AMENDMENT OF SOLICITATION/MODIFICATION OF CONTRACT

1. CONTRACT ID CODE

PAGE OF PAGES: 1 of 1

2. AMENDMENT/MODIFICATION NO.: 305

3. EFFECTIVE DATE: See Block 16C

4. REQUISITION/PURCHASE REQ. NO.: 13EM000218

5. PROJECT NO. *(If applicable)*

6. ISSUED BY — CODE 00901

Savannah River Operations
U.S. Department of Energy
Savannah River Operations
P.O. Box A
Aiken SC 29802

7. ADMINISTERED BY *(If other than Item 6)* — CODE 00901

Savannah River Operations
U.S. Department of Energy
Savannah River Operations
P.O. Box A
Aiken SC 29802

8. NAME AND ADDRESS OF CONTRACTOR *(No., street, county, State and ZIP Code)*

SAVANNAH RIVER NUCLEAR SOLUTIONS, LLC
Attn: LLOYD CLEVINGER
203 LAURENS ST SW
AIKEN SC 298012421

(x) 9A. AMENDMENT OF SOLICITATION NO.

9B. DATED *(SEE ITEM 11)*

X 10A. MODIFICATION OF CONTRACT/ORDER NO. DE-AC09-08SR22470

10B. DATED *(SEE ITEM 13)* 01/10/2008

CODE 798861048 — FACILITY CODE

11. THIS ITEM ONLY APPLIES TO AMENDMENTS OF SOLICITATIONS

☐ The above numbered solicitation is amended as set forth in Item 14. The hour and date specified for receipt of Offers ☐ is extended, ☐ is not extended.
Offers must acknowledge receipt of this amendment prior to the hour and date specified in the solicitation or as amended, by one of the following methods: (a) By completing Items 8 and 15, and returning ________ copies of the amendment; (b) By acknowledging receipt of this amendment on each copy of the offer submitted; or (c) By separate letter or telegram which includes a reference to the solicitation and amendment numbers. FAILURE OF YOUR ACKNOWLEDGEMENT TO BE RECEIVED AT THE PLACE DESIGNATED FOR THE RECEIPT OF OFFERS PRIOR TO THE HOUR AND DATE SPECIFIED MAY RESULT IN REJECTION OF YOUR OFFER. If by virtue of this amendment you desire to change an offer already submitted, such change may be made by telegram or letter, provided each telegram or letter makes reference to the solicitation and this amendment, and is received prior to the opening hour and date specified.

12. ACCOUNTING AND APPROPRIATION DATA *(If required)*

13. THIS ITEM ONLY APPLIES TO MODIFICATION OF CONTRACTS/ORDERS. IT MODIFIES THE CONTRACT/ORDER NO. AS DESCRIBED IN ITEM 14.

CHECK ONE	
	A. THIS CHANGE ORDER IS ISSUED PURSUANT TO: *(Specify authority)* THE CHANGES SET FORTH IN ITEM 14 ARE MADE IN THE CONTRACT ORDER NO. IN ITEM 10A.
	B. THE ABOVE NUMBERED CONTRACT/ORDER IS MODIFIED TO REFLECT THE ADMINISTRATIVE CHANGES *(such as changes in paying office, appropriation date, etc.)* SET FORTH IN ITEM 14, PURSUANT TO THE AUTHORITY OF FAR 43.103(b).
	C. THIS SUPPLEMENTAL AGREEMENT IS ENTERED INTO PURSUANT TO AUTHORITY OF:
X	D. OTHER *(Specify type of modification and authority)* Section I, DEAR 970.5211-1 Work Authorization (May 2007)

E. IMPORTANT: Contractor ☐ is not, ☒ is required to sign this document and return 1 copies to the issuing office.

14. DESCRIPTION OF AMENDMENT/MODIFICATION *(Organized by UCF section headings, including solicitation/contract subject matter where feasible.)*

A. The purpose of this modification is to incorporate Contract Work Authorization numbers APO #2013, HQ10001-0-SR, SR071801, and HO091101, see attachments 1 through 4, hereto (See pin and ink changes attachment 1, APO #2013).

B. This modification formally incorporates the above referenced contract work authorizations as part of the contract. Funds authorizations will continue to be allocated by separate modifications in accordance with the DOE-SR FIN PLANs. As stated under DEAR 970.5211-1 Work Authorization (May 2007), paragraph (b), the work authorization, whether issued bilaterally or unilaterally shall become a part of the contract.

C. The contract estimated value and all other terms and conditions remain unchanged.

Except as provided herein, all terms and conditions of the document referenced in Item 9A or 10A, as heretofore changed, remains unchanged and in full force and effect.

15A. NAME AND TITLE OF SIGNER *(Type or print)*: L.C. Clevinger II, Manager, Contracts

16A. NAME AND TITLE OF CONTRACTING OFFICER *(Type or print)*: Marie A. Garvin

15B. CONTRACTOR/OFFEROR: [signature] *(Signature of person authorized to sign)*

15C. DATE SIGNED: 11/6/12

16B. UNITED STATES OF AMERICA: [signature] *(Signature of Contracting Officer)*

16C. DATE SIGNED: 11/7/12

NSN 7540-01-152-8070
Previous edition unusable

STANDARD FORM 30 (REV. 10-83)
Prescribed by GSA
FAR (48 CFR) 53.243

Attachment 1

Contract Work Authorization

AOP #2013

Project Title: Solar Energy

U. S. DEPARTMENT OF ENERGY
CONTRACT WORK AUTHORIZATION

1a. Project Title	1b. Work Proposal Number
Solar Energy	AOP #2013

2. Headquarters Program Point of Contact

Name: Minh Le | Organization Code: | Telephone No. 202-287-1372

3. Headquarters Budget Point of Contact

Name: Kyra Humphreys | Organization Code: EE-3B | Telephone No. 202-586-8138

4. Responsible Program	5. Responsible Secretarial Officer
Office of Energy Efficiency and Renewable Energy	David Danielson

6. Responsible Field Organization

Savannah River Site Office

7a. Site and Facility Management Contractor	7b. Contractor Point of Contact
Savannah River Nuclear Solutions, LLC	Name: John W. Temple Telephone No. (803) 952- 7210

8. Work Authorization Number	9. Revision Number
SL-410003-12	1

10. Funds Authorized ($ in thousands)(See **NOTE** below)

NOTE: Funding obligated under most current contract modification and related approved financial plan executed under contract clauses B-4, Obligation of Funds, and I.53, DEAR 970.5232-4 Obligation of Funds (Dec 2000) applies.

Budget and Reporting Code:	Previous = Carry Over	Change = New BA	Current = TAC
EB2101010	$0	$1,000,000	$1,000,000

11. Performance Period Covered by Funds		12. Work Start Date	13. Expected Completion Date
From: 10/1/2012	To: 9/30/2013	10/1/2012	9/30/2013

14. Statement of Work (Includes attachments)

This revision provides further clarification to Attachment 1. Funding in the amount of $1,000,000.00 is authorized by the Solar Energy to perform work in the areas of: The U.S. Department of Energy (DOE) SunShot Initiatives and Solar Energy Technologies Program (SETP) authorizes funding in accordance with the program Annual Operating Plan (AOP). This operating plan authorizes specific funding amounts for each project and agreement, and required detailed performance milestones and deliverable be met or completed within the period of performance.

Please refer to Work Proposal Number (1b) to determine wich section(s) of the AOP for which this authorization provides funding. This funding will be split (Reference Attachment 2) between proposals titles "Low-Cost Metal Hydride Thermal Energy Storage Systems for Concentrating Solar Power Systems" and "Fundamental Corrosion Studies in High-Temperature Molten Salt Systems for Next Generation Concentrated Solar Power Systems," $581,725.00 and $418,275.00 respectively.

