

# **QUARTERLY PROGRESS REPORT**

July 1, 2011 to September 30, 2011

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

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## Introduction

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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 July 1 to September 30, 2011.

# Project 1

## Chemical Process Alternatives for Radioactive Waste

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**Project Manager: Dr. Dwayne McDaniel**

### **Project Description**

Florida International University has been conducting research on several promising alternative processes and technologies that can be applied to address several operational shortcomings in the current high-level waste processing strategy. The implementation of advanced technologies to address challenges faced with baseline methods is of great interest to the Hanford site. Specifically, the use of field or *in situ* technologies, as well as advanced computational methods can improve several facets of the retrieval and transport processes of HLW. FIU has worked with site personnel to identify three technology and process improvement needs that can benefit from FIU's core expertise in HLW. These needs are being addressed by the following tasks:

- Task 2: Pipeline Unplugging and Plug Prevention
- Task 12: Multiple-Relaxation-Time, Lattice Boltzmann Model for High-Density Ratio, Multiphase Flows
- Task 15: Evaluation of Advanced Instrumentation Needs for HLW Retrieval

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

#### Task 2 Overview

Over the past few years, FIU has found that commercial technologies do not meet the needs of DOE Sites in terms of their ability to unplug blocked HLW pipelines. FIU has since undertaken the task of developing alternative methods/technologies with the guidance from engineers at the national laboratories and site personnel. The new approaches that are being investigated include an asynchronous pulsing method and a peristaltic crawler. Both technologies utilize lessons learned from previous experimental testing and offer advantages that other commercially available technologies lack. The objective of this task is to continue efforts on the development of the two novel technologies for pipeline unplugging. The first phase of experimental testing conducted during the previous performance period demonstrated the technologies' potential for successful pipeline unplugging operations. The research that is being carried out during this performance period focuses on the experimental testing of the technologies on a larger scale.

#### Task 2 Quarterly Progress

- For the **peristaltic crawler**, a number of vendors were contacted who could provide the inner and outer bellows. There seems to be some difficulty finding a vendor who can assemble the units. We began constructing an FEA to determine if the bellows described by the vendors would have the strength and fatigue properties needed for the crawler.
- Validation of the FEA was completed for the peristaltic crawler. Experimental tests showed good correlation with the FEA data in terms of the obtained stiffness values. The FEA will next be used to optimize the bellow design with respect to bellow diameter and material thickness.

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- An FEA analysis was conducted to validate that the peristaltic crawler bellow can flex 90° and pass through a 90° elbow. The diameter of the bellow was also reduced to facilitate movement through the elbow. This reduction results in increased flexural stiffness. The FEA provides information regarding the bellow's response to the 90° turns and will assist in the design.
- We have been working with a vendor to obtain a quote for a reel to assist in deploying the crawler. The tubing for the reel will have the capability to connect with 4 ports - 3 pneumatic and 1 hydraulic.
- FIU has initiated a review of available instrumentation for the crawler to provide feedback on the internal pipe conditions. The instrumentation will have limitations regarding operation environment (HLW) and operating distance.
- For the **asynchronous pulsing system**, initial tests were repeated on the small scale test bed and a leak was found. After an extensive diagnosis, it was found that the Victaulic gaskets in the pipeline could not handle the vacuum pressures induced by the piston.
- An alternative testbed design was generated with the use of extended tees in place of the previously used couplings with pressure ports. This will allow for smaller gaskets and resolve the air leak issue.
- New tees and gaskets arrived and are currently being installed in the asynchronous pulsing testbed. The system will be checked for leaks to verify that new design can handle the pressure envelope required for testing. A revised test plan has also been developed and will be provided to the site contacts in October.

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

### Task 12 Overview

This task uses the knowledge acquired at FIU on implementing the Lattice Boltzmann Model (LBM) for multiphase flow modeling to create a multi-phase LBM using multiple-relaxation-time (MRT) collision models in three-dimensions having high performance computing capabilities. Focus is given to bubble dynamics in liquids, and the simulation results are being validated against the analytical and experimental data published in the literature for buoyant bubbles rising in liquid columns under the influence of gravity. The objective of this task is to provide the sites with mathematical modeling, validation, and testing of computer programs to support critical issues related to HLW retrieval and processing.

### Task 12 Quarterly Progress

- Finished development of 3D MRT LBM serial code based on the Lee and Lin model. Had numerous discussions with Dr. Deiterding at ORNL to incorporate an adaptive grid refinement method and sent him the 2D version of the code.
- The code currently has numerical instabilities due to the selection of the 19 relaxation parameters. There is limited information regarding these parameters in the literature for multiphase flow applications. The next step will be to run the code with a single value for

the 19 relaxation parameters which reduces the approach to the BGK method and will verify that the MRT code is correct.

- The relaxation parameters for the 3D MRT LBM code have been changed in accordance with a paper by D’humieres (2002). Stability results were improved but the accuracy is currently being tested for a static bubble case using the Laplace equation to determine the pressure difference across the bubble. In addition, the 2D BGK LBM code was run on a parallel computer cluster using the message passing interface library. The 2D MRT code is also in the process of being converted to run on a parallel computer.
- The 3D LBM MRT code has been run successfully for static bubble simulations using the relaxation parameters provided by D’Humieres (2002). Three different bubble diameters were tested at various surface tension values in order to calculate the pressure difference between the bubble and the surrounding fluid. The results were found to have 5-10% error compared to the analytical value obtained by the Laplace equation.
- A rising bubble simulation has been also conducted using the 3D LBM MRT code by imposing a buoyancy force on the bubble in the vertical direction. A spherical bubble shape was obtained. Periodic boundary conditions were used in all directions. Validation cases will be performed using experimental benchmark cases.
- A journal manuscript is being prepared regarding the experimental and computational analysis of NuVision wave erosion technology.

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

### Task 15 Overview

The purpose of this task is to evaluate the maturity and applicability of commercial and emerging technologies capable of addressing several instrumentation needs for HLW feed mixing and retrieval. During FY2011, this task continues the laboratory evaluation of the identified candidate technologies that began during the previous performance period. The objective of this year’s work is to continue laboratory investigations of the identified alternative and promising instrumentation for HLW mixing and retrieval. Specifically, the task continues the evaluation of the Ultrasonic Spectroscopy (USS) and the Coriolis-based as viable techniques for the measurement of bulk density directly within the tank. Also, FIU is assessing additional prototype and conceptual instrumentation alternatives in an infancy stage through modeling, computer simulation and laboratory evaluation.

