(VI) concentration of 4.4 mmol/L. The suspensions were slightly agitated at 60rpm in an incubator/shaker at 25 °C. A 0.3 mL sample of the solution was aseptically withdrawn from each bottle and filtered (0.2  $\mu$ m). Sample aliquots were then ashed on a hot plate with the addition of concentrate plasma grade nitric acid and hydrogen peroxide solutions. Wet digestion was continued until a dry white precipitate formed, and then dry ashing was performed in the furnace at 450°C for 15 min. Samples were allowed to cool at room temperature followed by the dissolution of the precipitate by the addition of 1 M nitric acid (HNO<sub>3</sub>). The bioleaching experiment will end at the beginning of May to line up with the previous experiment conducted on natural Ca-autunite.

### **Milestones and Deliverables**

The milestones and deliverables for Project 2 for FIU Year 3 are shown on the following table. The deliverable for task 1.1 was completed and a progress report was sent to DOE on 02/19/13.

FIU Year 3 Milestones and Deliverables for Project 2

Task	Milestone/	Description	Due Date	Status	OSTI

Period of Performance: January 1, 2013 to March 31, 2013

	Deliverable				
Task 1.1: Sequestering Uranium at the Hanford 200 Area Vadose Zone by <i>In Situ</i> Subsurface pH Manipulation Using NH3 Gas	2012-P2-M2	Completion of testing on the formation of U(VI)-bearing precipitates using various Si:Al ratios in the presence of bicarbonate	11/30/2012	Complete	
	Deliverable	Subtask 1.1 Progress report on over time morphological changes of U- bearing precipitates' via SEM/EDS.	1/11/2013	Complete	
Task 1.2: Investigation on Microbial-Meta- Autunite	2012-P2-M3	Completion of AFM assessment on bacteria exposed to U(VI) in bicarbonate-bearing solutions.	4/30/2013	Forecasted on 5/30/13 due to the issues with AFM instrument	
	Deliverable	Subtask 1.2 Progress report on AFM assessment on bacteria exposed to U(VI) in bicarbonate- bearing solutions	4/30/2013	Forecasted on 5/30/13 due to the issues with AFM instrument	
	Deliverable	Draft Project Technical Plan	6/18/2012	Complete	
Project-wide	2012-P2-M1	Waste Management Symposium 2013 abstract(s) submitted	8/17/2012	Complete	OSTI <sup>2</sup>
-	Deliverable	Draft Year End Report	6/28/2013	On Target	OSTI
	Deliverable	Quarterly Progress Reports	Quarterly	On Target	

### Work plan for next quarter

- All Tasks: Draft the Year End Report for DOE
- Complete testing on the formation of U-bearing precipitates.
- Complete manufacturing of the isopiestic chamber and initiate experiments for testing solubility of U-bearing precipitates.
- Conduct XRD analysis of precipitates.
- Obtain preliminary data with AFM on the bacterial surface properties in the presence of bicarbonate ions and prepare a progress report.
- Complete the revision of two manuscripts and resubmit to the peer-review journals.

<sup>&</sup>lt;sup>2</sup> Announcement of published journal or conference paper will be submitted to OSTI

### Project 3 Remediation and Treatment Technology Development and Support

### Project Manager: Dr. Georgio Tachiev

### Task 1: East Fork Poplar Creek Model Update, Calibration & Uncertainty Analysis

- Subtasks 1.1 & 1.2
  - Numerical instabilities previously present in the model (i.e. cross-sections, boundary conditions, Eco Lab settings) were resolved.
  - Successfully executed a 15 year simulation from 1991 2005 for water movement and water quality, including Eco Lab. Began processing simulations results and generating graphical output. Simulation outputs are shown below for the following station pairings:
    - Discharge downstream EFPC (an example is provided below):

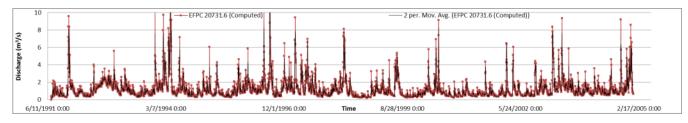
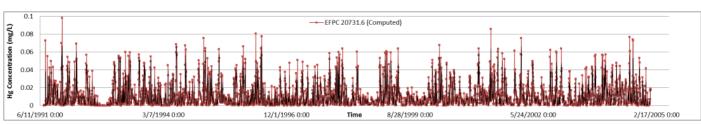


Figure 3-1 Discharge downstream EFPC



• Mercury Concentrations downstream EFPC and Bear Creek:

Figure 3-2 Mercury Concentrations downstream EFPC and Bear Creek

• Results for Bear Creek 7700.6 (computed) and 03538270 (observed)

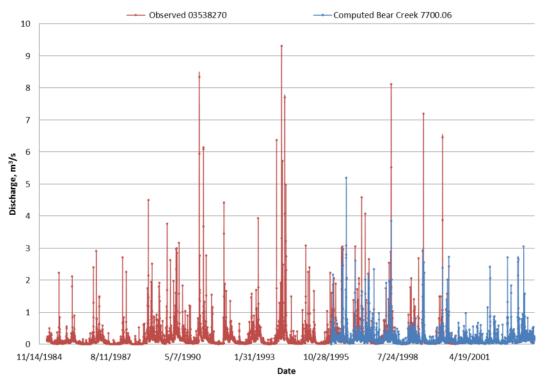


Figure 3-3 Comparison of flow duration curves for Bear Creek 7700.06 (computed) & 03538270 (observed)

 Comparison of computed discharges at Bear Creek 7700.06 & observed discharges at03538270

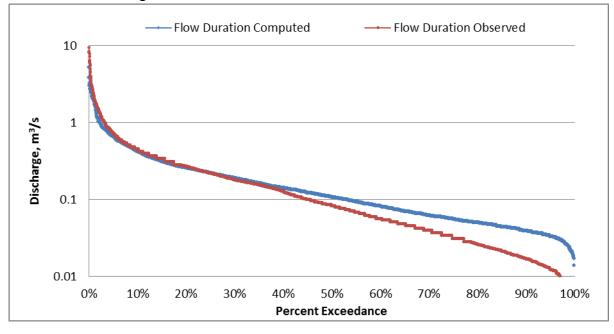


Figure 3-4 Comparison of flow duration curves for Bear Creek 7700.06 (computed) & 03538270 (observed)

• A set of one year simulations (2001 -2002) were conducted to identify the model's response to variations in the organic carbon partition coefficient (Kd). Kd values were

varied  $(0.025, 0.05, 0.5, 5, 50, and 500 \text{ m}^3/\text{g})$  and simulation results were compared to mercury concentrations at Sta. 17. The graphs below reveal that as the organic partition coefficient (Kd) increases the total mercury concentration and variability in data output decreases.

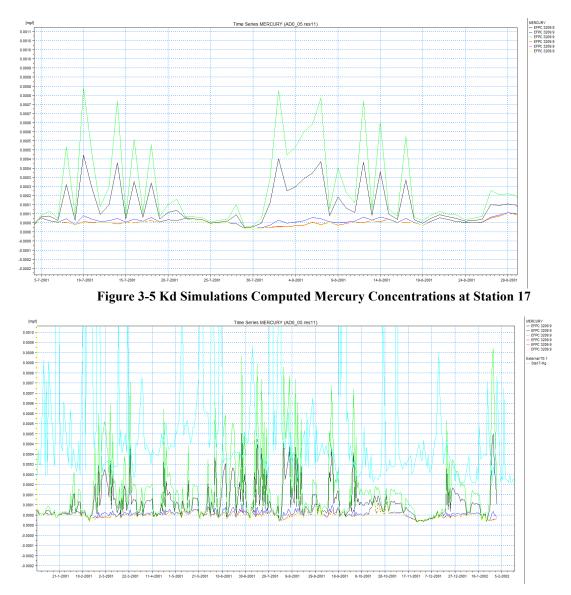


Figure 3-6 An example of varying Kd and comparison to observed mercury concentrations at Station 17

• Total suspended solids patterns were investigated for Station 17. The same process applied for analyzing the flow and mercury time-series, generating probability exceedance curves, and LDCs were implemented when evaluating total suspended solids. Figure 3-7 compares the observed and computed trends of TSS loads with the mercury loads at Station 17.

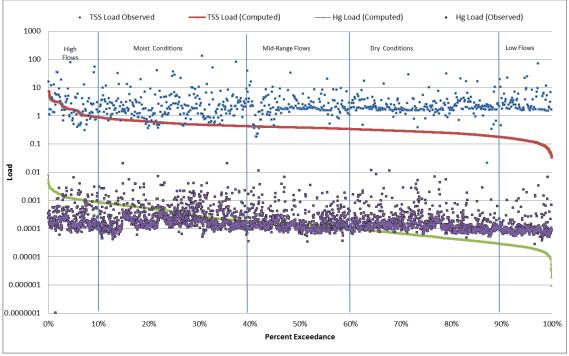


Figure 3-7 Observed and computed TSS load and mercury concentration load for Station 17

Profiles were generated for the major streams (East Fork Poplar Creek, Bear Creek, Gum Hallow Branch, Mill Branch, and Pinhook Branch) in addition to evaluating mercury concentrations and mercury loads downstream EFPC and Bear Creek. The profiles were used to analyze fluctuations in mercury concentrations as a function of time and identify how these fluctuations relate to hydrologic events. Figure 3-8 reveals a sample profile for EFPC. The subsequent images, Figures 3-9 and 3-10, protray the simulated mercury concentrations dowstream EFPC per corresponding hydrological event for time-step November 11, 1995 and January 6, 1996. The maximum mercury concentration reached within the simulated period is shown in red. A comparison of the mercury profile downstream of the selected branch with the precipitation pattern, reveals that during high flood events mercury concentration levels increase.

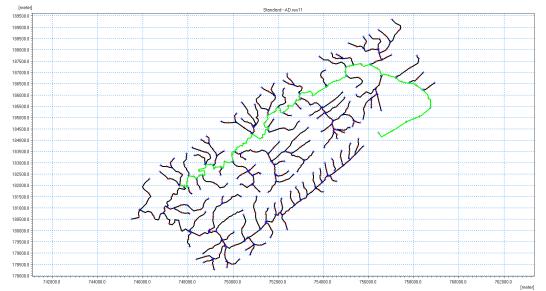


Figure 3-8 Model River network depicting physical paths within watershed of the mercury profile showcased in subsequent figure.