All work shall be conducted in accordance with this Modification. LGH 11/6/12 SL 11/6/12 HM 11/6/12

16. Work Authorization Program Official - Contracting Officer's Representative

Name (typed):	Signature:	Date:
Reference Attachment 1		

17. DOE-SR Budget Official (Field CFO)

Name (typed):	Signature:	Date:
Harold K. Nielsen	Harold K. Nielsen	9/11/12

18. Contractor's Authorized Representative		
Name (typed):	Signature:	Date:
John W. Temple	[signature] FOR JWT	10/25/12
19. DOE Contracting Officer (or delegated representative)		
Name (typed):	Signature:	Date:
James Lovett	[signature]	10-25-2012

U.S. DEPARTMENT OF ENERGY
CONTRACT WORK AUTHORIZATION

1a. Program Title: Solar Energy	1b. Work Proposal Number (if applicable): AOP #2013

2. Headquarters Program Point of Contact:

Name: Minh Le Organization Code: Telephone No: (202) 287-1372

3. Headquarters Budget Point of Contact:

Name: Kyra Humphreys Organization Code: EE-3B Telephone No: (202) 586-8138

4. Responsible Program:	5. Responsible Secretarial Officer:
Office of Energy Efficiency and Renewable Energy	David Danielson

6. Responsible Field Element:

Savannah River Site Office

7a. Site and Facility Management Contractor:	7b. Contractor Point of Contact:
Savannah River Nuclear Solutions, LLC	Name: Brenda Garcia-Diaz Telephone No: (803) 725-9978

8. Work Authorization Number:*

SL-410003-12	0

10. Funds Authorized:

Congressional Control Point	Previous	Change	Current
EB2100000-05460-1103953 (2011)	$0.00	$1,000,000.00	$1,000,000.00

11. Performance period covered by funds:	12. Work Start Date:	13. Expected Completion Date:
From:10/01/2011 To:09/30/2012	10/01/2011	09/30/2012

14. Statement of Work:

Funding in the amount of $1,000,000.00 is authorized by the Solar Energy to perform work in the areas of :
The U.S. Department of Energy (DOE) SunShot Initiative and Solar Energy Technologies Program (SETP) authorizes funding in accordance with the program Annual Operating Plan (AOP). This operating plan authorizes specific funding amounts for each project and agreement, and requires detailed performance milestones and deliverable be met or completed within the period of performance.
Please refer to the Work Proposal Number (1b) to determine which section(s) of the AOP for which this authorization provides funding.

•

15. Reporting Requirements (Status reports, scientific and technical information or similar):

16. Work Authorization Program Official:

Name (typed): Craig Connelly, Signing on behalf of Ramamoorthy Ramesh	Signature: 99952aaf-48d8-49a1-bc28-9b69073c5610	Date: 8/14/2012

17. DOE Field Organization Official:

Name (typed): Patrick R. Jackson	Signature: Patrick R. Jackson	Date: 9/11/12

18. Contractor's Authorized Representative:

Name (typed): Lloyd Clevenger III	Signature: [signature]	Date: 9/11/12

19. DOE Contracting Officer (or delegated representative):		
Name (typed): James Lovett Jr	Signature: [signature]	Date: 9/12/2012
* The work authorization number will consist of the program code, AFP code, and the fiscal year		

DOE EERE SunShotInitiative

SunShot Lab Proposal FY2012-2015
Concentrating Solar Power Subprogram

Lead Organization Submitting Proposal:
Savannah River National Laboratory
FFRDC

Low-Cost Metal Hydride Thermal Energy Storage System for Concentrating Solar Power Systems

Technical Contact:
Ragaiy Zidan
Advisory Scientist and Principle Investigator
Savannah River National Laboratory
Bldg 999-2W
Aiken SC, 29808
(803)646-8876
Ragaiy.Zidan@srnl.doe.gov

Business Contact:
Robert E. Peters
Contract Administration
730-1B Room 3040
Aiken SC, 29808
(803)952-8648
robert02.peters@srs.gov

This 3-year project seeks to address the cost and efficiency of thermal energy storage for concentrating solar power systems. It involves the development and evaluation of highly reversible, compact and environmentally safemetal hydride-based systems forthermal energy storage.

1. **Project Overview**

a. Background

Three of the major areas for Thermal Energy Storage(TES) system improvements are in lowering their costs, reducing their full charging time to less than 6 hours and increasing their temperature of operation to improve the CSP overall production efficiency. Metal hydride TES systems have the ability to enable all of these improvements. In addition, many of the high and even the new lower temperature metal hydrides are fairly inexpensive. Preliminary calculations indicate that existing metal hydride TES systems can approach $15-$25/kWh. Only 3-4 kg of material would be needed per kWh. Because of their very high thermal capacity (approximately 20 times that of current systems), the size of the overall TES system along with its associated BOP can be substantially reduced leading to additional capital cost savings. Metal hydride TES systems can also be made to be self-regulating, thereby simplifying their design and lowering not only their capital but their operating costs as well. Because of their high energy capacity and reasonable kinetics many metal hydride systems can be charged rapidly. Metal hydrides for vehicle applications have demonstrated charging rates in minutes and tens of minutes as opposed to hours.This coupled with high heat of reaction allows metal hydride TES systems to produce very high thermal power rates (approx. 1kW per 6-8 kg of material). Finally, many new metal hydride materials have recently become available. One of the problems with metal hydride TES systems in the past has been selecting a suitable high capacity low temperature metal hydride material to pair with the high temperature material.

b. Objectives

The objectives of this research will be to evaluate and demonstrate a metal hydride-based TES system for use with a CSP system. A unique approach will be applied to this proposed project that makes use of the hierarchal modeling methodology developed by the Savannah River National Laboratory(SRNL). This approach combines our modeling experience with the extensive material knowledge and expertise at both SRNL and Curtin University (CU) to screen several promising metal hydride candidate materials and then select the best candidates for more thorough evaluation through experiments and more detailed models. During the second year, material optimization, bench-scale testing and more detailed component and system models will lead to a proof-of-concept demonstration and a preliminary system design. The culmination of this proposed research will be the design, fabrication and evaluation of a prototype metal hydride energy storage system that is aimed at meeting the SunShot cost and performance targets for TES systems allowing CSP systems to further expand their role in the renewable energy marketplace.

c. Novelty

The main novelty of this research is the use of high capacity metal hydride materials for thermal energy storage. The amount of thermal energy that can be stored per kilogram of metal hydride is typically very large and often 15 to 20 times more than what can be stored in traditional molten-salt systems. The higher energy density provided by the use of metal hydride systems can substantially lower the size and the capital cost of many CSP TES systems.While a few investigations of metal hydride TES systems were undertaken in the past, today because of the recent research in hydrogen energy systems the choices of metal hydride materials are now better than ever. This will strongly increase the probability of these systems becoming successful.Another unique aspect of metal hydride TES systems is that many of these systems can be located on or near dish/engine collectors due to their high thermal capacity and small size. This will facilitate the use of TES systems on dish collectors where previously they were considered impractical and uneconomical.Many new hydrides have been recently discovered and can be implemented to achieve a cost effective thermal storage system.

2. Technical Work Plan

BUDGET PERIOD 1 (12 months)

Task 1.1: Obtain and Generate Preliminary Material Engineering Data

Both SRNL and CU will be actively involved in collecting and evaluating existing material property data for various proposed metal hydride candidate materials. This data, which will include physical, thermodynamic and kinetic properties of several candidate materials, will be used initially as input to into the screening tool/preliminary system model. Both SRNL and CU have extensive metal hydride and material characterization equipment to perform these analyses. The initial materials to be evaluated will be discussed among the partners and the material property collection and analyses work will be divided so as to make best use of each partner's capabilities and to avoid duplication of effort. SRNL and CU have worked with many of our proposed candidate materials, which include MgH_2, $MgFeH_6$, $NaAlH_4$, $NaMgH_3$, TiH_2, CaH_2, NaH, $LaNi_5$, TiFe, $TiCr_{1.8}$, $CaNi_5$and others. Relevant subtasks and milestones include:

- Task 1.1: Complete the generation of preliminary data on at least 10 candidate MH TES material pairs against targets for operating temperature, pressure and hydrogen capacity.
- **Milestone 1.1**: We will determine and present to DOE the temperature-dependent kinetic rate expression for each individual MH in the 10 MH TES material pairs. We will determine the thermodynamic properties for each MH material and use this value to generate temperature-dependent pressures-curves.

Task 1.2: Refine and Apply Material Screening Tool (Preliminary System Models)

The use of numerical screening tools based on preliminary system models that evaluate the material properties against SunShot CSP TES targets will allow us to screen various metal hydride materials early on in the project to come up with the best candidate materials for further testing. The screening tool is a one-dimensional model based on steady state energy balance of the storage system considering the hydrogen charging process in a selected time range. The heat released during the charging process causes a temperature increase inside the bed material, which is evaluated by the model considering the balance between the thermal diffusion process inside the bed and the heat produced during the hydrogen up-taking.

The tool will be modified to the operating conditions and environment for TES systems in CSP plants. SRNL has found that this approach not only helps to focus the materials property testing efforts on the most suitable materials but also helps to focus the experimentalist on what key properties are needed to arrive at the best overall solutions. Relevant subtasks and milestones include:

- Subtask 1.2.1: Refine material screening tool to apply it to CSP TES applications. The tool will be used by researchers to determine which properties the system needs to have (in terms of heat of reaction, thermal conductivity, hydrogen absorption capacity) to achieve SunShot TES targets (such as charging time, volumetric energy density, expected exergetic efficiency and preliminary material and system costs) and to compare different materials to each other.

- Subtask 1.2.2: Screen at least 10 material candidate pairs against targets, as defined in Task 1.2.1.