### Task 15 Quarterly Progress

- Began initial testing with the ultrasonic spectroscopy (USS) unit. Software and hardware issues were resolved after a number of discussions with and a visit from the manufacturer. Initial tests were to be conducted using Gibbsite, zirconium oxide and stainless steel powder to represent the various particle densities represented by the Hanford waste. Tests were conducted with various carry fluid densities and with Gibbsite using a range of percent solids from 2 to 20%.
- Before testing began with the zirconium oxide, the unit failed and would not provide accurate reflectance data. Poor ultrasonic echo capture by the system required additional

inspection by the vendor at their facility. Additional time will be needed to complete the testing which includes use of zirconium oxide and stainless steel powder.

- FIU completed the data analysis on the initial testing with the USS unit. A summary of the results was provided to Hanford site contacts. Results showed fairly good correlation with the Coriolis density meter readings. The technology vendor will provide thermal correction factors to address thermal noise drift in the baseline impedance/reflectance measurement.
- The USS vendor did provide a second unit for additional testing. This unit has been commissioned for testing with zirconium oxide and stainless steel powder.

### **Milestones and Deliverables**

The milestones and deliverables for Project 1 are shown on the following table. Due to hardware issues with the USS unit and unexpected leaks in the asynchronous pulsing testbed, two of the milestones and associated deliverables have been recast with a slightly modified schedule. Note that the overall scope of work has not changed for this year's performance period. A revised project task plan was sent to the Hanford site and EM-31 contacts.

### **Work Plan for Next Quarter**

- Draft Verification Test Plan for bench scale asynchronous pulsing (Task 2).
- Complete bench scale pipeline unplugging using the asynchronous pulsing system and develop summary document (Task 2).
- Development of the multiphase MRT LBM in 3D and develop summary document (Task 12).
- Verification of the multiphase SRT LBM in 3D for dynamic bubbles in closed domains and develop summary document (Task 12).
- Complete candidate technology testing at FIU and develop summary document (Task 15).

### Milestones and Deliverables for Project 1

Task	Milestone/ Deliverable	Description	Due Date	Status
Task 2: Pipeline Unplugging and Plug Prevention	Deliverable	Draft Verification Test Plan for bench scale asynchronous pulsing	10/12/2011	On target
	2011-P1-M2.1	Complete bench scale pipeline unplugging using the asynchronous pulsing system	12/9/2011	On target
	Deliverable	Summary Document for 2011-P1-M2.1	12/9/2011	On target
	Deliverable	Draft Verification Test Plan for engineering scale asynchronous pulsing	02/10/2012	On target
	2011-P1-M2.2	Complete experimental testing of third generation peristaltic crawler	5/06/2012	On target
	Deliverable	Summary Document for 2011-P1-M2.2	5/06/2012	On target
	2011-P1-M2.3	Complete engineering scale pipeline unplugging testing using the asynchronous pulsing system	5/11/2012	On target
	Deliverable	Summary Document for 2011-P1-M2.3	5/11/2012	On target
Task 12: Multiple-Relaxation-Time Lattice Boltzmann Model for Multiphase Flows in Three Dimensions	2011-P1-M12.1	Development of the multiphase MRT LBM in 3D	10/17/2011	On target
	Deliverable	Summary Document for 2011-P1-M12.1	10/17/2011	On target
	2011-P1-M12.2	Verification of the multiphase SRT LBM in 3D for dynamic bubbles in closed domains	12/22/2011	On target
	Deliverable	Summary Document for 2011-P1-M12.2	12/22/2011	On target
	2011-P1-M12.3	Parallelization of the 3D multiphase MRT LBM	05/09/2012	On target
	Deliverable	Summary Document for 2011-P1-M12.3	05/09/2012	On target
Task 15: Evaluation of Advanced Instrumentation Needs for HLW Retrieval	2011-P1-M15.1	Complete candidate technology testing at FIU	10/31/2011	On target
	Deliverable	Summary Document for 2011-P1-M15.1	10/31/2011	On target
Project-wide	Deliverable	Draft Project Technical Task Plan	09/17/2011	Complete
	Deliverable	Quarterly Progress Reports (all tasks and projects combined)	End of Q1, Q2, Q3, Q4	On target
	Deliverable	Draft Annual Task Progress Report (ALL TASKS)	06/17/2012	On target

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## **Project 2**

# **Rapid Deployment of Engineered Solutions to Environmental Problems**

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

### **Project Description**

This project focuses upon delivering solutions to environmental challenges at the DOE Hanford Site. During FY11, FIU ARC continues to provide support on uranium contamination and remediation at the Hanford Site with research under Project 2. This project includes two subtasks for FY11: continued research on uranyl mineral formation and co-precipitation by soil pH manipulation (Task 1.1) and microbial- uranium interactions that include dissolution of autunite mineral and bio-adsorption of uranium (VI) in the presence of bicarbonate and Ca ions (Task 1.2).

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

#### Task 1.1 Overview

The study under subtask 1 involves a series of batch experiments to evaluate the mechanisms and effectiveness of NH<sub>3</sub> gas injection, which has significant uncertainties under Hanford VZ site-specific conditions. The injection of a NH<sub>3</sub> gaseous mixture causes the formation of NH<sub>4</sub>OH and a subsequent increase in pH. This manipulation will significantly alter the pore water chemistry and promote the formation of various aluminosilicates during recrystallization of minerals followed by co-precipitation of U(VI) [as uranyl (UO<sub>2</sub><sup>2+</sup>)] and Al at higher pH conditions. These chemical reactions can potentially control the mobility of uranyl cations in soil systems since co-precipitated contaminants are less available for migration. This study is evaluating the role of major pore water constituents such as Al, Si, bicarbonate, and Ca on the formation and solubility of uranium – bearing precipitates created after NH<sub>3</sub> gas injection.