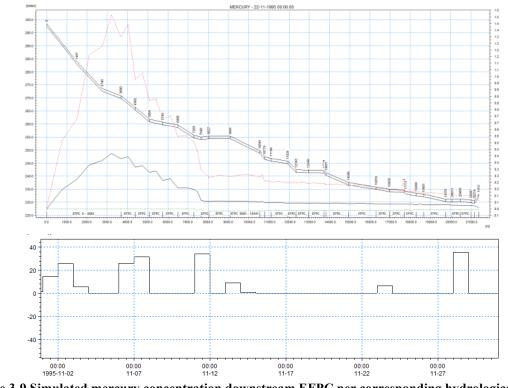


Figure 3-9 Simulated mercury concentration downstream EFPC per corresponding hydrological event for November 22, 1995

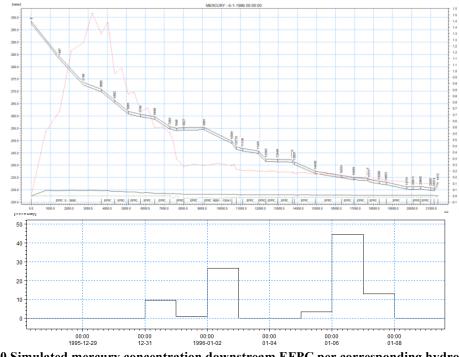


Figure 3-10 Simulated mercury concentration downstream EFPC per corresponding hydrological event for January 6, 1996

- Completed and submitted a technical report based on the research conducted for this task.
- A student poster entitled *Improvements of an Integrated Flow and Mercury Transport Model in East Fork Poplar Creek Watershed, Oak Ridge, Tennessee* was presented by Lilian Marrero (DOE Fellow) at the 2013 Waste Management Symposium Student Poster Competition. The poster showed an integrated surface and subsurface flow and transport model developed and implemented to determine the effect of hydrological and hydraulic parameters on mercury transport within the watershed.

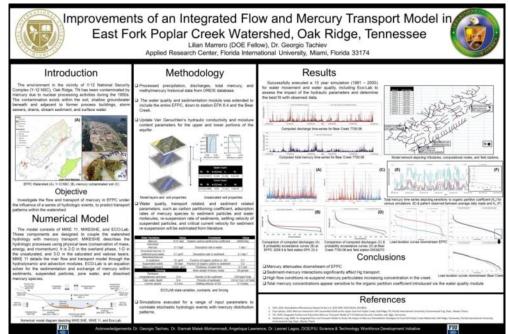


Figure 3-11 DOE Fellow student poster presented at the 2013 Waste Management Symposium

- A professional paper was also presented at the WM13 conference entitled *Recent* Approaches to Modeling Transport of Mercury in Surface Water and Groundwater – Case Study in Upper East Fork Poplar Creek, Oak Ridge, TN.
- Data results from the simulations conducted in February for this task are currently being reviewed and analyzed.
- The final technical report will then be updated with recently derived data.
- A student Master's thesis is being developed based on this research and will also be updated.

• Subtask 1.3a: Surface Water Flow and Contaminant Transport Model of ORNL 4500 Area

- Conducted additional calibration of model and sent to ORNL for review
- Ran additional simulations for the following conditions:
  - Groundwater interaction (4 variations)
  - $\circ$  Variation of percent imperviousness (+/-2 and 3%)
  - Introduced hypothetical conservative contaminant into system via Hydraulics mode (4 variations), Runoff mode (4 variations), and combination of the 2 (4 variations)
  - Design storms 5, 10, 25, 100 year design storms
- Produced MATLAB code to read 5 Manning's roughness coefficients variations, 2 infiltration variations, 5 percent imperviousness variations, 3 GW variations, and 4 design storms where the parameters: node elevation, node depth, link flow, link velocity, link USElev., and link DSElev. vs. time and their probability exceedance (PE) curves.

- There is an error when exporting data from XPSWMM where the conservative contaminant concentration data displays zeros when the polltographs indicate non-zero values. Currently troubleshooting with XPSWMM to resolve. To compensate for this error, data has been extracted per pipe per simulation, which is delaying data analysis for the transport portion of the work.
- Producing MATLAB code to read flow, concentration, create a load of the concentration and produce PE curves and fit them to the following probability density functions: extreme value, exponential, lognormal, Weibull.
- Analyzed the hydrographs and probability exceedance (PE) for the nodes and links within the network via MATLAB for the hydrology chapter of thesis.
- Produced the MATLAB code for the transport component to read flow rates, velocity, concentrations, and to create a load of the concentrations; produce hydrographs and pollutographs from the data; as well as produce PE curves. The flow rates, concentrations, and loads were then fit to the following distributions in order to characterize the data: Generalized Extreme Value, Exponential, Logistic, and Log-Logistic.
- Submitted final technical report to DOE.
- A student Master's thesis is also being developed based on this research. The hydrology chapter has been finalized and the transport chapter completed.
- Reran the transport analysis simulations by varying the conservative contaminant time series.
- Updated technical report with the revised XPSWMM hydrographs (flow versus time) and pollutographs (concentration versus time and load versus time).
- Reran MATLAB for the revised hydrographs and pollutographs and probability exceedance for flow, concentrations, and loads. These vary from the XPSWMM figures because all four scenarios are on one graph. Updated report.
- Fit the revised data to the EasyFit 5.5 tool to its 'goodness of fit' probability distribution. The following four tables indicate the results from the EasyFit 5.5 tool 'goodness of fit' probability distribution based on the following widely used probability distribution functions:
  - 1. Lognormal
  - 2. Log-Logistic
  - 3. Logistic
  - 4. Generalized Extreme Value (GEV)
  - 5. Inverse Gaussian
- Reran MATLAB for:
  - 1. Log-Logistic
  - 2. Logistic
  - 3. Generalized Extreme Value (GEV)
  - 4. Exponential

- Currently revising MATLAB code to produce consistent probability distributions with the 'goodness of fit' results, which means that the code will remove Exponential and add:
  - 1. Lognormal
  - 2. Inverse Gaussian
- *Subtask 1.3b: Surface Water Flow and Contaminant Transport Model of Y-12 NSC*The Y-12 model was expanded to cover more area of the site. The locations of outfalls were imported from the GIS file (Fig.3-12).





Figure 3-12 Location of Outfall: (a) outfalls 2-14; (b) outfalls 14-34; (c) outfalls 34-88; (d) outfalls 83-200

- The expanded Y-12 model was tested with the steady state rainfall and no loss occurred in the system (i.e. infiltration, evaporation). The model result was compared to the analytical calculation to verify the calculation capability of the model.
- The model results were identical to the analytical calculation results (mass balance). This indicates that the XPSWMM model has high accuracy and can be used for stormwater management for this site.

### Task 2: Simulation of TMDL for the Entire EFPC

- Developed spatial maps based on simulations that display flood patterns and mercury contamination patterns that include i) pore water, ii) sorbed mercury in soil, iii) and mercury in surface water.
- Developed mass balance calculations based simulations results and accounting for the major subdomains: surface, subsurface water, soil concentrations
- Presented a professional paper at WM2013 entitled *Recent Approaches to Modeling Transport of Mercury in Surface Water and Groundwater Case Study in Upper East Fork Poplar Creek, Oak Ridge, TN*, which focused on the research being conducted for this task and significant results as follows:.
  - Groundwater/surface water modeling was used to determine efficacy of stabilization in place (SIP) with hydrologic isolation for remediation of mercury contaminated areas in the Upper East Fork Poplar Creek (UEFPC) Watershed in Oak Ridge, TN.
  - SIP alternative could be less expensive than excavation, treatment, and disposal of mercury contaminated soil/sediment.
  - Modeling conducted on a watershed scale was used to determine the effect of removal of mercury contaminated soil sources on surface water concentrations at Station 17, a surface water integration point.
  - Modeling was conducted on a local scale to determine transport in groundwater from former Building 81-10 area, a site with liquid elemental mercury in soil.
  - The low solubility of mercury and high retardation factor in the soil near the former Building 81-10 minimize transport of mercury from soil to ground water. Simulations with a submodel extracted from the watershed model predict that low concentrations of mercury (defined by 10-6 mg/L) reached a steady state distribution in ground water 50 meters downgradient of the source within 50 years. However, concentrations in groundwater were below industrial risk levels (0.036 mg/L) by several orders of magnitude. Because the presence of humic acids and other strong ligands can modify the equilibrium concentration of mercury in groundwater and increase transport through groundwater pathways, additional research and modeling is needed to address this uncertainty.
  - Simulations of mercury contamination in soil did not create groundwater plumes above industrial risk standards where effective porous media conditions were present and would not influence concentrations in surface water at Station 17.
- Updated the MATLAB scripts used for model analysis and developed an additional script to allow automatic comparison between different simulations, including plotting of the main data results at selected locations (groundwater levels, contaminant concentrations, load duration curves, flow duration curves, model statistics on a daily, monthly and annual basis).
- Implemented a series of MATLAB scripts to allow hypothesis testing to show that the observed and computed data belong to the similar probability distributions.

- Downloaded the code and the manuals of SITEWISE<sup>TM</sup> which is used for analysis of remediation strategy and currently reviewing case studies.
- Prepared a presentation for the upcoming video teleconference.
- Worked on drafting annual report for the task.

### Task 3: Parameterization of Major Transport Processes of Mercury Species

- Experiments were conducted to check if elimination of oxygen during all the pretreatment procedures is necessary for conducting HgS dissolution experiments.
- A new technique, isotope dilutions (ID)-phenylation-purge and trap-ICP-MS have been developed for analyzing organomercury species at trace levels. Detection limit and recovery of this technique have been determined. Experiments are being conducted to validate the developed method by analyzing reference materials (sediment and fish).
- A paper regarding dissolution of HgS in aquatic environment is being drafted.
- Isotope tracer technique using enriched <sup>201</sup>Hg<sup>2+</sup> isotope was used to conduct experiments to investigate the role of mercury adsorption during mercury sulfide (HgS) dissolution and the experiments are ongoing.
- Experiments were conducted to determine the adsorption curves of <sup>201</sup>Hg<sup>2+</sup> onto HgS particles and further experiments are being designed and performed to link Hg adsorption to HgS dissolution.
- A paper on the dissolution of HgS in the aquatic environment was drafted and revisions are in progress to refine the manuscript.
- Adsorption curves of <sup>201</sup>Hg<sup>2+</sup> onto mercury sulfide (HgS) particles were measured by varying the concentrations of <sup>201</sup>Hg<sup>2+</sup> added to the testing systems.
- It was observed that, as expected, the adsorption of <sup>201</sup>Hg<sup>2+</sup> onto HgS particles affects the dissolution of HgS, as evidenced by the variations in the dissolved Hg concentrations in the testing systems.
- Data analysis and further experiments are being performed to correlate Hg adsorption to HgS dissolution by quantitatively determine the effect of Hg adsorption on HgS dissolution.