- Subtask 1.2.3: Submit a peer reviewed paper on proposed metal hydride CSP TES system and use of screening tool and criteria.

- **Milestone 1.2**: Screen a minimum of 10 material candidate pairs against targets to arrive at 2 to 3 preliminary candidate material pairs that meet all technical targets defined as: charging time of less than 6h, volumetric energy density ≥25kWh$_{th}$/m^3, cycle life demonstrates ≤5% degradationin thermal capacity over 1000 exercises with a plausible, scientifically valid pathway to less than 1% degradation, and exergetic efficiency ≥95% (as defined in the ARPA-E HEATS FOA). Cost estimation must demonstrate a viable path to TES cost of ≤$15/kWh$_{th}$,

Task 1.3: Design and Fabricate a Bench-Scale MH TES System

To further evaluate the top 2-3 candidate material pairs, SRNL will develop and fabricate abench-scale metal hydride TES system suitable for testing 10-20 g of material. The purpose of this system is to provide preliminary materials engineering data on the performance of the selected metal hydride material pair as well as to obtain longer-term performance data for the development of future TES systems. In addition to being able to augment the materials property data in Task 1.1, the bench-scale system will also be able to obtain preliminary operating data from the coupling of two metal hydride materials which will be needed by both system and detailed vessel design models. Based on the previous experience at both SRNL and CU in designing and evaluating metal hydride prototype and full-scale systems, it is believed that the data from this bench-scale system, when combined with the material property data and the engineering models developed in years 1 and 2, will be sufficient to design and fabricate a nominal 30kWh prototype system (which is described in more detail in section 3.2). Relevant subtasks include:

- Subtask 1.3.1: Complete 10-20g bench-scale MH TES design. One of the critical performance issues with a metal hydride TES system is the interaction of the metal hydride material pairs. The bench-scale system will be designed to provide valuable pressure, temperature and material flow data on the best candidate material pairings. The bench-scale system will also be designed to enable normal and accelerated material cycling data later in the program (see Tasks 2.1 and 3.1).
- Subtask 1.3.2: Complete bench-scale MH TES fabrication. The fabrication of the bench-scale designed in Task 1.3.1 will include materials of construction similar to the anticipated prototype system as well as advanced heat transfer and media compaction

techniques to ensure that this type of material engineering data is adequately evaluated and tested prior to the design and testing of the prototype system.

- **Milestone 1.3:** The majority of the SRNL MH system engineering team will agree that the design is appropriate for the collection of the relevant technical data for the MH system (i.e. Detailed kinetic data for at least for 3 pressures and temperatures; Additional thermodynamic data (pressure, temperature and composition data) suitable for more detailed transport models, and; Improved thermal conductivity, heat capacity, bulk density and preliminary cycling data for any media enhancement or additions required to better meet the DOE SunShot targets). SRNL in-house pressurized vessel safety operations will review and approve the bench-scale design.

Go/No-Go Decision Point 1: Successful completion of all milestones in Budget Period 1. Engineering materials property data evaluation is complete indicating that the performance of the MH TES system can meet the proposed system technical targets. Technical targets are defined as: charging time of less than 6h, volumetric energy density $\geq 25 kWh_{th}/m^3$, cycle life demonstrates $\leq 5\%$ degradation in thermal capacity over 1000 exercises with a plausible, scientifically valid pathway to less than 1% degradation, and exergetic efficiency $\geq 95\%$ (as defined in the ARPA-E HEATS FOA). Cost estimation must demonstrate viable path to TES cost of $\leq \$15/kWh_{th}$,Changes to the target numerical values for any milestone, including those shown to require adjustment based upon modeling resultsor other learning throughout the course of the phase, must receive DOE concurrence in order to be altered to a value other than listed in this document. Without DOE concurrence, the original target value remains the milestone and therefore will remain the go/no-go criteria by which the project will be evaluated for continuation.

As a result of the go/no-go or stage-gate or continuation reviews, DOE may, at its sole discretion, make any of the following determinations: (1) continue to fund the project, depending on the availability of appropriations; (2) recommend specific direction or redirection of work under the project; (3) place a hold on the project pending further supporting data, funding, or to evaluate other projects concurrently; or (4) stop funding the project due to noncompliance, insufficient progress, inadequate business plan, schedule slip, change in strategic direction, or other factors.

Patents and Publications: File patents for relevant intellectual property. Results of research published in high-visibility, high-impact, peer-reviewed journal(s). All publications resulting from the funded research are required to include an acknowledgement that the work was supported by the U.S. Department of Energy, SunShot Initiative, under the specific award number.

<u>BUDGET PERIOD 2 (12 months)</u>

Task 2.1: Generate Detailed Engineering Property Data for Most Promising Candidate Materials and Systems

Both SRNL and CU will be actively involved in evaluating and developing new engineering material property data for the proposed metal hydride candidate materials. This data will be used as input to the more detailed vessel and system models. While many properties for some of the materials already exist, some of the properties needed for the engineering models such as thermal conductivity and heat capacity do not always exist and if they do they are not always suitable for the conditions (i.e. higher temperatures) or media form (i.e. compacted etc.) needed for this work. Both SRNL and CU have extensive metal hydride and material characterization equipment to perform these analyses. The initial materials to be evaluated will be discussed among the partners and the material property collection and analyses work will be divided so as to make best use of each partner's capabilities and to avoid duplication of effort.Relevant subtasks and milestones include:

- Subtask 2.1.1: Complete the generation of engineering data on best 2-3 candidate material pairs. The engineering data to be collected includes: 1) Detailed kinetic data for at least for 3 pressures and temperatures; 2) Additional thermodynamic data (pressure, temperature and composition data) suitable for more detailed transport models; 3) Improved thermal conductivity, heat capacity, bulk density and preliminary cycling data for any media enhancement or additions required to better meet the DOE SunShot targets. The engineering data obtained in Task 2.1will be used in Task 2.2 below to develop more detailed models that will be applied to the design and evaluation of the performance and operation of the prototype MH TES system.

Task 2.2: Develop and Evaluate Transport and System MH TES Models

Following the development and application of the screening models, existing SRNL 3D metal hydride finite element models will be modified and evaluated for the TES application. Heat and mass transfer are critical to the operation and performance of metal hydride systems. Detailed metal hydride models have already been developed by SRNL for other applications and are available for this program. The modifications that need to be made involve coupling two metal hydride vessels together as well as the different operating and boundary conditions.

In addition, a higher level system model will be developed similar to what was done by SRNL on previous projects. These Simulink™ models will evaluate the overall performance of various metal hydride TES configurations along with inputs and outputs from various solar collectors and power generators (turbines, heat engines etc.). SRNL will work with NREL's Solar Advisory Model (SAM) and other SunShot partners to help develop these interfaces. Relevant subtasks and milestones include

- Subtask 2.2.1: Develop preliminary vessel design model.Operation of the metal hydride based thermal energy storage system depends on the temperature and pressure in the high and low temperature beds and the exchange of heat with a heat transfer fluid or heat pipe. A finite element heat and mass transport model will be developed that will predict the transient behavior of these parameters for the small-scale and prototype tests at locations that are critical to system performance.

- Subtask 2.2.2: Develop preliminary MH TES and CSP system model. The system-level MH model is based on suitably simplified transient mass and energy balance equations and will be included in SAM (or other similar programs) to interface the TES system with the other CSP equipment (power generators, solar concentrators, etc). In order to evaluate the performance of the integrated system, the key parameters from the MH model that will need to be exchanged with the interfaced components will include temperature, pressure and hydrogen concentration during the charging/discharging process. In addition the MH system size and material properties will also be included, to evaluate the costs related to the CSP system.

- Subtask 2.2.3: Submit a peer reviewed paper on the analysis and modeling of a metal hydride CSP TES system.
- **Milestone 2.2:** Complete detailed analysis of at least 1 MH TES system material pair that is capable of meeting all of the DOE CSP TES targets. These targets include TES cost of $\leq$\$15/kWh$_{th}$, charging time of less than 6h, volumetric energy density $\geq$25kW$_{th}$/m^3, cycle life demonstrates $\leq$2% degradation over 1000 exercises with a plausible, scientifically valid path towards $\leq$1% degradation, and process efficiency/exergy $\geq$95% (as defined in the ARPA-E HEATS FOA).

Go/No-Go Decision Point 2: Successful completion of all milestones in Budget Period 2. Using the best available engineering materials property data, evaluate the performance of the MH TES system and compare these predicted results to the proposed system targets.These targets include TES cost of $\leq$\$15/kWh$_{th}$, charging time of less than 6h, volumetric energy density $\geq$25kW$_{th}$/m^3, cycle life demonstrates $\leq$2% degradation over 1000 exercises with a plausible, scientifically valid path towards $\leq$1% degradation, and process efficiency/exergy $\geq$95% (as defined in the ARPA-E HEATS FOA). If the predicted system is shown that it can meet all of the SunShot CSP targets and DOE SunShot objectives then the program should continue.