#### Task 1.1 Quarterly Progress

- Completed batch experiments using Si/Al ratio up to 50 and the bicarbonate concentration of 100 mM; obtained results with KPA for U(VI) and Al & Si with ICP-OES. Completed limit of detection (LOD) for Si & Al with ICP-OES.
- Conducted data analysis for batch experiments carried out with 0.5 ppm and 2 ppm of U(VI), Si/Al ratio up to 50 and the bicarbonate concentration of 100 mM. Experimental runs with higher Si:Al molar ratios had relatively high removal efficiencies, reaching up to 95% -98% removal of U(VI) and Si concentrations and almost 100% removal of Al. At low ratios [Si/Al of 1.8 (5 mM Si+2.8 mM Al)], there was no observed reduction in the U(VI) concentrations in the supernatant solutions. However, at a ratio of 18 (50 mM Si +2.8 mM Al), the reduction of U was observed to increase at higher bicarbonate concentrations, starting from 50 mM. The formation of gel in the experimental tubes always correlated with the reduction of U(VI) and the removal of Si and Al from the



solution. If no Si polymerization and gel formation was observed, there was no U removal.

- Repeated data set for 25 mM of bicarbonate to obtain results for Al removal.
- Prepared samples and conducted SEM/EDS analysis for samples prepared in the presence of 3 mM of bicarbonate with 2 ppm of U(VI) at a Si/Al ratio of 35 (100 mM Si to 2.8 mM Al).
- Initiated work on U speciation using input parameters from experiments and Visual MINTEQ chemical speciation software. Graphed MINTEQ data using Sigma Plot software to obtain U speciation as a function of bicarbonate concentrations and Si/AL ratios.
- Conducted batch experiments using 2 ppm of U(VI), the bicarbonate concentration of 3 mM, and Si solution with no Al present. Conducted data analysis for the obtained results to evaluate the effect of Al on the Si precipitation reactions.
- Initiated XRD and FTIR analysis for the dried precipitates obtained from the experiment using 2 ppm of U(VI), 3 mM of bicarbonate at a Si/Al ratio of 20. Initiated a literature search for the XRD phase identification.
- Submitted abstract to the Waste Management 2012 Symposium.

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

#### Task 1.2 Overview

Research under subtask 2 continues to investigate the effect of bicarbonate on the autunite mineral microbial leaching and U(VI) biouptake by *Arthrobacter* sp., soil bacteria previously isolated from Hanford Site soil. The obtained data suggests that bacteria is responsible for autunite dissolution and is able to influence U(VI) leaching while are even not in direct contact with the mineral. The G975 strain U(VI) biouptake, found in the 83-90% range for the aqueous solutions at equilibrium with CO<sub>2</sub> atmospheric pressure, was shown to exponentially reduce as the bicarbonate concentration was increased. Experiments are exploring other *A. sp* strains on autunite bioleaching and U(VI) biouptake and determining possible mechanisms for their efficacy.

#### Task 1.2 Quarterly Progress

- Conducted EDS analyses of samples prepared on G975 bacteria cells cultivated in media amended with 20 ppb of U(VI) and 0, 5 and 10 mM of bicarbonate. Ran statistical tests on obtained results. Results showed that samples with added bicarbonate have less U(VI) content compared to the bicarbonate-free control (P<0.004).
- Completed preparations and conducted experiments to investigate the effect of Ca in the concentration of 5 mM at 0 and 2.5 mM of bicarbonate on biosorption of U(VI) by *Arthrobacter* G975 bacterial strain.
- Completed U(VI) speciation on obtained results on the effect of Ca in the concentration of 5 mM at 0 and 2.5 mM of bicarbonate on biosorption of U(VI) by *Arthrobacter* G975 bacterial strain using MINTEQ chemical speciation software.

- Completed preparations to redo autunite bioleaching experiments using culture ware with inserts and completed these autunite bioleaching experiments. To get statistically significant results, experiments were conducted using n=7 for each bicarbonate concentration.
- Repeated experiments on U(VI) reduction in concentration due to interactions with phosphorus media components. Measurements were conducted in triplicates using cell-free controls over duration of 7 days. The results indicated that over this period, the uranium concentration in abiotic control samples amended with 10 & 30 ppm of U(VI) deviated no more than  $6.9 \pm 2.6$  % of its initial value. Changes were made to the text of the manuscript prepared for the Geomicrobiology Journal.
- Received comments after peer-review for a manuscript based on this research that was submitted to the Geomicrobiology Journal. Resolution of the comments was completed and a revised manuscript prepared.

### **Milestones and Deliverables**

The milestones and deliverables for Project 2 are shown on the following table. The project is on schedule to meet all milestones and deliverables.

### **Work Plan for Next Quarter**

- Task 1.1: Complete experiments to investigate the effect of Al on the formation of precipitates. Experiments will be conducted without Al or at a higher Al concentration of 5mM at 3mM and 50mM of  $\text{HCO}_3^-$ . Continue evaluation of precipitates using EDS, XRD and FTIR methods. Prepare a manuscript for the WM conference proceedings.
- Task 1.2: Set up bioleaching experiments with *Arthrobacter* sp. G968 strain. Continue a study on the effect of Ca on biosorption and viability of *Arthrobacter* bacteria. Conduct microscopic studies on bacterial cells exposed to U in the presence of bicarbonate and Ca. Submit revised manuscript to the Geomicrobiology Journal. Finalize a manuscript on the effect of G975 strain on the bioleaching of U(VI) from autunite mineral.