### Task 4: Geodatabase Development for Hydrological Modeling Support

- A customized Python script was developed which adds files from the ORR geodatabase and clips them using the EFPC domain. The script was then added to the ArcGIS toolbox developed for the ORR project work being conducted.
- Continued modification and refinement of existing Python scripts to enhance model capabilities and versatility.
- Completed review and testing of downloadable GIS freeware that can be used for querying the ORR geodatabase.

- Completed and submitted milestone progress report to DOE on 2/1/13.
- Continued review and testing of downloadable GIS freeware that can be used for querying the ORR geodatabase and sharing maps and data based on findings of the literature and Internet search. Some of the products being reviewed include:
  - ArcReader
  - ArcGIS Explorer Online
  - ArcGIS Explorer Desktop
  - o Quantum GIS
  - Christine GIS
  - Geomatica Freeviewer
  - Geospatial Explorer
  - Natural Resources Database
  - ShapeViewer
  - o TatukGIS
    - TNTAtlas
- Although several products were reviewed, only software that was easy to find on the Internet, readily available, completely free, and simple to download and install were evaluated in depth. Aside from these characteristics, the software products selected also had to be able to perform certain operations and functions such as basic zooming and panning around the map; selection of features and querying of their attributes which contain project derived data stored in the existing ORR geodatabase; addition or removal of georeferenced vector layers and raster imagery to the map; addition of customized symbology and annotation; development, customization, export and printing of map layouts with the option to insert and edit map elements such as a north arrow, scale, legend, map title, etc. Tools for measuring distance and conducting simple buffer analyses were also a consideration.
- Although at this point of project development very simplistic operations and functions are required, scalable products were given preferential consideration to provide the option of more sophisticated editing and geoprocessing capabilities in the future, particularly with respect to timeseries and hydrological data.

Software	Version	Operating System	Free/Open Source	Website
ArcReader	10.1	Windows Mac OS	Free	http://www.esri.com/software/arcgis/arcreader
ArcGIS Explorer Desktop	2500	Windows Mac OS	Free	http://www.esri.com/software/arcgis/explorer
Quantum GIS	1.8.0	Windows Mac OS	Free/Open Source	http://www.qgis.org/
DIVA GIS	7.5	Windows Mac OS	Free/Open Source	http://www.diva-gis.org/
TatukGIS Viewer	4	Windows	Free	http://www.tatukgis.com/

• The following table shows the various products reviewed by ARC-FIU.

MapWindow	4.x	Windows	Free/Open Source	http://www.mapwindow.org/
HydroDesktop	1.5	Windows	Free/Open Source	http://hydrodesktop.codeplex.com/
GRASS GIS	6	Windows	Free/Open Source	http://grass.osgeo.org/

• Completed Final Technical Report due 4/1/13.

### Task 5: Student Support for Modeling of Groundwater Flow and Transport at Moab Site

- The boundary conditions of the existing model were extended to cover additional period of 50 years and using daily timeseries.
- Available data for stage, rainfall, evapotranspiration boundaries were used to develop an extended set of timeseries using a combination of available monthly averages for each specific month
- The model is currently revised and will be extended do use daily timeseries
- Output from the model using monthly averages is compared with results using daily values.
- Downloaded topography from USGS with increased resolution and updated the Moab model.
- Reviewed the previously developed model using FEFLOW and compared input data used for FEFLOW including topography, boundary conditions, and results.
- Developed comparative charts between the two models for the duration of the simulations.
- Worked on developing MATLAB scripts to read the arrays computed by the model. The scripts will be used to reduce manual processing of the model results and to automate the workflow of conducting simulations, data analysis and comparison between simulations.
- Prepared a presentation for the upcoming video teleconference.
- Worked on drafting the annual report.
- Presented the professional poster entitled *Long-term Performance of Uranium Tailings Disposal Cells*, shown in Figure 3-6, at the 2013 Waste Management Symposium.

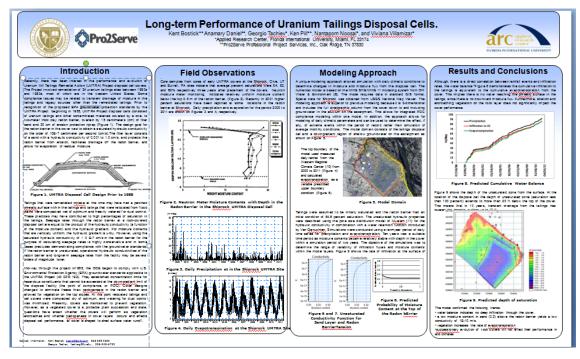


Figure 3-6 Poster presented at the 2013 Waste Management Symposium

### **Milestones and Deliverables**

The milestones and deliverables for Project 3 are shown in the following table. Milestone 2012-P3-M3.1 "Preliminary results summary of laboratory experiments" related to Task 3: Parameterization of Major Transport Processes of Mercury Species, was submitted to DOE on 1/18/2013.

Milestone 2012-P3-M4.1 "Sample Python scripts and ModelBuilder process workflow diagram" related to Task 4: Geodatabase Development for Hydrological Modeling Support was submitted to DOE on 2/1/2013, and the technical report associated with Task 3 for the Parameterization of Major Transport Processes of Mercury Species was submitted on 2/18/2013.

Also, the Technical Report deliverables for Tasks 1 and 5 were submitted to DOE on 3/1/2013 and 3/19/2013 respectively.

Task	Milestone/ Deliverable	Description	Due Date	Status	OSTI
Task 1: EFPC Model Update, Calibration, Uncertainty Analysis	2012-P3-M1.1	Finalize XPSWMM model preliminary configuration parameters	9/14/2012	Complete	
	2012-P3-M1.2	XPSWMM model preliminary results summary	11/16/2012	Complete	
	Deliverable	Technical Report for the EFPC Simulations	3/1/2013	Complete	OSTI
Task 2:	2012-P3-M2.1	Presentation overview to DOE	9/21/2012	Complete	OSTI

Simulation of NPDES- and		ORO/DOE HQ of the project progress and accomplishments		8/21/2012	
TMDL-Regulated Discharges from Non-Point Sources for the EFPC and Y-12 NSC	Deliverable	Technical Report for Simulation of NPDES and TMDL for EFPC and Y-12 NSC	4/16/2013	On Target	OSTI
Task 3: Parameterization	2012-P3-M3.1	Preliminary results summary of laboratory experiments	1/18/2013	Complete	
of Major Transport Processes of Mercury Species	Deliverable	Technical Report for the Parameterization of Major Transport Processes of Mercury Species	2/18/2013	Complete	OSTI
Task 4: Geodatabase	2012-P3-M4.1	Sample Python scripts and Model Builder process workflow diagram	2/1/2013	Complete	
Development for Hydrological Modeling Support	Deliverable	Technical Report for Geodatabase Development for Hydrological Modeling Support	4/1/2013	On Target	OSTI
Task 5: Student Support for	2012-P3-M5.1	Moab model preliminary results summary	10/19/2012	Complete	
Modeling of Groundwater Flow and Transport at the Moab Site, Utah	Deliverable	Technical Report for the Modeling of Groundwater and Flow and Transport at the Moab Site in Utah.	3/19/2013	Complete	OSTI
	Deliverable	Draft Project Technical Plan	6/18/2012	Complete	
Project-wide	2012-P2-M6.1	Waste Management Symposium 2013 abstract(s) submitted	8/17/2012	Complete	OSTI <sup>3</sup>
	2012-P3-M8.1	Submit publications to relevant journals	5/17/2013	On Target	$OSTI^4$
	Deliverable	Draft Year End Report	6/28/2013	On Target	OSTI
	Deliverable	Quarterly Status and Progress Summary Reports	Quarterly	On Target	

### Work Plan for Next Quarter

- All Tasks: Draft the Year End Report for DOE
- Task 1: Subtask 1.3a: Surface Water Flow and Contaminant Transport Model of ORNL 4500 Area
  - Analysis of data results after revision of MATLAB code to produce consistent probability distributions with the 'goodness of fit' results.
  - Update of final report.
- Task 1: Subtask 1.3b: Surface Water Flow and Contaminant Transport Model of Y-12 NSC

<sup>&</sup>lt;sup>3,4</sup> Announcement of published journal or conference paper will be submitted to OSTI

- Obtain the Y-12 site geometry (if it is possible with the security issue).
- If the site geometry is available, it will be input into the model (ground and pipe elevations, pipe sizing, location of outfalls, etc.).
- If the site geometry cannot be obtained, the Y-12 site geometry will be assumed based on the ground elevation and outfall locations (contour lines) obtained from GIS files of the area. The pipe sizing will be assumed based on ORNL data.
- Task 2: Simulation of NPDES- and TMDL-Regulated Discharges from Non-Point Sources for the EFPC and Y-12 NSC
  - Submission of Task 2 "Technical Report for Simulation of NPDES and TMDL for EFPC and Y-12 NSC", due 4/16/2013.
- Task 3: Parameterization of Major Transport Processes of Mercury Species
  - Isotope tracer technique using enriched <sup>201</sup>Hg<sup>2+</sup> isotope will be employed to conduct further experiments to measure the adsorption curves of Hg on HgS particles within a broader Hg concentration range, as previous results indicate that the dissolved Hg is related to the Hg adsorbed on the HgS particles;
  - Experiments will be designed and carried out to investigate possible processes (e.g., reduction in dissolved Hg and potential exchange reactions between Hg species) that are involved in simultaneous Hg adsorption and HgS dissolution to study how Hg adsorption affects HgS dissolution.
  - The paper on the dissolution of HgS in the aquatic environment will be further revised to refine the manuscript.
- Task 4: Geodatabase Development for Hydrological Modeling Support
  - Update of final report with findings from evaluation of downloadable GIS freeware that can be used for querying the ORR geodatabase.
  - Completion and submission of Task 4 "Technical Report for Geodatabase Development for Hydrological Modeling Support", due 4/1/2013.
- Task 5: Student Support for Modeling of Groundwater Flow and Transport at Moab Site, Utah
  - Update report and submit as part of end of year report.