Changes to the target numerical values for any milestone, including thosefound to require modification based upon modeling outputs or other learning throughout the course of the phase, must receive DOE concurrence in order to be altered to a value other than what is listed in this document. Without DOE concurrence, the original target value remains the milestone and therefore remains the go/no-go criteria by which the project will be evaluated for continuation.

As a result of the go/no-go or stage-gate or continuation reviews, DOE may, at its sole discretion, make any of the following determinations: (1) continue to fund the project, depending on the availàbility of appropriations; (2) recommend specific direction or redirection of work under the project; (3) place a hold on the project pending further supporting data, funding, or to evaluate other projects concurrently; or (4) stop funding the project due to noncompliance, insufficient progress, inadequate business plan, schedule slip, change in strategic direction, or other factors.

Patents and Publications: File patents for relevant intellectual property. Results of research published in high-visibility, high-impact, peer-reviewed journal(s). All publications resulting from the funded research are required to include an acknowledgement that the work was supported by the U.S. Department of Energy, SunShot Initiative, under the specific award number.

BUDGET PERIOD 3 (12 months)

Task 3.1: Operate the Bench-Scale MH TES System to Obtain Long-Term Operation Data

SRNL will operate the bench-scale metal hydride TES system during the third year to obtain longer-term performance data for the development of future TES systems. A major objective of this task is to obtain accelerated material cycling data attemperature and pressure conditions representative from both the pilot and future larger scale TES systems. Relevant subtasks and milestones include:

- Subtask 3.1.1: Begin long-term bench-scale accelerated thermal cycle testing of at least 1 to 2 MH pairs in order to be able to estimate 10 years of operational performance (i.e. 5,000 cycles). The thermal cycle testing will go from a temperature of ≤250°C to ≥650°C and use an appropriate ramp rate for the MH system being testing. The system will be held at the minimum and maximum temperature for 15 min before ramping begins again.

- **Milestone 3.1:** Submit a peer reviewed paper on the bench-scale and proof-of-concept operation of a metal hydride CSP TES system The report will contain data from long-term bench-scale testing of at least 1 metal hydride pair that demonstrates the satisfactory performance for an estimated 10 year of operation (accelerated cycling of 5,000 cycles with no more than 5% loss of performance, with performance defined as the energy storage capacity of the system after 5,000 cycles divided by the original energy storage capacity). The report will also provide long term performance resultsincluding operating temperature, pressure, and gas transfer rates for preliminary validation of the vessel and component designs.

Task 3.2: Design and Fabricate Prototype MH TES Vessel and Components

Using the results from the vessel and system models along with the preliminary bench-scale results, CU will design and fabricate a suitable sized MH TES prototype system. The size and scale will be guided by the SRNL modeling results and the resources available at CU.The anticipated scale for the prototype will be on the order of 30kWh for a minimum of 6 hrs. SRNL will assist in the design of the prototype vessels and main components. CU will perform the final design and fabrication. Relevant subtasks and milestones include:

- Subtask 3.2.1: Design and fabricate prototype MH TES vessels that are capable of demonstrating all of DOE SunShot MH TES targets. These targets include TES cost of ≤$15/kWh$_{th}$, charging time of less than 6h, volumetric energy density ≥25kW$_{th}$/m^3, cycle life demonstrates ≤2% degradation over 1000 exercises with a plausible, scientifically valid path towards ≤1% degradation, and exergetic efficiency ≥95% (as defined in the ARPA-E HEATS FOA). Preliminary estimates show that approximately 2 kg of hydrogen would need to be cycled back and forth for a 30kWh scale prototype. The actual sizes of the prototype vessels will depend on the final metal hydrides selected but a nominal 5% capacity metal hydride material would require approximately 40 kg of metal hydride material to be contained in the vessel.

- Subtask 3.2.2: Design and fabricate key as-needed prototype MH TES components (includes heat exchangers, thermocline etc.). In addition to the metal hydride vessels themselves, SRNL and CU will design internal heat exchangers and/or heat pipes capable of removing or adding sufficient heat to maintain the operation of a nominal 30kWh prototype system for 6 hours.

Milestone 3.2: Complete design of a nominal 30kWhprototype metal hydride TES system capable of demonstrating and validating the SunShot CSP TES targets. These targets include TES cost of ≤$15/kWh$_{th}$, charging time of less than 6h, volumetric energy density ≥25kW$_{th}$/m^3, cycle life demonstrates ≤2% degradation over 1000 exercises with a plausible, scientifically valid path towards ≤1% degradation, and process exergetic efficiency ≥95% (as defined in the ARPA-E HEATS FOA). The majority of the SRNL MH system engineering team will agree that the design is appropriate to demonstrate the relevant technical milestones (i.e. TES cost of ≤$15/kWh$_{th}$, charging time of less than 6h, volumetric energy density ≥25kW$_{th}$/m^3, cycle life demonstrates ≤2% degradation over 1000 exercises with a plausible, scientifically valid path towards ≤1% degradation, and exergetic efficiency ≥95% (as defined in the ARPA-E HEATS FOA)). SRNL in-house pressurized vessel safety operations will review and approve the prototype design.

Task 3.3: Test and Evaluate Prototype Components and Vessels

Using the results from the vessel and system models along with the preliminary bench-scale results, CU will test and evaluate a suitable sized MH TES prototype system.A testing and evaluation plan will be developed between the experimentalists and the modelers to ensure that the right quantity and right quality of data is obtained during the prototype testing. The results need to be adequate to validate the models for later use for full-scale TES systems. Due to the time available for this project, long term material performance data will be obtained from the bench-scale testing where accelerated material cycling should be possible. The operation and data collection will be guided by the SRNL modeling results and the resources available at CU. Relevant subtasks and milestones include:

- Task 3.3: Complete 6-12 months of testing and evaluation of prototype components and vessels. Operation of the metal hydride based thermal energy storage system depends on the temperature and pressure in the high and low temperature beds and the exchange of heat with a heat transfer fluid or heat pipe. Transient measurements of these parameters will be made for the prototype tests at locations that are critical to system performance. Transient parameters will be measured and subsequently compared to model predictions. Key parameters that will be measured will include: operating temperatures, pressures, gas transport rates and cycle times. Results for steady-state, startup and shutdown operations will be demonstrated. Additional data measurements to support complete system and component mass and energy balances will also be obtained.

- **Milestone 3.3:** Submit a peer-reviewed journal publication that describes the operation and performance of the nominal 30kWh prototype MH TES system. The results of the testing described in the report will be of sufficient duration and quality so that when combined with the modeling and the bench-scale results they can be used to demonstrate and validate the SunShot CSP targets. These targets include TES cost of ≤$15/kWh$_{th}$, charging time of less than 6h, volumetric energy density ≥25kW$_{th}$/m^3, cycle life demonstrates ≤2% degradation over 1000 exercises with a plausible, scientifically valid path towards ≤1% degradation, and exergetic efficiency ≥95% (as defined in the ARPA-E HEATS FOA).

Task 3.4: Update and Validate Transport and System MH TES Models

Following the completion and analysis of the bench-scale and prototype performance results both the more detailed vessel transport model as well as the system level Simulink™ models will be updated and validated. Model validation consists of ensuring that the models accurately predict experimentally measured values. This effort requires not only that that experimental data are properly measured, but that experimental conditions are also recorded to be used as input to the models.

Relevant subtasks and milestones include:

- Subtask 3.4.1: Validate final vessel design model.Operation of the metal hydride based thermal energy storage system depends on the temperature and pressure in the high and low temperature beds and the exchange of heat with a heat transfer fluid or heat pipe. Transient measurements of these parameters will be made for the small-scale and prototype tests at locations that are critical to system performance. Validation of the detailed model will consist of running a model that simulates the experiments, using appropriate material data together with the boundary and initial conditions that existed for the experiments. Transient parameter values predicted by the model(s) will be compared against measured values. The model will be considered successfully validated if the error between measured and predicted parameter values is less than 10% throughout the transient.

- Subtask 3.4.2: Validate final MH TES and CSP system model. Temperatures, pressures and hydrogen concentrations data available from the system-level MH model will be validated against data available from the prototype design and testing the model to experimental validation should be within 10%. MH system cost analysis estimates are expected to be within 20% of the mass produced cost (based on future large-scale, approx.1000 units/yr. production).

- Subtask 3.4.3: Submit a peer reviewed paper on the operation and model validation for a 30 kWh prototype metal hydride CSP TES system.

- **Milestone 3.4**: Complete final analysis of a 30kWh MH TES system versus targets and validate that the error between measured and predicted parametervalues is less than 10%. Also provide future recommendations and develop a commercial partnership/technology transfer plan for a metal hydride based TES system At least 2 commercial companies (at least one U.S.) will be identified during the course ofthis project that with be willing to further develop and test commercial metal hydride based TES systems.