### Milestones and Deliverables for Project 2

Task	Milestone/ Deliverable	Description	Due Date	Status
Task 1: Sequestering Uranium at the Hanford 200 Area Vadose Zone by In Situ Subsurface pH Manipulation Using NH <sub>3</sub> Gas	2011-P2-M1	Completion of testing on the removal efficiency of U(VI) using various Si:Al ratios in the presence of bicarbonate	2/28/2012	On target
	Deliverable	Progress report on results on biosorption and bacterial tolerance to uranium in the presence of bicarbonate ion	1/11/2012	On target
Task 2: Effect of bicarbonate on the autunite mineral bioleaching and U(VI) biouptake by <i>Arthrobacter</i> sp	2011-P2-M2	Completion of assessment of the role of bacteria on U(VI) leaching from autunite using <i>Arthrobacter</i> sp. strains	4/30/12	On target
Project-wide	Deliverable	Draft Project Technical Plan	6/17/2011	Complete
	Deliverable	Draft Year End Report	6/18/2012	On target

# **Project 3**

## **Remediation and Treatment Technology Development and Support**

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**Project Manager: Dr. Georgio Tachiev**

### **Project Description**

The overall objective of this project is to provide technical assistance and perform research in support of the remediation efforts at the Oak Ridge Reservation. Student support for research at the Moab Site will also be provided. Research efforts will be executed in collaboration with DOE EM and DOE ORO and will be closely aligned with the ASCEM program objectives. The numerical modeling and experimental work will provide a better understanding of the fate and transport of inorganic and organic pollutants.

### **Task 1: EFPC model update, calibration & uncertainty analysis**

#### Task 1 Overview

The main objectives of this task are to extend the existing EFPC model by adding a reactive transport and sedimentation module, and use the model to perform numerical simulations. The simulations will provide a better understanding of the flow and transport within the watershed on a regional scale. Simulations will be conducted using historic observations of rainfall, evapotranspiration, and contaminant distribution, within the watershed to determine transport patterns within the domain. During FY11, the focus is on extending the sedimentation module to include the entire EFPC and Bear Creek. In addition, the proposed research will provide stochastic modeling of the system and will include an analysis of the spatial and temporal patterns as a result of the stochastic variations of selected properties of the sub domain.

#### Task 1 Quarterly Progress

##### *Model Extension:*

- Completed the addition of the sedimentation module to the entire watershed.
- Prepared a series of MATLAB scripts for statistic analysis of the observed and computed data. Outfall added to the hydrodynamic (HD) and advection (AD) module of MIKE11.
- Revised the HD and AD module and used the additional observed data to recalibrate the model.
- Obtained recently added environmental data from the OREIS database for EFPC including water quality parameters and spatial data for groundwater, surface water, sediment, and soil. This process is performed to ensure the inclusion of all monitoring stations and sample locations that may have relevant and up-to-date information required for the model simulations.



## **Task 2: TMDL Analysis for the entire EFPC**

### Task 2 Overview

The numerical model of the EFPC will simulate fate and transport of mercury and VOC plumes within the EFPC watershed, and will assist in analyzing the TMDL requirements for surface water and groundwater within the EFPC watershed. The main objectives of this task are to:

- Develop a TMDL methodology for analysis of flow and load duration exceedance probabilities for key monitoring stations along Bear Creek and the EFPC from numerical simulations and observed data; and
- Provide analysis of the relative contribution of point and non-point sources to mercury pollution in the watershed including the contributions from the floodplain of the two watershed creeks (EFPC and Bear Creek), the remobilization of stream sediments during stormwater events, the groundwater exchange with the creeks, and the transport within the creeks.

### Task 2 Quarterly Progress

- Reviewed the recent TMDL documents by EPA and TDEC. Collected and organized the hydrological and pollution data including flow, water level, and groundwater depth, temporal and spatial distribution of pollutant sources in soil, water, and sediments from OREIS, DOE reports, and literature.
- Summarized the steps and requirements of TMDL analysis into a report, including information on identifying sources and setting TMDL targets and watershed characteristics by reviewing recent TMDL documents by EPA and TDEC.
- Organized the flow and stream pollution data for the entire East Fork Poplar Creek (i.e., filtered data, removed outliers and invalid data points).
- Performed spatial analysis of the flow and pollution data along the creek to verify the logical alteration of the flow and contamination, and to identify any spatial trend in the mercury concentration values along the creek.
- Began preparation of TMDL report which currently includes some project background information as well as information on the Water Quality Criteria and TMDL Target, Water Quality Assessment and Deviation from the TMDL target, and Water Quality Data Analysis.
- Water quality data analysis has been completed including graphical presentations of temporal and spatial variations of data points, seasonal analysis of data points, and removal of data outliers and anomalies using methods suggested by EPA.
- Prepared a set of timeseries files which are used in the model simulation.
- A scientific paper entitled “Simulation of Flow and Mercury Transport in Upper East Fork Poplar Creek, Oak Ridge, TN” was submitted to the Remediation Journal and accepted for publication in January 2012.

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

#### Task 3 Overview

The overall objective of this task is to provide laboratory measurements for critical mercury transport, transformation, and exchange processes (i.e., methylation/demethylation, exchange of mercury species between soil, pore water in the sediment, colloidal particles, and the water column, mercury desorption rate in water and sediment, and the organic carbon partitioning coefficient) to be used in the numerical model. The laboratory experimental work will provide insight on parameters relevant to the Oak Ridge Reservation (ORR) and which are required in the numerical model, such as desorption rates of mercury in different media. In addition, experimental work will be conducted to analyze the effect of significant environmental factors (pH, pE, light mediated processes) on methylation and demethylation processes.

In collaboration with the Oak Ridge National Laboratory (ORNL), under this task we will systematically investigate the stability, reactivity, and mobility of the aged mercury species in the soils and sediments of the DOE Oak Ridge site. A special focus will be placed on the aged mercury beads, which have often been observed at this site and are thought to be recalcitrant mercury species with limited contributions to the aquatic mercury cycling and bioaccumulation. Two processes, i.e., oxidation-reduction, and complexation with organic ligands (e.g., low molecular weight thiols such as cysteine and glutathione and large molecular NOM), will be particularly investigated for their role in mobilizing the aged mercury species.

#### Task 3 Quarterly Progress

##### *Photomethylation of Hg(II) in natural water:*

- A kinetic model was developed to calculate the photomethylation rate of Hg(II) in natural water by using data from double stable isotope ( $^{199}\text{Hg}^{2+}$  and  $\text{Me}^{201}\text{Hg}$ ) addition experiments. Methylation of  $\text{Hg}^{2+}$  in water was observed. However, its influence on MeHg cycling is supposed to be minor as its rate was found to be only about 0.04% of MeHg photodemethylation rate.
- Completed the measurement of the photomethylation rate of Hg(II) in natural water by using double stable isotope ( $^{199}\text{Hg}^{2+}$  and  $\text{Me}^{201}\text{Hg}$ ) addition experiments.