# Project 4

# Waste and D&D Engineering & Technology Development

## **Project Manager: Dr. Leonel E. Lagos**

#### Task 1: Waste Information Management System (WIMS)

A professional poster entitled, *Waste Information Management System with 2012-13 Waste Streams*, was presented at the Waste Management Symposium 2013 (Figure 4-1). This poster presented WIMS with the current 2012 dataset of wastestream and transportation forecast information from the various DOE sites and facilities. The objectives of WIMS was addressed as well as the results to date for the DOE complex-wide, high performance, n-tier web-based system for generating waste forecast information, disposition maps, GIS maps, successor stream relationships, and custom reports. FIU also demonstrated WIMS to interested conference attendees at the FIU exhibitor booth during the conference.



Figure 4-1 Poster entitled *Waste Information Management System with 2012-13 Waste Streams*, presented at the Waste Management Symposium 2013

FIU discussed the upcoming new dataset for integration with WIMS with Doug Tonkay (DOE). DOE has the data from the field sites and will perform quality checks on the data prior to sending it to FIU for integration with WIMS.

Period of Performance: January 1, 2013 to March 31, 2013

FIU began making preparation for receiving the 2013 data set for incorporation into WIMS. Data is still anticipated to be reviewed and ready for transmittal to FIU in the near future. No data format changes from last year are expected. FIU will integrate the new dataset within 60 days of receipt.

Performed database management, application maintenance, and performance tuning to the online Waste Information Management System (WIMS) in order to ensure a consistent high level of database and website performance.

# Task 2: D&D Support to DOE EM for Technology Innovation, Development, Evaluation and Deployment

An oral presentation entitled, *Application and Removal of Strippable Coatings via Remote Platform*, was given at the Waste Management Symposium 2013 (Figure 4-2). This presentation reviewed the results of FIU's work with the International Climbing Machine (ICM) technology vendor in demonstrating a remote platform technology for remotely applying fixatives, strippable coatings, and decontamination gels. The presentation further presented the results of the feasibility study with ICM on using the remote platform for remotely removing strippable coatings.



Figure 4-2 Peggy Shoffner presenting *Application and Removal of Strippable Coatings via Remote Platform* at WM13

Also, FIU made a presentation at the Waste Management Symposium in Session #109 entitled *ER Challenges – Sensor Network Demonstration for In Situ Decommissioning (ISD)* (Figure 4-3). Many attendees were interested in the results of the research efforts, as implementation strategies were defined for a heterogeneous sensor network that can assist many of the ER challenges faced within the Complex.

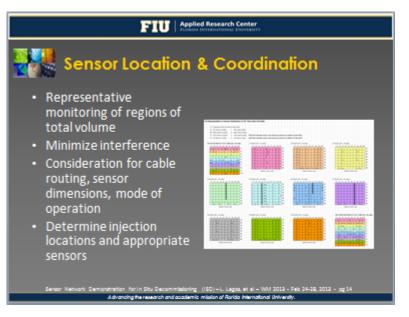


Figure 4-3 Screenshot of presentation at the Waste Management Symposium in Session #109 entitled *ER* Challenges – Alternative Approaches to Achieving End State

The sensor data network is currently operational, and continues logging system(s) data. The network virtual instruments (VI) are still being modified to improve communication, memory management and power management. The VI's are being tested using an object-oriented programming (OOP) approach in labview that will allow improved runtime execution and memory management.

FIU completed several modifications to the network virtual instruments (vi) developed for the shared data network. In particular, the data parsing vis were improved for performance and variable acquisition rates. In preparation for the planned fluid injection studies to occur on the Meso-Scale Test Bed (MSTB) in the summer months, FIU completed the troubleshooting and testing of the INL systems. The TC-AT system was completely operational, with no acquisition issues or systemic errors in the collected data. FIU also arranged for the ERT system to be shipped back to FIU facilities after repair, and be setup and tested. The TC-AT and ERT wiring configuration was verified as a QA check for INL's final efforts in completion of a final test report.

FIU is also performing a paper study of wireless charging technologies that could be integrated as part of this current MSTB, to evaluate its potential for operation with a commercial acquisition and logging systems.

FIU supported the removal and packaging of sensor systems from UH. This activity was performed by UH personnel that had come to Miami in order to collect the equipment. FIU provided site personnel for access, verification of system operational performance while at FIU, equipment handling and storage, and a final inventory check. FIU has disconnected the controller used for the shared data network node for power and weather data in the interim, while the other sensor systems are either removed or prepared for fluid injection trials. This controller will be reconnected before the end of the next performance period.

#### Carryover funding activity

The Phase II feasibility study for the remote removal of strippable coatings is complete and ICM prepared the Phase II feasibility report.

Conclusions of the report include:

1) The brush with vacuum capture was effective at removing both manufacturers' materials tested and at removing them from both concrete and metal surfaces (Figure 4-4). This method is reliable and the average productivity of 45 square feet an hour for the small size brush tested was reasonable for field expectations. A larger, more powerful production brush would yield greater productivity.



Figure 4-4 ICM remote platform using a brush with a vacuum shroud to remove strippable coating from vertical surface.

2) The gripper / scraper method was also effective at removing both manufacturers' materials and at removing them from both concrete and metal (Figure 4-5). This method is particularly fast after an edge has been lifted and, duplicating the actions of a human manually removing the strippable coating, it can be pulled up in sheets. Thus, the average productivity of this method of 75 feet per hour was quite impressive. A tool designed with two gripper / scrapers and possibly an air ejector to help manipulate the sheets of strippable coating being removed will be features built onto a production unit. These features will address certain shortcomings noted in the testing and increase productivity.



### Task 3: D&D Knowledge Management Information Tool (KM-IT)

An oral presentation entitled, *Knowledge Framework Implementation with Multiple Architectures*, was given at the Waste Management Symposium 2013 (Figure 4-6). This presentation discussed the various development and deployment architectures like n- tier architecture, web/client server architecture and service oriented architecture. It explained the features and advantages/disadvantages of each of the various architectures and the development of knowledge framework. All the modules of the D&D KM-IT framework were discussed and demonstrated. Attendees were encouraged to sign up as a registered user and subject matter specialist in D&D KM-IT.

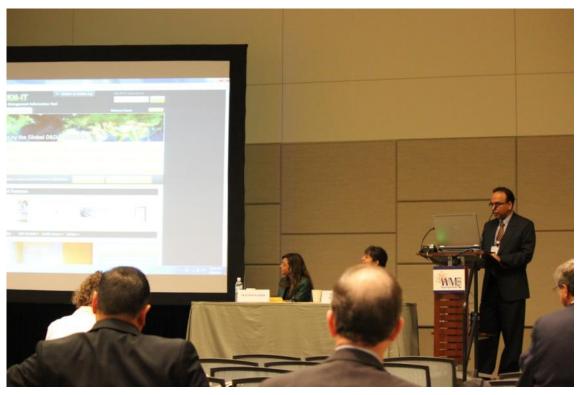


Figure 4-6 Himanshu Upadhyay presenting *Knowledge Framework Implementation with Multiple Architectures* at WM13

During the WM13 Conference, FIU hosted a booth (#635) in the exhibiters' hall to provide conference attendees with additional information on the DOE-EM applied research being conducted at ARC. Projects fact sheets were made available, as well as DVD and CD containing description of the DOE-EM applied research as well as results of the research conducted. Also, a live demonstration of the D&D Knowledge Management Information Tool (Figure 4-7) was conducted at the ARC booth. Conference attendees were encouraged and assisted with registering as users on D&D KM-IT.



Figure 4-7 Some of the FIU Staff attending WM13

The following three posters related to KM-IT were presented at the WM13 conference (Figures 4-8 to 4-10).

A student poster entitled *D&D Technology Services Development using Windows Communication Foundation on Cloud* was presented by Revathy Venkataraman (DOE Fellow) at the 2013 Waste Management Symposium Student Poster Competition.

This poster presented the technology services module provides comprehensive information on D&D related technologies, demonstrations and benefits including characterization, decontamination, dismantlement, worker health and safety and commercial vendors. The technology server module is being developed using Microsoft windows communication foundation services to study its performance, flexibility, implementation cost, scalability, interoperability and security of data when hosted in a cloud environment.

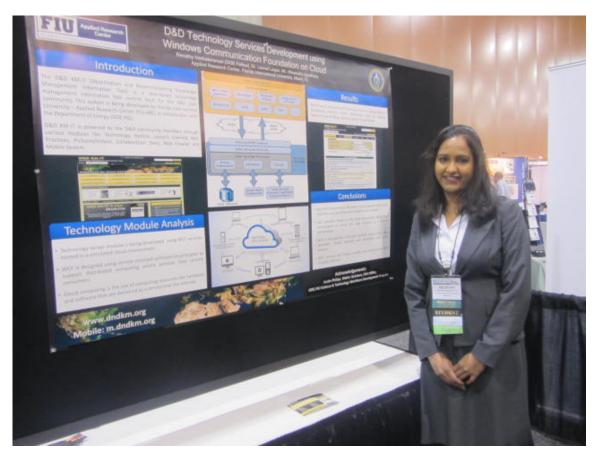


Figure 4-8 DOE Fellow, Revathy Venkataraman, presenting student poster titled *D&D Technology Services* Development using Windows Communication Foundation on Cloud at WM13.

A student poster entitled *Applications for Mobile Devices using Cloud Computing on Service Oriented Architecture* was presented by Justin Phillips (FIU Student) at the 2013 Waste Management Symposium Student Poster Competition.

This poster presented three applications (based on jQuery, ASP.NET C#, and the Android Operating System environment) were created to test the performance and viability of service-oriented architecture in the mobile development task to ensure that it meets the standards and requirements for the D&D Knowledge Management Information Tool Mobile Application.