Final Deliverables:

- Final Deliverable 1: Publication of an article in a peer-reviewed journal that contains a completed and validated vessel model against prototype testing data that demonstrates and validates the model with respect to all DOE CSP TES SunShot targets. The final design package will also include future vessel recommendations, improvements and scale up options.

- Final Deliverable 2: A completed and validated system model, against date from the prototype, that agrees to experimental data to within 10%.
- Final Deliverable 3: A thoroughly tested nominal 30kWhprototype metal hydride TES system that demonstrates a MH system can meetthe SunShot CSP TES targets. These targets include TES cost of $\leq$\$15/kWh$_{th}$, charging time of less than 6h, volumetric energy density $\geq$25kW$_{th}$/m^3, cycle life demonstrates $\leq$2% degradation over 1000 exercises with a plausible, scientifically valid path towards $\leq$1% degradation, and process exergetic efficiency $\geq$95% (as defined in the ARPA-E HEATS FOA).

Patents and Publications: *File patents for relevant intellectual property. Results of research published in high-visibility, high-impact, peer-reviewed journal(s). All publications resulting from the funded research are required to include an acknowledgement that the work was supported by the U.S. Department of Energy, SunShot Initiative, under the specific award number.*

Changes to the target numerical values for any milestone, including those found to require modification based upon modeling outputs or other learning throughout the course of the phase, must receive DOE concurrence in order to be altered to a value other than what is listed in this document. Without DOE concurrence, the original target value remains the milestone and therefore remains the go/no-go criteria by which the project will be evaluated for continuation.

DOE EERE SunShot Initiative

Concentrating Solar Power Research and Development
SunShot Lab Proposal Development Process FY2012-2015

Lead Organization Submitting Proposal:
Savannah River National Laboratory
FFRDC

Fundamental Corrosion Studies in High-Temperature Molten Salt Systems for Next Generation Concentrated Solar Power Systems

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This project seeks to reduce corrosion at high operating temperature in concentrating solar power systems through the identification of heat transfer fluid systems and corrosion protection strategies to predict and control corrosion rates with common heat transfer materials.

1. **Project Overview**
   a. *Background*

Concentrating solar power (CSP) systems are projected to need to produce energy with a cost of $0.06 / kWh when implemented on a very large scale. It is generally believed that temperatures of the heat transfer fluids (HTFs) will need to be higher than 800°C to drive an advanced Brayton cycle or Rankine cycle with superheated steam to reach this target. To make this system technically feasible, HTFs need to be developed that can operate at these temperatures for long periods of time without significant degradation of either the HTF or the materials of construction for the system. Increasing the lifetime and operating temperature of HTFs in CSP systems will allow capital costs to be amortized over longer time periods and, hence, reduce the cost of energy generation. Decreasing materials corrosion will lower system maintenance costs due to less frequent component failure and replacement.

   b. *Objectives*

The objective of this research is to improve materials durability in CSP systems in the presence of high operating temperature (HOT) HTFs that can be used with advanced power production processes. Improvements in materials durability will be achieved by creating an integrated experimental and numerical approach that will allow identification of optimal combinations of HOT HTFs with materials of construction and corrosion protection schemes that maintain the HTFs good heat transfer properties, achieve low corrosion rates, and indicate good performance in CSP system simulations. This objective will be achieved by combining: 1) experimental determination of corrosion rates in model HOT HTF systems and identification of critical parameters of corrosion mechanisms 2)thermodynamic property modeling for HOT HTFs3) risk mitigation methods for the identified corrosion mechanisms, 3) demonstrating the effectiveness of corrosion mitigation methods and 4) modeling of corrosion and corrosion in heat transfer systems.

   c. *Novelty*

While materials durability studies have been conducted for lower temperature HTFs that are common in industry, detailed characterizations of molten salt systems capable of high temperature operation at temperatures routinely exceeding 800°C have either not been performed or not been extensive. The corrosion management strategies employed with higher temperature salts is often drastically different when compared to those for the lower temperature nitrate salts that can utilize well known oxide passivation layers for corrosion prevention. Whereas at higher temperatures, activity gradient driven mass transfer and thermal gradient driven mass transfer are often dominant, especially in many chloride and fluoride salt systems that are among the most promising HOT HTFs. This research will characterize corrosion and material degradation at these conditions and compare corrosion rates and mechanisms with state-of-the-art systems. In addition, thermodynamic properties of binary and higher order mixtures will be calculated because data for these more complex systems is not readily available in the literature.

2. Technical Work Plan

BUDGET PERIOD 1 (12 months)

Task 1.1: Measure the Corrosion Properties of State of the Art HOT HTFs in Static and Isothermal Systems

We will design and refine test equipment for accurate, reproducible measurement of corrosion rates for containment materials in contact with hot molten salts at temperatures up to 1000°C in static environments with no fluid flow. We will determine the corrosion rates of state of the art HTFs with common containment materials including stainless steels, superalloys, refractory alloys, and ceramics, or other advanced materials agreed upon with SunShot Program Management. The testing in Task 1.1 will include electrochemical testing such as linear polarization resistance (LPR) determination, polarization testing, electrochemical impedance spectroscopy (EIS), and cyclic potentiodynamic polarization (CPP) scans to determine susceptibility to localized corrosion. Potentiostatic experiments may also be conducted in specific regions of interest in tests to accelerate corrosion mechanisms. The following subtasks will be performed:

- Subtask 1.1.1: Development of an experimental apparatus capable of isothermal and static corrosion testing and temperatures up to 1000°C under varying environments (argon gas, nitrogen, ammonia, etc.). The apparatus will include the capability for a static electrochemical potential hold device for rapid corrosion measurements and long-term static corrosion cells (for testing up to 1000 hours).
- Subtask 1.1.2: Perform post testing microscopic, spectroscopic and analytical characterization of corrosion samples with state-of-the art HTF systems. Specific techniques to be used may include: SEM and TEM for surface morphology characterization, EDS for surface elemental analysis and element mapping, Raman, Auger, and XPS for oxidation state characterization, XRD for phase identification, and scanning electrochemical microscopy (SECM) for corrosion inspection and localized surface characterizations including electrochemical impedance spectroscopy (EIS). Salt composition and corrosion product composition may also be analyzed using ICP-AES, ICP-MS, AA or other techniques.
- **Milestone (Subtask 1.1.1)**: Commissioning of high temperature isothermal and static corrosion apparatus system capable of measurements at temperatures up to 1000°C and proof of operation by validation with typical corrosion rates in chloride and fluoride salts. The system will be capable of temperature control within 4°C of the set point temperature and will be capable of operation from vacuum up to 15 psig with controlled atmosphere and gas flow rates up to 50 sccm. The reactor will be capable of sustained ramp rates of a minimum of 5°C / minute.
- **Milestone (Subtask 1.1.2)**: Measurement of the general corrosion rates and trends for Incoloy-800H, Hastelloy-N (if available, other alloy with Cr level ~10% if not), and Ni-201 in FLiNaK at 850°C will be compared with values of 29 mg/cm^2, 13 mg/cm^2, and 0 mg/cm^2, at 500 hours from Olson (2009) to demonstrate proper operation of the system. Weight-loss will not exceed that seen from Olson (2009) for each particular alloy by more than 25%, and will be correlated to mean alloy Cr content.

Task 1.2: Numerical Simulations of Corrosion in State of the Art HOT HTFs

Corrosion mechanisms will be identified and preliminary models will be developed to predict corrosion rates observed in state of the art molten salt heat transfer systems. These corrosion models will account for the effect of mass transport and will be used to predict corrosion rates in systems with fluid flow. A framework for incorporation of general corrosion reactions with soluble products at a containment surface will be developed later and incorporated into computational fluid dynamics (CFD) models.

- Subtask 1.2.1: Identification of relevant corrosion reactions, reactants, and mechanisms. Development and application of 0-D and/or 1-D corrosion models that are capable of analyzing and predicting the local chemical environment, corrosion rates, and corrosion mechanisms for state of the art systems and advanced HOT HTFs. Validation of predictions requires data from, and will be accomplished in, year 2.
- Subtask 1.2.2: Development of a 3-D CFD-based modeling platform capable of predicting local chemical environment and corrosion rates based on corrosion models developed in Subtask 1.2.1.
- **Milestone (Subtask 1.2.1)**: Identify two corrosion mechanisms that explain prominent localized and general corrosion phenomena and that correlate with electrochemical and physical characterizations of results in Tasks 1.1 and 1.4
- **Milestone (Subtask 1.2.2)**: Demonstration of a CFD-based 3-D numerical modeling platform capable of calculations over a surface area greater than 50 cm^2 that incorporates relevant physiochemical mechanisms to the dominant corrosion mechanisms to allow for the prediction of key system variables such as localized concentration and electrochemical potential. The numerical model will agree with published values from the literature to within +/- 10%.