##### *Estimation of the bioavailability of Hg(II) and methylmercury for methylation and demethylation in natural sediment:*

- A kinetic model was developed to calculate the bioavailability of Hg(II) and methylmercury for methylation and demethylation in natural sediment. By simulating data obtained from double stable isotope ( $^{199}\text{Hg}^{2+}$  and  $\text{Me}^{201}\text{Hg}$ ) addition experiments, percentage of bioavailable Hg(II) and MeHg for methylation/demethylation was calculated.
- Ongoing estimation of the bioavailability of Hg(II) and methylmercury for methylation and demethylation in natural sediment.

##### *Summarization of current studies on mobility of mercury beads in soil:*

- Current studies on mobility of mercury beads in soil were summarized. An experimental plan was developed to study the mobility of mercury beads in the soil of Oak Ridge.

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- Ongoing investigation of absorption/desorption of Hg(II) and MeHg and affecting factors in soil.
- Ongoing investigation of dissolution of mercury in soil and sediment.

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

##### Task 4 Overview

The main objective of this task is to create a geodatabase to support hydrological model development and simulation of contaminant fate and transport at Oak Ridge Reservation (ORR), TN. The geodatabase will serve as a centralized data management system which facilitates storage, editing, and versioning of model parameters. A working prototype was developed by FIU ARC during FY 2010. As FIU ARC continues to conduct model simulations to support the D&D remediation activity at ORR, there will be an ongoing need for the update of the geodatabase and the utilization of the integrated GIS-hydrological modeling system developed.

The two objectives for this task for FY 2011 are:

- Configuration of the database to provide remote access to input and output files.
- Import of simulation input and output files for the Y-12 NSC, WOC and EFPC models into the geodatabase along with versioning.

##### Task 4 Quarterly Progress

- Created Moab geodatabase and generated feature datasets and raster catalogs. The database used the same data structure as the ORR geodatabase and it is based on the ArcHydro and ArcGIS Basemap data models. Customization of the geodatabase will be made according to model input data specifications.
- Customized and populated the ORR Geodatabase with relevant model data.
- Completed "GIS & Hydrological Modeling Data Server Management" document.
- Conducting ongoing customization of geodatabases to facilitate import/export of model data.
- Conducting ongoing import/export of spatial data into geodatabases and execution of geoprocessing tasks as necessary for model simulations.

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

##### Task 5 Overview

FIU, in collaboration with DOE's Moab site project director, will use an existing groundwater numerical model to evaluate the tailings pore-water seepage in order to assist in effective dewatering of the tailings pile and to optimize the groundwater extraction well field as part of the DOE Uranium Mill Tailings Remedial Action (UMTRA) for the Moab site.



The two main objectives of Task 5 are to:

1. Use an existing groundwater numerical model to simulate the fate and transport of contaminants including uranium and ammonia in the subsurface at the Moab, Utah site.
2. Perform numerical simulations of remedial scenarios proposed by DOE including pumping of contaminated groundwater from the shallow plume to an evaporation pond on top of the tailings pile, and injecting the diverted Colorado River water into the alluvial aquifer in order to predict the outcome of each remedial action and to investigate the effectiveness of each scenario. Numerical simulation of remedial actions assists DOE in deciding their effectiveness.

#### Task 5 Quarterly Progress

- Obtained and organized the hydrological data for the analysis and modeling.
- Conducted simulations with the existing hydrological model (developed by a DOE consultant). The model is currently being reconfigured with more current spatial and timeseries data to simulate fate and transport of contaminants including uranium and ammonia in the subsurface domain at the Moab site in Utah.
- Completed the analysis of available groundwater quality data from wells. Prepared water quality contour maps by using analyzed results to assess the pattern of contaminant transport.
- Compared results obtained from carrying out simulations using the existing model with the results presented by the sub contractor.
- Extracted pumping test data and regular monitoring data from literature, which will be used in the model to show the natural seasonal variations and responses to other stresses.
- Ran simulations with the Moab air dispersion model for the new location of the landsharks and created a report which included the new results.

#### **Milestones and Deliverables**

The milestones and deliverables for Project 3 are shown on the following table. One of the milestones (2011-P3-M4) has been re-forecast; the report on project coordination with the applied field research center (ORNL) & ASCEM will be completed after a site visit.

#### **Work Plan for Next Quarter**

- Prepare Task 1 progress report on “EFPC model update, calibration, uncertainty analysis.”
- Prepare Task 5 progress report on “Student support for modeling of groundwater flow and transport at Moab, UT site.”

### Milestones and Deliverables for Project 3

Task	Milestone/ Deliverable	Description	Due Date	Status
Task 1: EFPC Model Update, Calibration, Uncertainty Analysis	2011-P3-M5	Task 1 progress rpt on “EFPC model update, calibration, uncertainty analysis”	11/17/2011	On target
Task 2: Simulation of TMDL for the Entire EFPC	2011-P3-M7	Task 2 progress rpt on “Simulation of TMDL for entire EFPC”	2/1/2012	On target
Task 3: Laboratory experiments for methylation/demethylation and transport parameters of mercury	2011-P3-M1	Task Plan for Prof. Cai (after visit & coordination with ORNL)	8/1/2011	Complete
	2011-P3-M11	Task 3 technical report entitled, “Parameterization of major transport processes of mercury species”	5/17/2012	On target
Task 4: Geodatabase Development for Hydrological Modeling Support	2011-P3-M9	Task 4 progress on “Geodatabase development for hydrological modeling support”	3/1/2012	On target
Task 5: Student Support for Modeling of Groundwater Flow and Transport at the site of Moab, Utah	2011-P3-M3	Student summer internship at Moab Site	9/23/2011	Complete
	2011-P3-M6	Task 5 progress report on “Student support for modeling of groundwater flow and transport at Moab, UT site”	12/1/2011	On target
	2011-P3-M10	Finalize model and its configuration according to ASCEM specifications (after visit to Moab Site)	03/17/2012	On target
Project-wide	2011-P3-M2	Submit 2 abstracts to Waste Management Symposium 2012	8/19/2011	Complete
	2011-P3-M4	Rpt on project coordination w/ applied field research center (ORNL) & ASCEM (after site visit)	9/28/2011	Re-forecast 11/18/2011
	2011-P3-M8	Presentation overview to DOE HQ of the project and accomplishments	2/17/2012	On target
	2011-P3-M12	Submit publications to relevant journals	5/17/2012	On target
	Deliverable	Draft Technical Task Plan	08/12/11	Complete
	Deliverable	Quarterly Status and Progress Summary Reports	Quarterly	On target
	Deliverable	Year End Report	06/15/2012	On target