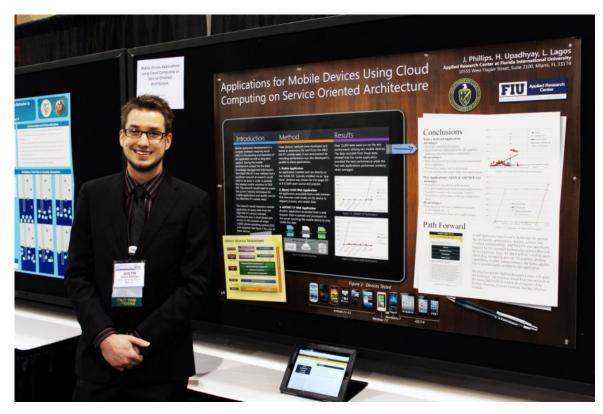


Figure 4-9 Justin Phillips presenting student poster titled *Application of Mobile Devices using Cloud Computing using Service Oriented Architecture* at WM13

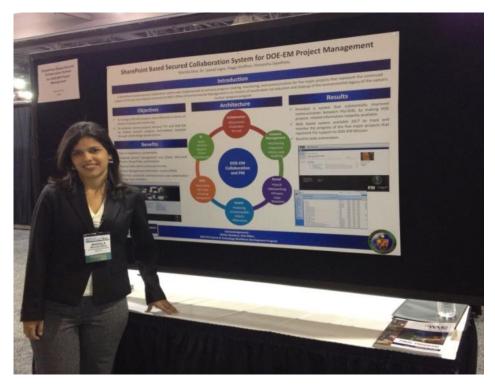


Figure 4-10 Mariela Silva presenting poster titled *SharePoint Based Secured Collaboration System for DOE*-EM Project Management at WM13

A student poster entitled *SharePoint Based Secured Collaboration System for DOE-EM Project Management* was presented by Mariela Silva (DOE Fellow) at the 2013 Waste Management Symposium Student Poster Competition.

This poster presented a SharePoint-based secured collaboration system was implemented to enhance progress tracking, monitoring, and communication for five major projects that represent the continued support of Florida International University to DOE's Office of Environmental Management in its mission of accelerated risk reduction and cleanup of the environmental legacy of the nation's nuclear weapons program.

Held bi-weekly teleconferences with DOE on project task status and action items.

Added new vendors to the D&D KM-IT vendor module. As of March 20, the Vendor module includes a total of 587 vendors. Also continued adding technologies to the Technology module from technologies identified in the SRS ISSC newsletters and industry publications. The Technology module includes 583 technologies as of March 20, 2013.

Search Engine Optimization process continues to be deployed on the D&D KM-IT web application.

A quarterly report (October to December 2012) on the D&D KM-IT web analytics was completed and sent to DOE on 1/24/13.

Completed the development and deployment of the picture lite mobile application (Milestone 2012-P4-M3.6) on 1/18/13.

Completed the development and deployment of the technology lite mobile application (Milestone 2012-P4-M3.7) on 2/15/13.

Coordination and testing was performed to prepare for televideo conferencing between FIU and DOE HQ.

### *Carryover funding activity*

The D&D KM-IT team requested an audit of the system application and infrastructure by the FIU security team for vulnerability and issues with the system. An audit report was provided by the team And FIU has resolved all of the issues identified. A followup audit by FIU was initiated in January and was completed in February. A report was generated by FIU security team on the audit results and is undergoing ARC review.

DOE granted approval for the new website template. The new website look will be implemented and deployed on the public server by the due date of April 12, 2013 (Milestone 2012-P4-M3.8). As the D&D KM-IT team implements the new website look on the KM-IT modules, DOE Fellows are performing QA testing. Specifically, they are testing that the functionality works as intended, that every browser is functional, and that the design looks consistent across browsers and modules.

The new look is based on new HTML5 standards, machine semantic friendly HTML structure, dynamic meta data, and a more intuitive layout with element placement

based on Google Analytic data. The data descriptors used are compatible with Google, Yahoo, and Bing search engines. The HTML5 standard used will help future proof the tool as well as provide a more dynamic user experience, such as animations, few page loading events, access to sharing tools, and so on. The new templatewill create a unified look and feel, a more dynamic user experience, and better search engine indexing. The new template features more dynamic logins, faster access to other modules via a module list dropdown, greater page width, and larger fonts with type enhancements for more readability.

### Milestones and Deliverables

The milestones and deliverables for Project 4 for FIU Year 3 are shown on the following table.

During this reporting period, FIU completed the development and deployment of the picture lite mobile application (Milestone 2012-P4-M3.6) and the technology lite mobile application (Milestone 2012-P4-M3.7) on 1/18/13 and 2/15/13 respectively.

Task	Milestone/ Deliverable	Description	Due Date	Status	OSTI
Task 1: Waste Information Management System (WIMS)	2012-P4-M1.1	Import 2012 data set for waste forecast and transportation data	Within 60 days of receipt of data from DOE	Complete	
	2012-P4-M1.2	Import 2013 data set for waste forecast and transportation data	Within 60 days after receipt of data from DOE	On Target	
	2012-P4-M1.3	Waste Management Symposium 2013 abstract submitted	08/17/2012	Complete	OSTI <sup>5</sup>
	2012-P4-M2.1	Completion of Meso-Scale Testbed System Demonstration	09/30/2012 Re-forecasted to 11/23/2012	Complete	
Task 2: D&D Support to DOE EM for	2012-P4-M2.2	Completion of preliminary prototype technology evaluation for remote removal of strippable coatings	04/26/2013	On Target	
Technology Innovation,	2012-P4-M2.3	Waste Management Symposium 2013 abstract submitted	08/17/2012	Complete	OSTI <sup>6</sup>
Development, Evaluation, and	Deliverable	Lessons Learned and Best Practices	30 days after final DOE/EFCOG approval	On Target	
Deployment	Deliverable	Draft technical reports for demonstrated technologies	30-days after evaluation/demo	On Target	OSTI
	Deliverable	Draft Tech Fact Sheet for technology evaluations/ demonstrations (ICM crawler)	30-days after evaluation/demo	On Target	
Task 3: D&D Knowledge Management Tool (D&D	2012-P4-M3.1	Deployment of SRS ISSC report integration to DOE for review/testing	07/13/2012	Complete	
	2012-P4-M3.2	Deployment of global search feature to DOE for review/testing	08/17/2012	Complete	
KM-IT)	2012-P4-M3.3	Waste Management Symposium 2013 abstract	08/17/2012	Complete	OSTI

#### FIU Year 3 Milestones and Deliverables for Project 4

<sup>&</sup>lt;sup>5,6</sup> Announcement of published journal or conference paper will be submitted to OSTI

		submitted			
	2012-P4-M3.4	Deployment of D&D dictionary module to DOE for review/testing	09/28/2012	Complete	
2012-P4-M3.5		Deployment of the multiple SMS support for the D&D Hotline	11/16/2012	Complete	
	2012-P4-M3.6 Deployment of picture lite mobile application to DOE for review/testing		01/18/2013	Complete	
	2012-P4-M3.7	Deployment of technology lite mobile application to DOE for review/testing	02/15/2013	Complete	
	2012-P4-M3.8 User interface enhancement completion		04/12/2013	On Target	
	2012-P4-M3.9	Help videos development complete and sent to DOE for review	05/17/2013	On Target	
	Deliverable	Draft Summary Report for Mobile Development Research	12/14/2012	Complete	
	Deliverable	D&D KM-IT Performance Analysis Report	Quarterly	On Target	
	Deliverable	Draft Tech Fact Sheet for new modules or capabilities of D&D KM-IT	30-days after new module deployed	On Target	
	Deliverable	Draft Project Technical Plan	06/18/2012	Complete	
Project Wide	Deliverable	Draft Year End Report	06/28/2013	On Target	OSTI
	Deliverable	Quarterly Progress Reports	Quarterly	On Target	

#### Work Plan for Next Quarter

- All Tasks: Draft the Year End Report for DOE.
- Task 1: Perform database management, application maintenance, and performance tuning to WIMS.
- Task 1: Integrate new waste forecast data into WIMS within 60 days of receiving a new dataset from DOE.
- Task 2: Complete feasibility evaluation for remote removal of strippable coatings and decon gels.
- Task 2: FIU will test the shared data network with the ERT and TC-AT system if the ERT system arrives to FIU in time. In addition, FIU will also complete the power network literature review that evaluated the possible energy infrastructure approaches for such a deployed sensor network.
- Task 3: Complete design, development, and deployment of website interface enhancement.
- Task 3: Complete development of help videos for KM-IT.

# Project 5 DOE-FIU Science & Technology Workforce Development Initiative

## **Project Manager: Dr. Leonel E. Lagos**

Fellows continue their support to the DOE-FIU Cooperative Agreement by actively engaging in EM applied research and supporting ARC staff in the development and completion of the various tasks. Also, the program director continues to work with DOE sites and HQ to fully engage DOE Fellows with research outside ARC where Fellows provide direct support to mentors at DOE sites, DOE-HQ, and DOE contractors.

Coordinated travel for DOE Fellows to attend Waste Management 2013 Symposium.

DOE Fellows participated in the Waste Management 2013 Conference (WM13) in Phoenix, AZ, from February 24 to February 28, 2013. A total of twenty-two (22) FIU students, including 21 DOE Fellows, participated in WM13 and twenty (20) presented technical posters during Session 31 (Student Poster Competition: The Next Generation – Industry Leaders of Tomorrow) based on the hands-on research that they have performed at ARC and during their summer internships at DOE sites, national laboratories, and site contractors (Figures 5-1 and 5-2). Poster presenters and titles included:

DOE	Poster Title / Brief description			
<b>Fellow/Student</b>				
Jennifer	High-Level Waste Pipeline Unplugging Technologies: Asynchronous Pulsing			
Arniella	System. The asynchronous pulsing method creates pressure waves in a flooded			
	pipeline from both ends of a blocked section. The waves are created			
	asynchronously in order to break the mechanical bonds between the blockage			
	and pipe wall. We are currently working on understanding how the air and the			
	geometry of the pipeline affect the pressure waves. (Figure 5-3)			
Francisco	Computer Simulations of Multiphase Flow Systems Applied to Transfer of			
Bolanos	High-Level Waste. This work presents computer simulations dealing with 2D			
	and 3D multiphase Lattice Boltzmann Method for high density ratio systems.			
	The method is intended to accurately represent and predict fluid fluids in high			
	level waste storage tanks. Simulations of computer model are presented and			
	compared to benchmark case. (Figure 5-4)			
Claudia	The Effect of Ca Ions on the Removal of U(VI) at the Hanford Site Area.			
Cardona	Injection of NH3 is an innovative technology that targets uranium			
	contamination in the vadose zone to reduce radionuclides mobility in			
	subsurface. The effect of porewater constituents such as Si, Al, Ca, HCO3 on			
	the U(VI) co-precipitation process is unknown. The research investigates the			
	effect of porewater constituents on the removal of U(VI). (Figure 5-5)			
Dania Castillo	Computational Simulation and Evolution of High-Level Waste Pipeline Plugs			
	at Hanford. A multi-physics module is being developed to efficiently simulate			
	and predict the formation of a plug in a high level waste pipeline. The			