Task 1.3: Prediction solubility and stability of species in advanced molten salt systems

Use Gibbs energy minimization to calculate thermodynamic solubility of species in molten salts and thermal stability of molten salts in equilibrium with container and heat exchanger materials. Species solubility modeling will be useful for corrosion analysis and modeling to determine whether corrosion products are likely to passivate metal surfaces and reduce corrosion. Solubility data can aid identification of corrosion inhibitors, as well as identify key contaminants that may play an active role in determining corrosion susceptibility in the localized electrochemical environment. Solubility data will feed into models as bounding conditions to approximate the local electrochemical environment, which may be very different from the predicted bulk composition. Understanding corrosion product stability may allow for prediction of likely corrosion species formed for various molten salt combinations with alloys.

- Subtask 1.3.1: Prediction of the solubility of alloy components and corrosion products in molten salts. This work will focus on calculating the solubility of fluorides from alloy or ceramic constituents in all materials proposed for use with high temperature molten salt systems. Of specific interest are metals selectively attacked by dissolution such as Cr or involved in forming passive layers such as Ni. Modeling will identify the most stable corrosion products for the alloys and their solubility in the molten salt mixtures to be studied.

- Subtask 1.3.2: Prediction of corrosion potential at the alloy surface. Thermodynamic simulation results will be compared with SRNL experimental data. Specific determined corrosion potential data, and potentially modify the thermodynamic model if necessary. The effect of variables such as temperature and composition of the salt media and containment materials will be assessed.
- Subtask 1.3.3: Prediction of thermal stability and decomposition of molten salt in contact with the alloy. Research will be conducted utilizing temperatures and atmospheres in the proposed window of operation and where salts or dissolved species may be unstable.
- **Milestone (Subtask 1.3.1)**: The species solubility from the alloys in molten salts will be predicted using a Gibbs energy minimization method. The solubility will be predicted to within a maximum deviation of $\leq$ 10% of the values reported in the literature or experimentally determined values. The species composition in molten salt predictions will be carried out at various temperatures (>800°C). Molten salt composition and alloy composition will be input variables for the thermodynamic predictions. Equilibrium species concentrations will be predicted using equilibrium constants and activity coefficients.
- **Milestone (Subtask 1.3.2)**: The stable solid corrosion products formed at the alloy or ceramic surface in equilibrium with molten salt and alloy will be evaluated using the Gibbs energy minimization method. These products will be evaluated with the species non-ideality in the solution. Subsequently, the Gibbs energy for the reaction in the actual working condition can be determined by using the activity of each substance. The thermodynamic potentials (U_{corr}) for corrosion (which are used with electrochemical kinetics for prediction of E_{corr}) calculated from the Gibbs energy will be compared with the experimentally determined corrosion potential measured in Task 1.1 to illustrate (by subtraction) the extent of kinetics and mass transfer in those measurements. The most stable corrosion products will be suggested from the comparison with E_{corr}. The values for E_{corr} (calculated) will be compared to E_{corr} (experimental, SRNL) and the error will be $\leq$ 10%
- **Milestone (Subtask 1.3.3)**: The composition change for the molten salt at temperatures above >800°C will be calculated using Gibbs energy minimization method. The vapor pressure of the individual salt components and decomposition to other liquid and solid components will determined to guage the stability of the salt mixture. Stability is defined as a weight loss of $\leq$1%. Interaction among the different species in the molten salt in equilibrium with the alloys or ceramics will be considered in evaluations.

Task 1.4: Isothermal Performance Qualification Testing in Advanced HOT HTFs

A set of performance qualification tests will be carried out by UTRC on a minimum of six test coupons of each containment material type including stainless steels, superalloys, refractory alloys, and ceramics. For each material, static testing for corrosion will be carried out under isothermal conditions. Pretreated test coupons will be immersed in the HOT molten salt systems (placed in crucibles and under an inert gas environment) and the weight-change due to corrosion will be measured at different intervals of time and up to 10,000 hours total testing time. In these tests, high-purity molten salt will be used to establish a baseline for each material at a pre-specified temperature.

Multiple samples will be tested for extended times to provide statistical information needed to provide quantitative corrosion data required for use of HOT HTF / container material combinations in commercial systems. It should be noted that Task 1.1 focuses on short-term corrosion characterization and aims to determine corrosion mechanisms using electrochemical testing techniques designed to accelerate corrosion and elucidate corrosion mechanisms. Testing under Task 1.4 will mostly focus on flat test coupons submerged into the corrosive environment and held at the desired isothermal temperature for extended times followed by post testing characterization of the test coupons. This will allow for validation of mechanisms determined by Task 1.1 and ensure potential errors are not propagated in other tasks. In this task multiple samples will be tested for at least an order of magnitude longer times to provide statistical information needed to provide quantitative corrosion data required for use of HOT HTF / container material combinations in commercial systems. Comparison of results between Tasks 1.1 and 1.4 will be essential in determining the long-term importance of corrosion mechanisms observed and quantified in short-term electrochemical characterization, and shorter-term static corrosion tests.

- Subtask 1.4.1: Baseline long-term performance qualification testing for HOT HTFs under isothermal and static conditions
- Subtask 1.4.2: Develop physics-probabilistic-based models to predict service lifetime of containment materials. Employed physics-probabilistic-based models will include the Arrhenius model and/or the Eyring model. The constants in either of these two models will be determined empirically based on results from testing in subtask 1.4.1.
- Subtask 1.4.3: Identification of degradation mechanisms and mitigation methods. Examples of potential failure mechanisms that may be uncovered during the execution of the experiments in Subtask 1.4.1 may include: a) Dealloying of metals (such as Cr) from the containment material that contacts the hot molten salt system by direct chemical reactions between the containment material and the salt, b) The products of dealloying may completely dissolve in the molten salt system but at lower temperatures these dealloying products may reprecipitate, and c) Impurity-driven corrosion where the hot molten salt system react with impurities in the containment material. Sometimes, these reaction products deposit as a corrosion-resistant layer on the surface of the containment material. For each identified failure mechanism, risk mitigation methods will be developed. Examples of the proposed risk mitigation methods may include: the addition of corrosion inhibitors and the use of protective surface coating for the containment material.
- **Milestone (Task 1.4)**: By the end of this reporting period, Task 1.4 milestones to be delivered are: 1) Determine long-term weight loss by corrosion due to contact of the molten salt (at temperatures above >800°C) with each of the selected containment materials [Task 1.4.1]. 2) Physics-probabilistic models to predict the time-dependent material loss by corrosion [Task 1.4.2]. 3) Demonstration of effectiveness of proposed risk mitigation methods for the identified corrosion mechanisms As shown by a corrosion rate of less than 3mpy. Cost/benefit analysis will also be undertaken.

Go/No-Go Decision Point 1:

The GO criterion at the end of this reporting period signifies that all the milestones listed for Budget Period 1 above are fully met.

Changes to the target numerical values for any milestone, including those indicated to be adjusted based upon modeling outputs or other learning throughout the course of the phase, must receive DOE concurrence in order to be altered to a value other than what is listed in this document. Without DOE concurrence, the original target value remains the milestone and therefore the go/no-go criteria by which the project will be evaluated for continuation.

As a result of the go/no-go, stage-gate, or continuation reviews, DOE may, at its sole discretion, make any of the following determinations: (1) continue to fund the project, depending on the availability of appropriations; (2) recommend specific direction or redirection of work under the project; (3) place a hold on the project pending further supporting data, funding, or to evaluate other projects concurrently; or (4) stop funding the project due to noncompliance, insufficient progress, inadequate business plan, schedule slip, change in strategic direction, or other factors.

Patents and Publications: File patents for relevant intellectual property. Results of research published will be directed towards high-visibility, high-impact, peer-reviewed journal(s). All publications resulting from the funded research include an acknowledgement that the work was supported by the U.S. Department of Energy, SunShot Initiative, under the specific award number.