## **Project 4**

### **Waste and D&D Engineering & Technology Development**

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

#### **Project Description**

This project focuses on delivering solutions under the decontamination and decommissioning (D&D) and waste areas in support of DOE HQ EM and includes support of the Office of Innovation and Technology Development R&D Plan. This work is also relevant to D&D activities being carried out at other DOE sites such as Oak Ridge, Savannah River, Hanford, Idaho and Portsmouth or international efforts being conducted by EM-30 with the Nuclear Decommissioning Authority (NDA) in England and the International Atomic Energy Agency (IAEA). Efforts on this project include the following tasks:

- Task 1: Waste Information Management System (WIMS)
- Task 2: D&D Support to DOE EM for Technology Innovation, Development, Evaluation and Deployment
- Task 3: D&D Knowledge Management Information Tool (KM-IT)
- Task 4: IT Support to EM and DOE Sites

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

##### Task 1 Overview

This task provides direct support to DOE EM for the management, development, and maintenance of a Waste Information Management System (WIMS). WIMS was developed to receive and organize the DOE waste forecast data from across the DOE complex and to automatically generate waste forecast data tables, disposition maps, GIS maps, transportation details, and other custom reports. WIMS is successfully deployed and can be accessed from the web address <http://www.emwims.org>. The waste forecast information is updated at least annually. WIMS has been designed to be extremely flexible for future additions and is being enhanced on a regular basis.

##### Task 1 Quarterly Progress

- New waste forecast data is imported into WIMS on an annual basis. The 2011 waste forecast dataset was imported into WIMS and made available to the public on the WIMS website on April 19, 2011.
- Performed database management, application maintenance, and performance tuning to WIMS in order to ensure a consistent high level of database and website performance.
- Submitted an abstract on WIMS to the Waste Management 2012 Symposium.

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

### Task 2 Overview

This task provides direct support to DOE EM for D&D technology innovation, development, evaluation and deployment. The objective of Task 2 is to use an integrated systems approach to develop a suite of D&D technologies (D&D Toolbox) that can be readily used across the DOE complex to reduce technical risks, improve safety, and limit uncertainty within D&D operations. FIU directly supports DOE-EM's Office of Innovation and Technology Development and affiliated DOE sites, national laboratories, and institutions contributing to the development of innovation in D&D. This task will also collaborate with DOE-EM's international partnerships and agreements by providing D&D expertise, knowledge and support when requested to do so by DOE EM. The technical approach for this task is to identify and demonstrate new technologies, methodologies, and approaches to support EM's collaborative international activities.

### Task 2 Quarterly Progress

- Held teleconference with the technology provider on a feasibility study for the removal of strippable coatings using a remote controlled platform. Began preliminary benchscale testing of potential end tools.
- In an effort to aid the various in-situ decommissioning projects at SRS, a meso-scale concrete test bed has been designed and is being installed at FIU-ARC in order to test various sensors imbedded in grout. This experiment consists of using various sensors including Electrical Resistivity Tomography, Advanced Tensiometers, Piezoelectric Sensors, and Fiber Optic Sensors (ERT, AT, PES, FOS) to measure various parameters including strain, crack detention, corrosion, fluid mobility, moisture, as well as a variety of others. Principal Investigators (PIs) from Idaho National Laboratory (INL), Mississippi State University (MSU), University of Houston (UH), and University of South Carolina (USC) will be providing the sensors as well as testing them. The main purpose is to recognize the limitations of these sensors for their future use in monitoring closed nuclear facilities. Figures showing the assembly of the ISDSN sensor racks are shown below.
- Participated in bi-weekly conference calls with the ISDSN working team. Conference calls are led by SRNL with participation of team members INL, Mississippi State University (MSU), University of Houston (UH), and University of South Carolina (USC), and Florida International University (FIU).



**Assembly of ISDSN Sensor Racks and Sensor Racks Support Assemblies**

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

#### Task 3 Overview

The D&D Knowledge Management Information Tool (KM-IT) is a web-based system developed to maintain and preserve the D&D knowledge base. The system was developed by Florida International University's Applied Research Center (FIU-ARC) with the support of the D&D community, including DOE-EM (EM44 & EM72), the ALARA centers at Hanford and Savannah River, and with the active collaboration and support of the DOE's Energy Facility Contractors Group (EFCOG). The D&D KM-IT is a D&D community driven system tailored to serve the technical issues faced by the D&D workforce across the DOE Complex. D&D KM-IT can be accessed from web address <http://www.dndkm.org>.

#### Task 3 Quarterly Progress

- Completed and deployed Vendor Management module to the staging server for DOE to review/test on July 29.
- Integrated a new web site look to the staging server for review by DOE.

- Added Innovative Technology Summary Reports (ITSR) module to D&D KM-IT on the staging server with extensive collection of ITSR documents for DOE review. Located all ITSRS with an archive search engine, categorized and integrated them. Updated file names on the staging server.
- Began development of the Collaboration Tools module on D&D KM-IT. Evaluated the feasibility of 3<sup>rd</sup> party open source solutions. Established the Sharepoint Foundation server as the solution which will map with the collaboration tools features.
- Search Engine Optimization process is being deployed on the D&D KM-IT web application.
- Completed analysis of website analytics on a monthly basis and prepared reports on the results.
- Updating vendor information for new Vendor Module, adding new vendor descriptions as well as areas of expertise for each vendor.
- Adding D&D technology information to the Technology Module.
- An abstract on D&D KM-IT was submitted to the Waste Management 2012 Symposium.
- Dr. Lagos, attended and presented KM-IT at the ICEM conference held in Reims, France. The DOE-FIU web-based tool was presented at a panel session on Knowledge Management and attracted the attention of several conference attendees.