simulations will demonstrate the relationship between plug formation and
critical flow velocity, pipeline geometry and the physical properties of the
waste stream during the transfer process. (Figure 5-6)
Battery-less Wireless Sensors for Structural Health Monitoring for In-Situ
Decommissioning of DOE Facilities. Design considerations for monitoring
using batteryless RFID sensing platforms inside grout, used for
decommissioning DOE's nuclear facilities, include several key areas (e.g.,
materials characterization, transmission losses, sensor placement, etc.). These
design considerations for structural monitoring using wireless sensors are
applied to the detection of temperature, humidity and strain inside building
structures. (Figure 5-7)
Hydrogen in Pipes and Ancillary Vessels in Waste Treatment Plant at the
Hanford Site. An evaluation, based on various research and testing, that
determines the validity and dangers involved with a possible hydrogen
explosion event which can possibly occur within the pipes in the "black cells"
and "hot cells" of the waste treatment plant being built at DOE's Hanford
Site. (Figure 5-8)
Storm Water Management Model Analysis of the Oak Ridge Storm Water
Collection System Up To Outfall 211. A hydrologic-hydraulic model of the
ORNL 4500 Area's stormwater collection system has been developed in order
to quantify flow rates within the system. The resulting flow rates from the
model may be utilized in conjunction with contaminant data to assess
contamination within the system. (Figure 5-9)
Single Pass Flow-Through Testing of Metals for Hanford 200 Area Vadose
<i>Zone.</i> This study investigates the effects of variables on the morphology and
composition of U-bearing precipitates created as a result of ammonia gas pH
manipulation in the Hanford 200 Area vadose zone conditions. The analysis
of samples by scanning electron microscopy and energy dispersive
spectrometry gauged the impact of variables such as time, bicarbonate
concentration, and calcium concentration. (Figure 5-10)
Improvements and Modifications of an Integrated Flow and Mercury
Transport Model for East Fork Poplar Creek, Oak Ridge, Tennessee. Portions
of the East Fork Poplar Creek watershed were heavily contaminated with
mercury as a byproduct of nuclear processing activities. An integrated surface
and subsurface flow and transport model was developed and implemented to
determine the effect of hydrological and hydraulic parameters on mercury

Jose Matos	Development of Improved Bodies for a Peristaltic Crawler for Unplugging of
	Hanford Waste Transfer Pipelines. Limitations in speed and force output of
	current peristaltic crawler robot designs limit their viability as an unplugging
	tool for DOE Hanford Site pipelines. The study described in this poster covers
	a new design of the crawler device which incorporates powerful, micro
	pneumatic cylinders in order to address these shortcomings. (Figure 5-12)
Joel McGill	Degradation of Grout: Compressive Strength Comparative Analysis. This
	research assists the Savannah River Site in their planned monitoring of the P
	and R reactor sites which have been decommissioned via in situ
	decommissioning. This project will help aid in the monitoring of the longevity
	of the compressive strength of the grout used to entomb the sites'
	underground portions. (Figure 5-13)
Joshua Midence	Saltstone Processing of Low-Level Waste at Savannah River Site. The process and
	safe storage of low-level radioactive waste at Savannah River site is of
	concern. The Saltstone formulation (a cementitious mixture) must produce a
	grout waste form that meets both placement and performance properties.
	Saltstone is a breakthrough process that not only encloses the tanks, but
	absorbs some of the damaging chemicals to be transported offsite. (Figure 5-
Jaime Mudrich	14) A Lattice Boltzmann Method for the Analysis of Gas Behavior in Hanford
Jaime Muunen	<i>Tanks.</i> In this work, computer simulations are presented based on the 3D
	multiphase lattice Boltzmann method for high density ratio systems. The
	method is capable of incorporating complex geometries generated in CAD
	software. The geometries are voxelized and then imported for use in
	multiphase flow simulations. Surface wetting features enable accurate
	simulation of contact angles. (Figure 5-15)
Lucas	Acoustic Pulse Reflectometry For Identifying Pipeline Properties At Hanford
Nascimento	Site. The U.S. Department of Energy's Hanford Site waste retrieval and
	transfer process can lead to pipeline plugging and corrosion. Acoustic pulse
	reflectometry (APR) is a technique that measures reflections from a volume to
	estimate plug formation and changes in pipeline geometry. This technique
	can be used to select unplugging technologies. (Figure 5-16)
Raul Ordonez	Sensor Network Energy Demand for In-situ Decommissioning Applications at
	Savannah River Site. The electrical resistance tomography (ERT) system is
	used to gain a better understanding of the performance of cementitious
	materials used for in situ decommissioning (ISD) at the Savannah River Site.
	The ERT system consumes too much power in the sensor network; therefore,
	other sources of energy or alternate methods were researched to diminish
	consumption. (Figure 5-17)
Justin Phillips	Mobile Device Applications using Cloud Computing on Service Oriented
	Architecture. Three applications (based on jQuery, ASP.NET C#, and the
	Android Operating System environment) were created to test the performance
	and viability of service-oriented architecture in the mobile development task
	to ensure that it meets the standards and requirements for the D&D
Vincena	Knowledge Management Information Tool Mobile Application. (Figure 5-18)
Ximena Prugue	Development of a Mechanical based System for Dry Retrieval of Single-Shell

	<i>Tank Waste at Hanford</i> . This study explores the development of a mechanical
	based system to retrieve single-shell tank waste at Hanford without the
	addition of water. Focusing on leaking tanks and tanks with significant in-
	tank obstruction and utilizing existing risers in Hanford's tanks, commercially
	available technologies are evaluated for cost and efficiency. (Figure 5-19)
Mariela Silva	SharePoint Based Secured Collaboration System for DOE-EM project
	management. A SharePoint-based secured collaboration system is being
	implemented to enhance progress tracking, monitoring, and communication
	for five major projects that represent the continued support of Florida
	International University to DOE's Office of Environmental Management in its
	mission of accelerated risk reduction and cleanup of the environmental legacy
	of the nation's nuclear weapons program. (Figure 5-20)
Gabriela	Improved Third Generation Peristaltic Crawler for Removal of High-Level
Vazquez	Waste Plugs in Hanford Site Pipelines. The improved third generation
	pneumatic/hydraulic operated peristaltic crawler propels itself by a sequence
	of pressurization/depressurization of cavities used for unplugging clogged
	radioactive waste transport lines. The third generation crawler showed speed
	and maneuverability restrictions. The new design incorporates pneumatic
	valves to reduce cycle time, inspection camera for visual feedback, and a thin
	walled outer bellow for improved maneuverability. (Figure 5-21)
Revathy	D&D Technology Services Development using Windows Communication
Venkataraman	Foundation on Cloud. The Deactivation and Decommissioning Knowledge
	Management Information Tool (D&D KMIT) is a web-based tool custom
	built for the D&D user community. Its technology server module is being
	developed using Microsoft windows communication foundation services to
	study its performance, flexibility, implementation cost, scalability,
	interoperability and security of data when hosted in a cloud environment.
	(Figure 5-22)



Figure 5-1 DOE Fellow Gabriela Vazquez presenting her research at the 2013 Waste Management Symposium

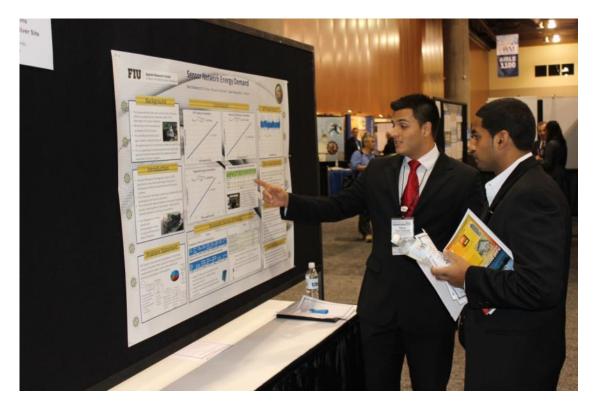


Figure 5-2 DOE Fellow Raul Ordonez presenting his research at the 2013 Waste Management Symposium

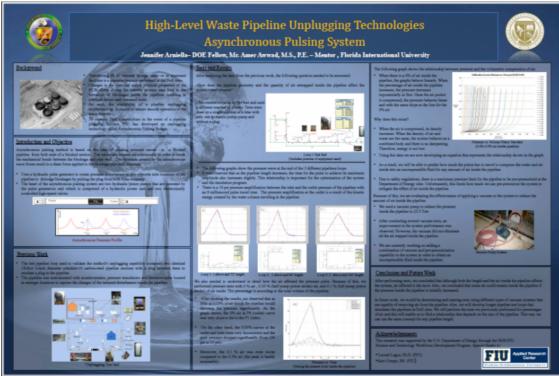


Figure 5-3 High-Level Waste Pipeline Unplugging Technologies: Asynchronous Pulsing System

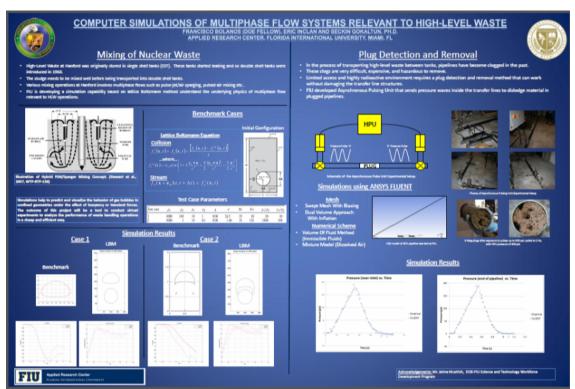


Figure 5-4 Computer Simulations of Multiphase Flow Systems Applied to Transfer of High-Level Waste

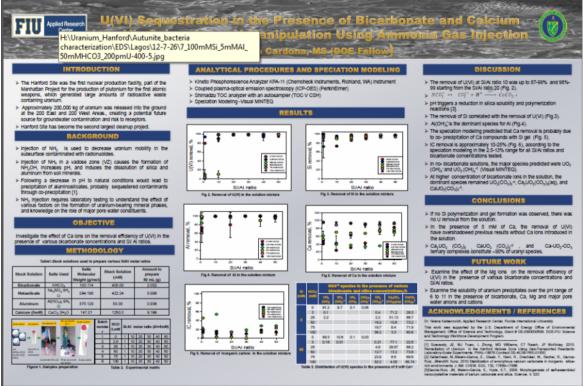


Figure 5-5 The Effect of Ca Ions on the Removal of U(VI) at the Hanford Site Area