BUDGET PERIOD 2 (12 months)

Task 2.1: Measure the Corrosion Properties of State of the Art HOT HTFs in Systems with Fluid Flow and Thermal Gradients

In most fluid heat transfer systems, fluid flow and thermal gradients are intrinsic system design parameters. Non-isothermal systems cause distributions in alloy-salt thermodynamic equilibriums that manifest as temperature dependent corrosion rates, temperature dependent equilibrium corrosion product concentrations, and material stresses that can aggravate corrosion mechanism. Fluid flow can enhance corrosion by continually interrupting the formation of temperature dependent thermodynamic equilibriums and can cause erosion-corrosion mechanisms. SRNL will design and refine test equipment for accurate, reproducible measurement of corrosion rates in environments with thermal gradients and fluid flow. The testing in Task 2.1 will mirror that performed in Task 1.1. The following subtasks will be performed:

- Subtask 2.1.1: Development of an experimental apparatus capable of corrosion testing with temperature gradients and fluid flow at temperatures up to 1000°C under varying environments (argon gas, etc.). The apparatus may consist of either a natural convection flow loop, or thermosiphon for the study of thermal gradient driven mass transfer measurements.
- Subtask 2.1.2: Perform post testing characterization identical to Subtask 1.1.2 but for samples from Subtask 2.1.1.
- **Milestone (Subtask 2.1.1)**: Commissioning of high temperature corrosion apparatus system capable of measurements with fluid flow and thermal gradients at temperatures up to 1000°C. The system will be capable of operation with minimum temperature gradients

of 50°C between the hot and cold legs and will be capable of naturally convective flows generated by these temperatures. The temperatures of the hot leg of the system will be capable of having temperatures varied at a minimum of 5°C / minute. Fluid flow will be verified by direct measurements or a combination of temperature measurement and CFD.

- **Milestone (Subtask 2.1.2)**: Observation and quantification of the changes in corrosion mechanisms and corrosion rates in the presence of high, intermediate, and low thermal gradients and fluid flow. Experiments will allow quantification of the average and standard deviation for sample weight-change at specific locations in the natural convection system with the presence of thermal gradients and fluid flow. We will deliver a rank ordered list of the best alloys (at least of those measured) for corrosion resistance with the HTF used at the temperature and flow conditions.

Task 2.2: Numerical Simulations of Corrosion in State of the Art HOT HTFs

Corrosion models that include thermal gradients and fluid flow will be developed to predict corrosion rates and mechanisms observed in state of the art molten salt heat transfer systems. These corrosion models will account for the effect of heat and mass transport and will be used to predict local electrochemical environment and corrosion rates in systems with fluid flow. Coupling of non-isothermal experiments with CFD modeling of systems with thermal gradients and natural convection will allow enhanced evaluation of corrosion on samples. Changes in corrosion mechanisms and rates compared with isothermal cases with no fluid flow will be evaluated. The impact of dimensionless parameters such as Rayleigh number and Grashof number on corrosion in systems with natural convection will be characterized.

- Subtask 2.2.1: Extend 0-D and 1-D models of year 1 (Task 1.2) to 2-D and 3-D platforms. Analyze and predict corrosion rates and mechanisms in the presence of thermal gradients, concentration gradients, and fluid flow.
- Subtask 2.2.2: Application of CFD modeling to understand heat and mass transport in experiments with thermal gradients and fluid flow. Integration of corrosion modeling with CFD thermal and mass transport modeling to predict corrosion phenomena observed in non-isothermal experiments.
- **Milestone (Subtask 2.2.1)**: Prediction of local electrochemical environment for materials at 800°C, 850°C and 900°C based on corrosion potential values, calculation of Tafel and Butler-Volmer kinetic parameters from polarization at 800°C, 850°C and 900°C. Compare of long-term corrosion rates with linear polarization resistance values at 800°C, 850°C and 900°C. Incorporation of CPP experimental results and thermodynamic modeling results at 800°C, 850°C and 900°C for evaluation of localized corrosion susceptibility. The numerical model will agree with published values from the literature or experimentally determined values to within +/- 10%.
- **Milestone (Subtask 2.2.1)**: Use models to evaluate local electrochemical environment for cases with high, medium, and low thermal gradients and fluid flow experiments conducted at high temperature. Quantify kinetic parameters using Tafel and Butler Volmer kinetic expressions. Evaluation of CPP experiments to determine significance of localized corrosion mechanisms in systems with thermal gradients and fluid flow.
- **Milestone (Subtask 2.2.2)**: CFD-based 3-D numerical model of the flow and thermal gradients in the SRNL experimental apparatus from Task 2.1.1 for non-isothermal

corrosion testing without externally forced electrochemical reactions to support understanding of fluid flow and thermal gradients on corrosion phenomena. The numerical model will agree with published values from the literature or experimentally determined values to within +/- 10%.

Task 2.3: Prediction of corrosion products and suggestion of corrosion inhibiting modifications to advanced molten salt systems

Measurements of corrosion potential at SRNL will be compared to the thermodynamic predictions and the predicted local chemical compositions will then be provided to USC for modeling of corrosion systems. The effect of variables such as temperature, changes to composition of the salt media, and containment materials on corrosion potential will be theoretically predicted. The corrosion potential is related to Gibbs energy of the system and is calculated as a function of temperature and composition. This modeling will be used to predict molten salt mixtures that may bring about superior corrosion resistance through the addition of corrosion inhibitors to proposed HOT HTFs. Corrosion inhibitors such as ZF_4 can be used to react with oxide, moisture, and other impurities [1, 2] or adjust the acidity or basicity of the molten salt to alter the solubility of corrosion products such as CrF_3 [3]. The success of the use of corrosion inhibitors in different molten salt mixture families such as molten fluorides, molten chlorides, has been shown to be broadly applicable by [1-4]. The corrosion properties of these novel HOT HTF mixtures will be tested.

- Subtask 2.3.1: Prediction of corrosion products from U_{corr} data. Using the Gibbs energy model, the U_{corr} for container and heat exchanger material combinations with different molten salts will be evaluated. These will be compared with the experimentally determined corrosion potentials, E_{corr}, that are generated from Tasks 1.1 and 2.1. If the plot of calculated U_{corr} for the molten salt system shows linear dependence with the experimental data, this indicates that the calculated U_{corr} is proportional to the E_{corr} value and the kinetics and mass transfer mechanism are similar.
- Subtask 2.3.2: Prediction of properties of the molten salts with the addition of corrosion inhibitors. The thermodynamic modeling approach based on Gibbs energy of fusion and interaction among salt components will be used to predict properties such as eutectic compositions and temperatures.
- **Milestone (Subtask 2.3.1)**: Predict principle corrosion products for all Year 1 and Year 2 experiments based on corrosion potential data. Compare predicted corrosion products with analytical results to determine corrosion products from the samples. Work with USC researchers to incorporate U_{corr} predictions into CFD models The values for E_{corr} (calculated) will be compared to E_{corr} (experimental, SRNL) and the error will be $\leq 10\%$.
- **Milestone (Subtask 2.3.2)**: Calculate the thermodynamic stability of salt/corrosion inhibitor mixtures under a variety of temperatures and pressures to ensure the eutectic liquid is going to be stable. Stability is defined as a weight loss of $\leq 1\%$. These calculations will be used to predict salt/corrosion inhibitor mixture heats of fusion, heat capacity, and eutectic points for inclusion in models. The model will have a maximum deviation of $\leq 10\%$ of the values reported in the literature or experimentally determined values.

Task 2.4: Thermal Cycling Performance Qualification Testing in Advanced HOT HTFs

Tests for quantifying the corrosion behavior under thermal cycling and thermal gradients with the coupons immersed in the molten salts will be carried out. At a minimum 6 coupons of each material type will be tested at each specified high temperature. The main objective of this series of tests is to identify how thermal cycling and the potential for thermal gradient driven mass transfer affects the corrosion rate compared to isothermal conditions, as well as the effect of thermal cycling on brittle materials such as ceramics or composites. Thermal cycling protocols will determine the effects of repeated heating and cooling of the samples in the molten salt on corrosion rates and corrosion mechanisms. A set of specific performance qualification tests will be carried out by UTRC on test coupons of each containment material type of interest. Weight-change due to corrosion will be measured after specific time intervals and up to 10,000 hours total testing time.

- Subtask 2.4.1: Cyclic long-term qualification testing for HOT HTFs (pure molten salts). With respect to identifying the acceptable performance of materials exposed to highly corrosive environments, UTRC performed comprehensive reviews of the industry's operating experience of best-corrosion-resistant materials. UTRC reviewed the requirements of corrosion-resistant materials per applicable industry codes and standards such as ASME, ASTM, API, NACE and EN standards. The insights of these reviews indicate that materials with maximum allowable corrosion rates below 3 mpy (mils per year; where 1 mpy is equivalent to 0.025 mm/yr) are typically recommended and materials with corrosion rates above 20 mpy are not recommended for highly corrosive environments. In our materials qualification testing, our target maximum allowable corrosion rate will be at ≤ 3 mpy.
- Subtask 2.4.2: Develop physics-probabilistic-based models to predict the service lifetime of the containment materials. Employed physics-probabilistic-based models will include the Arrhenius model and/or the Eyring model. The constants in either of these two models will be determined empirically based on results from testing in subtask 2.4.1.
- Subtask 2.4.3: Identification of degradation mechanisms and mitigation methods. Identical to task 1.4.3 but for cyclic long-term qualification tests performed in Subtask 2.4.1.
- **Milestones (Task 2.4)**: By the end of this reporting period, the following milestones will be delivered: 1) Results of impact of the long-term cycling tests on corrosion rates for the selected containment materials [Task 2.4.1]. 2) Physics-probabilistic based models for predicting weight loss by corrosion and with parameters empirically estimated from tests performed under Task 2.4.1 [Task 2.4.2]. 3) Demonstration of effectiveness of risk mitigation methods for the corrosion mechanisms identified in Task 2.4.1 [Task 2.4.3] as shown by a corrosion rate of less than 3mpy. Cost/benefit analysis will also be undertaken.