#### **Task 4: IT Support to EM and DOE Sites**

##### Task 4 Overview

DOE EM expressed a need for enhancing the DOE EM website and developing a system of knowledge management, similar to our current Knowledge Management Information Tool (KM-IT) being developed for EM-44, to allow sharing of DOE EM information among the DOE community. To address this need, FIU-ARC subsequently received additional funding toward the end of FIU's FY10; due to the late arrival of this additional funding, DOE and FIU agreed to treat this funding as carryover funding with the expectation that the scope of work delineated in the proposal document would be carried out during FIU's FY11 period of performance. FIU-ARC proposed 3 subtasks as described in the Task 4 section of this document. A fourth subtask, separate from the additional \$500K scope was added to provide support to SRS with data acquisition through wireless sensors and access through the D&D KM-IT system.

##### Task 4 Quarterly Progress

- Completed design of a static prototype for EM knowledge base and sent to DOE on Aug. 31. Further activities on the DOE EM Website and Knowledge Base for Environmental Management are currently being maintained in standby pending further input from EM-72.
- For the ISDSN IT subtask, the Sensor Remote Access System (SRAS) is being administered to provide access through KM-IT. Users from all 3 universities (Mississippi

State University, University of Houston, University of South Carolina), Idaho National Lab and Savannah River National Lab are registering with the D&D KM-IT framework to get access to SRAS. Test process is being developed to provide access to the ISDSN users through a VPN connection to access their data logger system from remote locations.

- Developed, and deployed Data Import Process for Sensor data of all 3 universities (Mississippi State University, University of Houston, University of South Carolina) and Idaho National lab.
- Designed, developed and deployed SRAS (Sensor Remote Access System) for ISDSN project which provides stakeholders access to sensor raw data, processed and analyzed reports.

### **Milestones and Deliverables**

The milestones and deliverables for Project 4 are shown on the following table. The project is on schedule to meet all milestones and deliverables.

### **Work Plan for Next Quarter**

- Perform database management, application maintenance, and performance tuning to WIMS (Task 1).
- Complete and submit paper on WIMS to the Waste Management 2012 Symposium (Task 1).
- Continue feasibility study for remote removal of strippable coatings and decon gels (Task 2).
- Continue work with university PIs and SRNL and INL in the development of a test site and testing of remote sensors at FIU for in situ decommissioning.
- Complete development and deployment of Collaboration Tools module to DOE for review/testing (Task 3).
- Complete and submit paper on D&D KM-IT to the Waste Management 2012 Symposium (Task 3).
- Draft DOE EM website analysis report (Task 4) – on standby pending input from EM-72.
- Continue installation of the meso-scale concrete test bed for the ISDSN subtask (Task 2).

### Milestones and Deliverables for Project 4

Task	Milestone/ Deliverable	Description	Due Date	Status
Task 1: Waste Information Management System (WIMS)	2011-P4-M1.1	Import 2011 data set for waste forecast and transportation data	Within 60 days after receipt of data from DOE	Complete
Task 2: D&D Support to DOE EM for Technology Innovation, Development, Evaluation, and Deployment	2011-P4-M2.1	Complete In-Situ Decommissioning Experiments	04/30/12	On target
	Deliverable	Draft technical report for review of mercury D&D issues at Oak Ridge	One month after receiving documents	On target
	Deliverable	Draft Tech Fact Sheet for in-situ decommissioning experiments	One month after experiments are completed	On target
	Deliverable	Draft Feasibility Report for remote removal of strippable coatings	4/20/2012	On target
Task 3: D&D Knowledge Management Tool (D&D KM-IT)	2011-P4-M3.1	Deployment of Vendor Management module to DOE for review/testing	7/31/2011	Complete
	2011-P4-M3.2	Deployment of Collaboration Tools to DOE for review/testing	10/31/2011	On target
	2011-P4-M3.3	Deployment of mobile application for vendor and specialist modules to DOE for review/testing	1/31/2012	On target
	2011-P4-M3.4	Deployment of training module to DOE for review/testing	4/30/2012	On target
	2011-P4-M3.5	D&D KM-IT data mining	5/17/2012	On target
	Deliverable	Draft report of internal C&A audit findings and responses	30-days after internal audit	On target
	Deliverable	Draft report of external C&A audit findings and responses	30-days after external audit	On target
	Deliverable	Draft Tech Fact Sheet for new modules or capabilities of D&D KM-IT	30-days after deployment of new module or capability	On target
Task 4: IT Support to EM and DOE Sites	2011-P4-M4.1	Draft static prototype for EM knowledge base to DOE for review	8/31/2011	Complete
	Deliverable	Draft DOE EM website analysis report	11/28/2011	On target
	Deliverable	Draft knowledge base requirements document for EM	2/28/2012	On target
Project-wide	Deliverable	Draft Project Technical Plan	6/17/2011	Complete
	Deliverable	Draft Year End Report	06/18/2012	On target
	Deliverable	Quarterly status and progress summary reports	Quarterly	On target



## **Project 5**

### **DOE-FIU Science & Technology Workforce Development Initiative**

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

#### **Project Description**

The DOE-FIU Science and Technology Workforce Development Initiative has been designed to build upon the existing DOE/FIU relationship by creating a “pipeline” of minority engineers specifically trained and mentored to enter the Department of Energy workforce in technical areas of need. This innovative program was designed to help address DOE’s future workforce needs by partnering with academic, government and DOE contractor organizations to mentor future minority scientists and engineers in the research, development, and deployment of new technologies, addressing DOE’s environmental cleanup challenges.

#### **Project Overview**

The main objective of the program is to provide interested students with a unique opportunity to integrate course work, Department of Energy (DOE) field work, and applied research work at ARC into a well structured academic program. Students completing this research program would complete the M.S. or Ph.D. degree and immediately be available for transitioning into the DOE EM’s workforce via federal programs such as the Student Career Experience Program (SCEP) or by getting directly hired by DOE contractors.