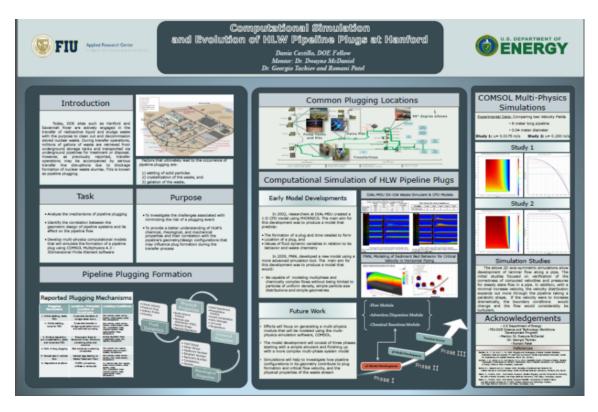


Figure 5-6 Computational Simulation and Evolution of High-Level Waste Pipeline Plugs at Hanford

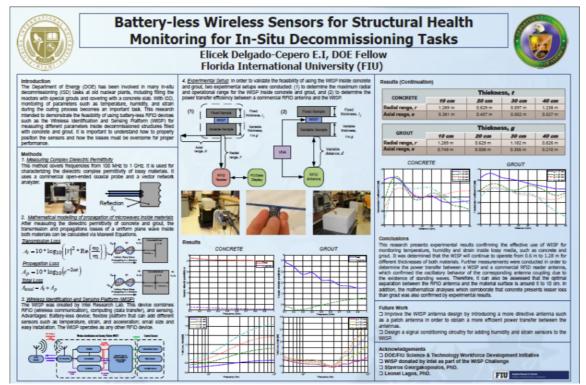


Figure 5-7 Battery-less Wireless Sensors for Structural Health Monitoring for In-Situ Decommissioning of DOE Facilities

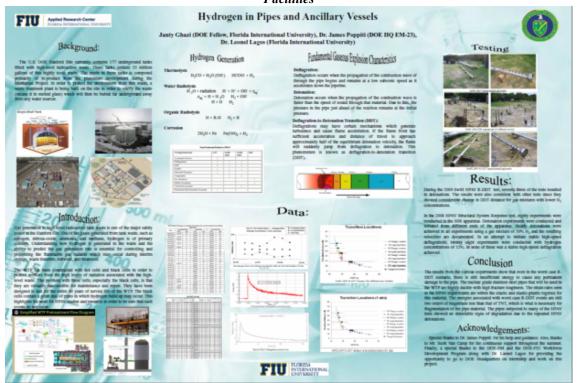


Figure 5-8 Hydrogen in Pipes and Ancillary Vessels in Waste Treatment Plant at the Hanford Site

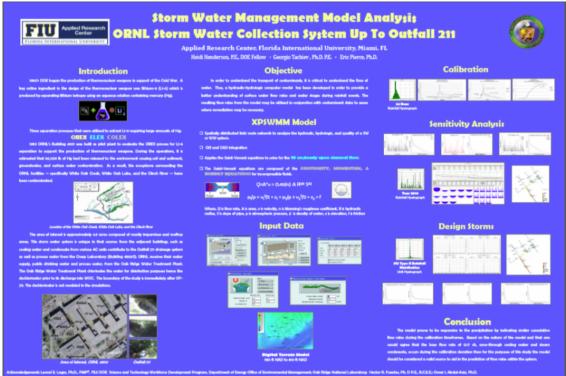


Figure 5-9 Storm Water Management Model Analysis of the Oak Ridge Storm Water Collection System Up To Outfall 211

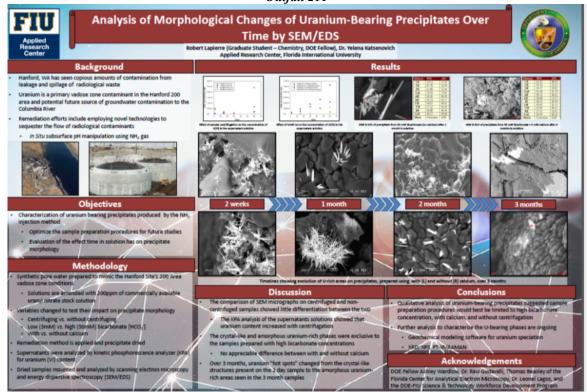


Figure 5-10 Single Pass Flow-Through Testing of Metals for Hanford 200 Area Vadose Zone

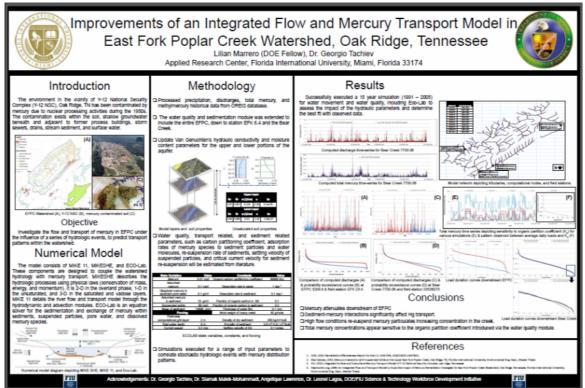


Figure 5-11 Improvements and Modifications of an Integrated Flow and Mercury Transport Model for East Fork Poplar Creek, Oak Ridge, Tennessee

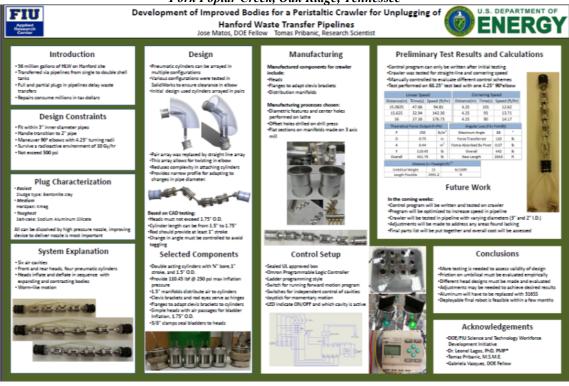


Figure 5-12 Development of Improved Bodies for a Peristaltic Crawler for Unplugging of Hanford Waste Transfer Pipelines

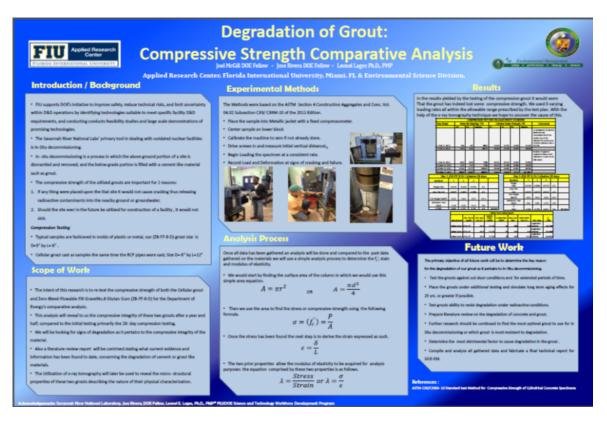


Figure 5-13 Degradation of Grout: Compressive Strength Comparative Analysis

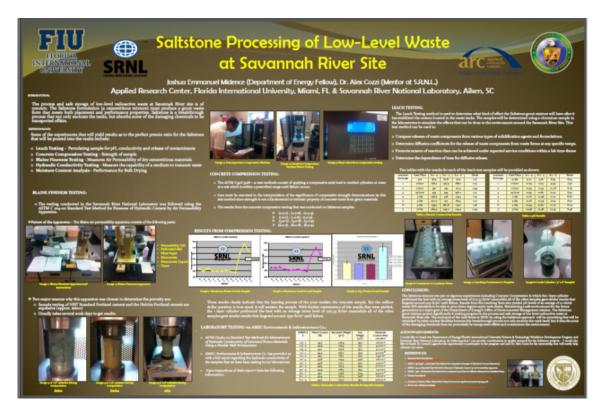


Figure 5-14 Saltstone Processing of Low-Level Waste at Savannah River Site

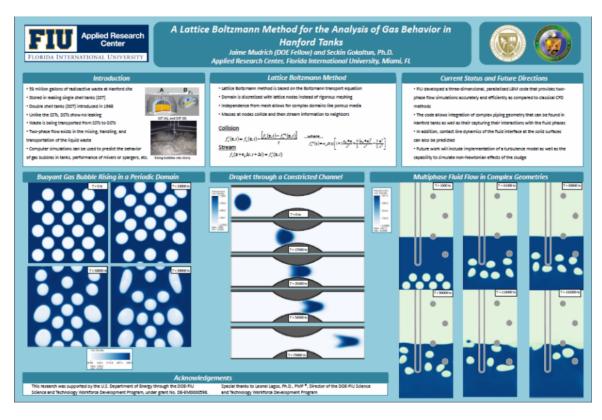


Figure 5-15 A Lattice Boltzmann Method for the Analysis of Gas Behavior in Hanford Tanks

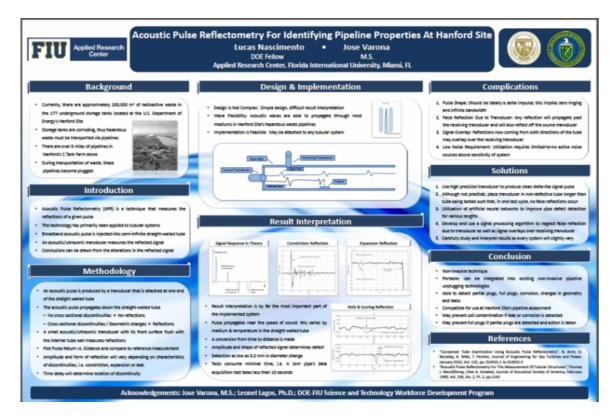


Figure 5-16 Acoustic Pulse Reflectometry For Identifying Pipeline Properties At Hanford Site

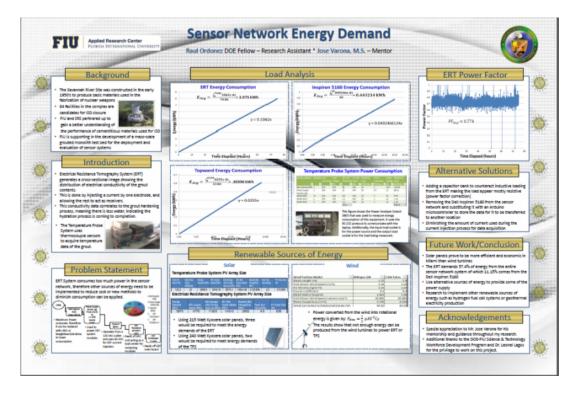


Figure 5-17 Sensor Network Energy Demand for In-situ Decommissioning Applications at Savannah River Site



Figure 5-18 Mobile Device Applications using Cloud Computing on Service Oriented Architecture



Figure 5-19 Development of a Mechanical based System for Dry Retrieval of Single-Shell Tank Waste at Hanford

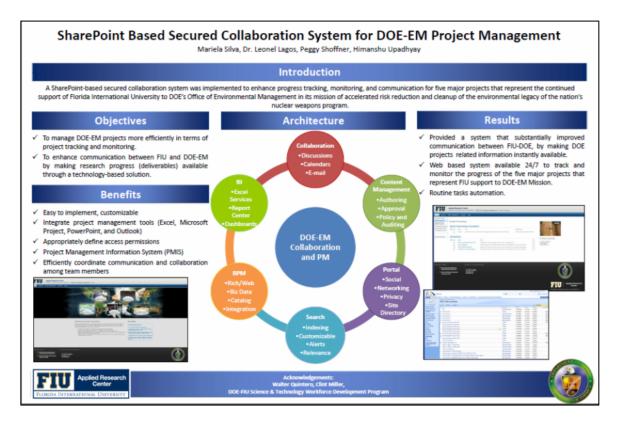


Figure 5-20 SharePoint Based Secured Collaboration System for DOE-EM project management

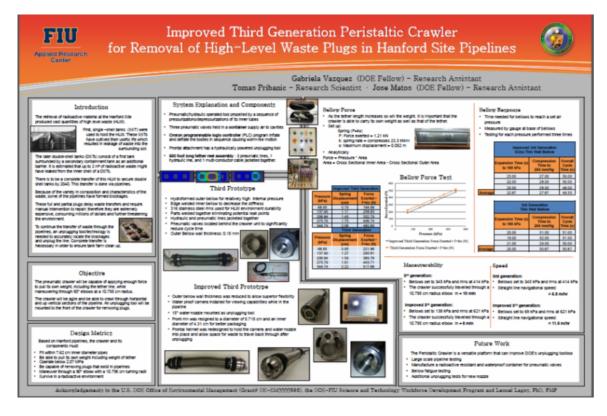


Figure 5-21 Improved Third Generation Peristaltic Crawler for Removal of High-Level Waste Plugs in Hanford Site Pipelines

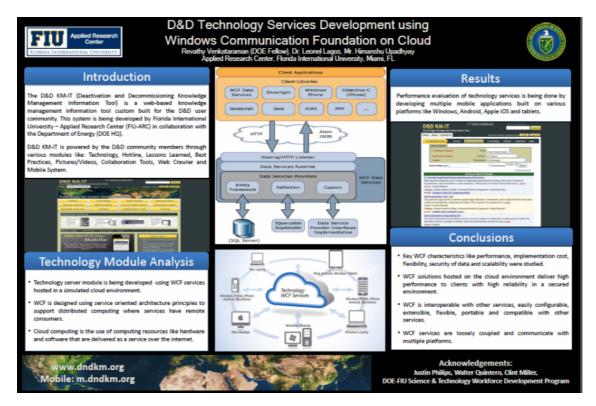


Figure 5-22 D&D Technology Services Development using Windows Communication Foundation on Cloud

Period of Performance: January 1, 2013 to March 31, 2013

In addition, 2 DOE Fellows (Paola Sepulveda and Lilian Marrero) presented their DOE-EM research during the professional oral sessions.

The DOE Fellows also had the opportunity to meet Mr. David Huizenga (DOE's Senior Advisor for Environmental Management) and had a chance to describe their EM applied research work at FIU's Applied Research Center and the work they have performed during their internships at DOE HQ, DOE sites and national laboratories (Figure 5-23).



Figure 5-23 Mr. Dave Huizenga and DOE Fellows at WM13]

In addition, one (1) DOE Fellow (Ximena Prugue) participated in a panel session at the conference, Session 62 on "Graduating Students and New Engineers – Their Wants and Needs." During this panel session, students and industry and government representatives shared their perspectives of the newer generation entering a workforce primarily occupied by workers nearing retirement age (Figure 5-24). A former DOE Fellow, Rosa Elmetti (DOE EM), participated in a second panel session at WM13, Session 63 on "Young Professionals." Ms. Elmetti described her experience as a DOE Fellow and as a young professional working for DOE EM's International Program.



Figure 5-24 DOE Fellow Ximena Prugue presenting in the panel session *Graduating Students and New* Engineers – Their Wants and Needs.

The FIU students also had the opportunity to participate as Student Assistants at the conference and helped conference organizers and presenters during the technical sessions. In addition, interested DOE Fellows attended the Women of Waste Management panel and had a chance to interact with a working group of professional women in the industry.

DOE Fellows Program Director (Dr. Lagos) performed as the lead organizer for the student poster session (session 31) and co-chaired the panel discussions (sessions 62 and 63) on "Graduating Students and New Engineers – Their Wants and Needs" and "Young Professionals" (Figure 5-25). Dr. Lagos also made a professional oral presentation on "Training and Mentoring the Next Generation of Scientists and Engineers to Secure Continuity and Successes of the US DOE's Environmental Remediation Efforts."



Figure 5-25 Panel discussions on "Graduating Students and New Engineers – Their Wants and Needs

The DOE Fellows program director continued to coordinate placement of DOE Fellows for summer 2013 internships. DOE Fellows prepared biographies and resumes to send to site representatives. Summer internships opportunities are being coordinated with DOE-HQ, Moab site, Hanford site, Savannah River National Laboratory, Pacific Northwest National Laboratory, Oak Ridge National Laboratory and Y-12 Security Complex.

DOE Fellow Elicek Delgado-Quintana prepared her poster titled *Structural Health Monitoring (SHM) inside Concrete and Grout using the Wireless Identification and Sensing Platform (WISP)* based on her research on RFID, for the 7<sup>th</sup> Annual Institute of Electrical and Electronics Engineers International (IEEE) Conference on RFID. This conference, known as IEEE RFID 2013, will be held at the Orange County Convention Center in Orlando, FL, from April 30 to May 2, 2013. RFID stands for radio-frequency identification and is the wireless non-contact use of radio-frequency electromagnetic fields to transfer data.

DOE Fellows Spring recruitment efforts started during the month of March. During this period, the current DOE Fellows and program director will host an Information Session for potential candidates, conduct recruitment campaigns by placing recruitment tables at College of Engineering, participate in the FIU College of Arts and Science's Job and Internship Fair, and make short presentations at targeted classes within the College of Engineering and College of Arts and Sciences.

DOE Fellows continued to assist EFCOG in developing Lessons Learned and Best Practices documents. A total of 7 the Best Practices and Lessons Learned documents are final, two have recently been reviewed by DOE and are undergoing revision, and three are in development and review at FIU.

Doc	BP/LL	Title	РОС	Status as of 3/30/2013
1	BP	Explosive Demolition of Buildings 337, 337B, and the 309 Stack at the Hanford's 300 Area	Daniel Beckworth, Bob Smith, and Thomas Kisenwether	FINAL
2	BP	Open Air Demolition of Asbestos Gunite by Using a Track Mounted Wet Cutting Saw	Rob Vellinger	FINAL
3	BP	185-3K Cooling Tower Demolition	Bill Austin	FINAL
4	BP	Historical Hazard Identification Process for D&D	Paul Corrado	FINAL
5	LL	Closure of the Reactor Maintenance, Assembly, and Disassembly Facility and the Pluto Disassembly Facility at the Nevada National Security Site	Annette Primrose	Reviewed by DOE HQ. In revision.
6	LL	Unanticipated High Dose During the Removal of Wire Flux Monitor Cabling from the HWCTR Reactor Vessel	Bill Austin	FINAL
7	LL	Radiological Contamination Event during Separations Process Research Unit (SPRU) Building Demolition	Brad Smith	Reviewed by DOE HQ. In revision.
8	BP	Structural Code Guidance for D&D Activities at DOE Facilities	Kirk Dooley	FINAL
9	BP	Electrical Code Guidance for D&D Activities at DOE Facilities	Kirk Dooley	FINAL

10	BP	SRS R and P -Reactor Disassembly Basin In Situ Decommissioning	Bill Austin	Under development and review at FIU.
11	BP	Use of Earthen Benches and other Technologies to Support River Structures' Demolition Activities	Brad Smith	Drafted. Under review at FIU.
12	BP	327 Facility Source Term Stabilization and/or Removal Prior to Demolition	Brad Smith	Drafted. Under review at FIU.

#### **Milestones and Deliverables**

The milestones and deliverables for Project 5 for FIU Year 3 are shown on the following table. No milestones or deliverables were due during this period.

Milestone/ Deliverable	Description	Due Date	Status	OSTI
2012-P5-M1	Selection of new DOE Fellows - Spring 2012	05/30/12	Complete	
Deliverable	Draft Project Technical Plan sent to DOE	06/18/12	Complete	
Deliverable	List of 2012 Student Summer Interns and their research assignment	06/29/12	Complete	
2012-P5-M2	Waste Management Symposium 2013 abstract submitted	8/17/2012	Complete	OSTI <sup>7</sup>
2012-P5-M3	DOE Fellows Complete Summer Internships	08/31/12	Complete	
2012-P5-M4	Summer Internships Reports Completed	10/05/12	Complete	
Deliverable	Deliver Summer 2012 Interns reports to DOE	10/19/12	Complete	OSTI
2012-P5-M5	Selection of new DOE Fellows – Fall 2012	10/30/12	Complete	
Deliverable	List of identified/recruited DOE Fellow (Class of 2012)	10/31/12	Complete	
2012-P5-M6	Conduct Induction Ceremony – Class of 2012	11/13/12	Complete	
2012-P5-M7	Waste Management Symposium 2013 (submittal of student abstracts)	12/31/2012	Complete	OSTI
Deliverable	Draft Year End Report	06/28/13	On Target	OSTI

FIU Year 3	<b>Milestones</b>	and Deliver	ables for	Project 5
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#### Work Plan for Next Quarter

- Draft the Year End Report for DOE.
- Complete Spring 2013 campaign to recruit new students into the DOE Fellows program.
- Complete coordination of internship placements for summer 2013, including travel and housing. DOE Fellows will begin summer internships in June 2013.
- Participate in IEEE RFID 2013 conference scheduled for the end of April 2013.

Period of Performance: January 1, 2013 to March 31, 2013

<sup>&</sup>lt;sup>7</sup> Announcement of published journal or conference paper will be submitted to OSTI