#### **Quarterly Progress**

- Coordinated the placement of summer internship assignments by DOE Fellows.
- This past summer, ten (10) DOE Fellows participated in summer internships across the DOE Complex:
  - Amaury Betancourt – Savannah River National Laboratory (SRNL)
  - Givens Cherilus – Savannah River Site (SRS)
  - Janty Ghazi – Washington River Protection Solutions (WRPS)
  - Rinaldo Gonzalez – Pacific Northwest National Laboratory (PNNL)
  - Heidi Henderson – DOE HQ EM-30
  - Alex Henao – Moab Site
  - Jose Matos – Washington River Protection Solutions (WRPS)
  - William Mendez – Savannah River Site (SRS)
  - Sheidyn Ng – DOE HQ EM-20
  - Mario Vargas – Lawrence Livermore National Laboratory (LLNL)
- Conducted weekly teleconferences with DOE Fellows, including Fellows participating in summer internships experiences.
- Conducted DOE Fellows weekly meeting and summer internships student presentations.

- Amaury Betancourt presented his summer internships results obtained during summer internship at SRNL working under the supervision of Dr Brian Looney.
- Rinaldo Gonzalez presented his summer internship work conducted at PNNL under the supervision of Mr. Kenneth Johnson.
- William Mendez presented his summer research accomplished during summer internship assignment at SRS under the supervision of Mr. Luther Reid and Mr. Dale Marzolf.
- Sheidyn Ng presented her summer internship work conducted with DOE HQ EM-20 under the supervision of Mr. Kenneth Picha.
- Heidi Henderson presented her summer internship work conducted with DOE HQ EM-30 under the supervision of Ms. Ana Han.
- Worked with DOE Fellows summer interns to complete Technical Summer Internship reports based on their summer internship experiences.
  - Amaury Betancourt – *Tin Distribution and Fate in Tims Branch at the Savannah River Site*
  - Givens Cherilus – *Saltstone Liquid Permeability and Formed Core Grout Sampler*
  - Janty Ghazi – *Electrical Upgrades for Hanford Supporting Facilities*
  - Rinaldo Gonzalex – *Soil Mesh Optimization and Preliminary FEA Study of Tank-to-Tank Interaction for Hanford Type IV SST*
  - Heidi Henderson – *Office of Environmental Management International Program*
  - Alex Henao – *Preliminary Studies of Nitrogen Concentration in Wells 0437, 0438, and 0439*
  - Jose Matos – *Agitated Thin-Film Evaporator*
  - William Mendez – *Formed Core Sampler*
  - Sheidyn Ng – *U.S. Department of Energy Headquarters Environmental Management (EM-20) Office of Safety and Security Program*
  - Mario Vargas – *Air Flow Calculations for the Centralized Waste Processing Line Glovebox*
- Coordinated Fall 2011 recruitment process to attract and select new DOE Fellows (Fall 2011). Received a total of 11 application packages that are currently being reviewed by the DOE Fellows Selection Committee.
- Coordinated DOE Fellows Poster Exhibition & Competition. DOE Fellows prepared 16 posters that will be showcased at the annual event scheduled for mid-October.
- Worked with DOE sites and HQ to fully engage DOE Fellows with research outside ARC.
- DOE Fellows prepared and submitted professional abstracts to Waste Management Symposia 2012 (WM12).

- During a recent visit to Miami, Florida on September 27, 2011, former New Jersey Governor Christine Whitman met with leaders at the Florida International University (FIU) College of Engineering and at FIU's Applied Research Center (ARC). Gov. Whitman is currently a co-chair of the *Clean and Safe Energy Coalition* (CASEnergy), founded in 2006 to promote nuclear energy. Gov. Whitman spoke with the Department of Energy (DOE) Fellows at the Applied Research Center about career opportunities in the nuclear energy industry. New nuclear reactors planned by Progress Energy and Florida Power & Light would produce 1,400-1,800 jobs during construction and 400-700 jobs during operation. Six of our Fellows had the opportunity to present posters showcasing their EM research conducted at ARC or during summer internships at DOE sites.



**Gov. Whitman and Dr. Ines Triay (former DOE's Assistant Secretary for Environmental Management) with DOE Fellows and program director, Dr. Lagos**



**Gov. Whitman and DOE Fellow Mr. Jose Matos showcasing his summer internship work conducted at DOE's Hanford Site**

- Dr. Lagos, Program Director, submitted a DOE-FIU Science and Technology Workforce Development Program abstract to WM12.
- Dr. Lagos attended and presented the DOE Fellows Program at the ICEM conference held in Reims, France. The DOE Fellows program was presented at the Young Generation Network (Y-Gen) and Professional Development Programs panel session organized by UK's NDA.

### **Milestones and Deliverables**

The milestones and deliverables for Project 5 are shown on the following table. The project is on schedule to meet all milestones and deliverables.

### **Work Plan for Next Quarter**

- Complete summer internship reports and deliver to DOE.
- Select new Fall 2011 DOE Fellows and provide list of recruited DOE Fellows to DOE.
- Plan, coordinate, and conduct Induction Ceremony (Class of 2011).

### Milestones and Deliverables for Project 5

Task	Milestone/ Deliverable	Description	Due Date	Status
Task 4: Selection of DOE Fellows	2011-P5-M1	Selection of new DOE Fellows - Spring 2011	06/30/11	Complete
	2011-P5-M4	Selection of new DOE Fellows – Fall 2011	10/31/11	On target
	Deliverable	List of identified/recruited DOE Fellow (Class of 2011)	10/31/11	On target
Task 6: Summer Internship Program (SIP)	Deliverable	List of 2011 Student Summer Interns and their research assignment	06/06/11	Complete
	2011-P5-M2	DOE Fellows Complete Summer Internships	08/31/11	Complete
	2011-P5-M3	Summer Internships Reports Completed	10/03/11	Complete
	Deliverable	Deliver Summer 2011 Interns reports to DOE	10/14/11	On target
Task 8: Program Presentations/ Communication/ Conferences	2011-P5-M5	Conduct Induction Ceremony – Class of 2011	11/30/11	On target
Program-wide	Deliverable	Draft Technical Task Plan	06/17/11	Complete
	Deliverable	Quarterly Status and Progress Summary Reports	Quarterly	On target
	Deliverable	Draft Year End Report	06/17/12	On target
	Deliverable	Update Technical Fact Sheet	30 days after end of project	On target