Go/No-Go Decision Point 2:

The GO criterion at the end of this reporting period signifies that all the milestones listed for Budget Period 2 above are fully met.

Changes to the target numerical values for any milestone, including those indicated to be adjusted based upon modeling outputs or other learning throughout the course of the phase, must receive DOE concurrence in order to be altered to a value other than what is listed in this document. Without DOE concurrence, the original target value remains the milestone and therefore the go/no-go criteria by which the project will be evaluated for continuation.

As a result of the go/no-go, stage-gate, or continuation reviews, DOE may, at its sole discretion, make any of the following determinations: (1) continue to fund the project, depending on the availability of appropriations; (2) recommend specific direction or redirection of work under the project; (3) place a hold on the project pending further supporting data, funding, or to evaluate other projects concurrently; or (4) stop funding the project due to noncompliance, insufficient progress, inadequate business plan, schedule slip, change in strategic direction, or other factors.

Patents and Publications: File patents for relevant intellectual property. Results of research published in high-visibility, high-impact, peer-reviewed journal(s). All publications resulting from the funded research are required to include an acknowledgement that the work was supported by the U.S. Department of Energy, SunShot Initiative, under the specific award number.

BUDGET PERIOD 3 (12 months)

Task 3.1: Measure the Corrosion Properties of Advanced HOT HTFs including Corrosion Inhibitors and Protective Surface Coatings

We will investigate and characterize corrosion and document the impact of more complex molten salt mixtures with corrosion inhibitors in advanced HOT HTFs. For the HOT HTFs, such as binary and ternary systems composed of chlorides or fluorides like $MgCl_2$-KCl or FLiNaK, research will focus on adding trace corrosion inhibitors to the HOT HTF salts that will act to either 1) reduce the solubility of the metallic component of the piping alloys in the salt through the use of redox agents or buffers that will reduce the basicity of the salt and its corrosion potential, 2) reduce active alloy component dissolution by reducing the solubility thermal dependence, 3) react with the alloy to help form or stabilize a passive layer in contact with the salt, making a spontaneously-generated, self-healing corrosion inhibiting layer, and 4) interfere with common corrosion mechanisms. For example, carburizing and nitriding components could potentially address 3) in chloride salts, while 1) could potentially work in chloride and fluorides salts by contacting them with metallic Zr, Na, or K. This project will also incorporate molten salt systems and alloys under study on other programs and in consultation with SunShot program management.

- Subtask 3.1.1: Characterization and determination of bulk, intergranular, and pitting corrosion rates and mechanisms of alloy and ceramic materials of interest at temperatures >800°C in HOT HTFs with corrosion inhibitors. Testing will focus on determining the effect of changes in salt composition, corrosion inhibitor additives, cathodic protection, and coatings on reducing corrosion. This testing will integrate corrosion management concepts developed by the project team over prior years of the project. Testing will mix isothermal and non-isothermal testing and will focus on materials and conditions determined to be of the most interest to the SunShot Program and assist in supporting peer reviewed publications.

- Subtask 3.1.2: Perform post testing characterization identical to Subtasks 1.1.2 and 2.1.2 but for samples from Subtask 3.1.1.
- **Milestone (Subtask 3.1.1)**: Submission of an article for publication in a peer reviewed journal detailing corrosion rates and mechanisms in HOT HTFs and the impact of corrosion on high temperature CSP system economics.
- **Milestone (Subtask 3.1.1 and Subtask 3.1.2)**: Develop a detailed evaluation of corrosion mitigation strategies including: changing salt composition, addition of corrosion inhibitors, cathodic protection schemes, and coating of metals. Provide recommendations for the best state-of-the-art corrosion reduction strategies. The corrosion rate for tests with corrosion inhibitors will be quantified and compared with baseline results from Year 1 and Year 2 of the project to determine the overall reduction in the corrosion rate. Corrosion mitigation strategies will be deemed viable if they can deliver corrosion rates of $\leq$3mpy with less than 20% additional cost to the salt or to the heat transfer system materials, or less than or equal to 170 $/kW$_{Th}$ (estimated cost of HTF system divided by heat transport capability) given in the Feb. 2012 SunShot Vision Study as the 2020 Tower Roadmap HTF System cost.

Task 3.2: Numerical Simulations of Corrosion in Advanced HOT HTFs

Corrosion models will be developed to explain corrosion rates and mechanisms observed in advanced HOT heat transfer systems and roles and impact of corrosion inhibitors. These corrosion models will include the effect of mass transfer and will be used to predict corrosion rates in systems with fluid flow. Sensitivity analysis will be used to determine how variation in specific fluid parameters affects corrosion rates. CFD models will be used and subroutines will be developed for cases where corrosion products are not soluble in solution and create passivating and non-passivating coatings.

- Subtask 3.2.1: Perform a sensitivity analysis on HOT HTF fluid properties to determine the properties that most affect corrosion rates. Sensitivity analysis will investigate fluid properties including heat capacity, viscosity, density, fluid velocity, and temperature as well as concentration of impurities including oxide species, chromium, and corrosion inhibitors. Other key parameters to be studied include the equilibrium and kinetic parameters associated with chemical and electrochemical reactivity of the species in solution, and parameters controlling mass transfer such as diffusion coefficients of species.
- Subtask 3.2.2: Perform CFD modeling of CSP systems that include non-soluble corrosion products, cathodic protection schemes, and corrosion inhibitors.
- Design cathodic protection scheme for chosen heat exchanger and container configuration and materials using CFD model which includes relevant corrosion mechanism.
- **Milestone (Task 3.2)**: Sensitivity analysis detailing the impact of system conditions and salt properties on system corrosion. The sensitivity analysis will outline how system conditions can be optimized to reduce corrosion in CSP heat transfer systems while operating in the optimal range for CSP power plants using high temperature power cycles. The sensitivity analysis will be based on the corrosion models developed as part of this project.

- **Milestone (Task 3.2.2)**: Submission of an article for publication in a peer reviewed journal detailing modeling of corrosion in HOT HTFs and integration of corrosion modeling with CFD tools.

Task 3.3: Prediction of corrosion rates, inhibitors and surface coatings of Advanced Molten Salt Systems

Use Gibbs energy minimization to evaluate the corrosion rates, corrosion inhibitors and surface coatings of molten salt and container materials systems for the HOT HTFs. The effect of variables such as temperature and composition of the salt media and system (i.e., containment and heat exchanger) materials on corrosion thermodynamics will be theoretically predicted. Team interactions will allow for estimation of corrosion kinetics for these inhibitors and coatings. Calculated corrosion rates will be compared to experimentally determined data. Modeling will predict corrosion rates of materials in molten salts and identify allowable container materials for HOT HTFs. UA will corroborate with SRNL on experimentally determined corrosion rates, CFD model development with USC and UTRC's long term thermal cyclic corrosion rates and corrosion system mechanisms.

- Subtask 3.3.1: Predict the corrosion resistance in the molten salts from E_{corr} and I_{corr} using thermodynamic modeling. The corrosion resistance is evaluated from the E_{corr} and I_{corr} for the molten salt and alloy system. The resistance value is calculated for each temperature at fixed salt and alloy compositions and for various corrosion environments. The calculated resistance value R is obtained from the slope of E_{corr} vs I_{corr} plot. The predicted i_{corr} value can be expressed as the equation $I_{corr} = -K\cdot(\Delta G^{o} - RTlna)/(nF\cdot R)$.
- Subtask 3.3.2: Prediction of suitable corrosion inhibitors and corrosion resistant surface coatings for the container materials and molten salt system. The Gibbs energy minimization approach will be adopted in predicting suitable corrosion inhibitors and corrosion resistant surface coatings for the molten salt system as a function of temperature, composition and static and dynamic corrosion environment.
- Subtask 3.3.3: Prediction of corrosion rates. Corrosion rates will be predicted from the predicted I_{corr} using Gibbs energy expressions as proposed in sub task 3.3.1. The corrosion rate at a specific temperature is dependent on the corrosion current I_{corr}. The predicted corrosion rate at a specific temperature can be determined as a function of Gibbs energy equation: $r = A \cdot \Delta G_T$. The A is derived for specific composition, temperature and corrosion environment. Thus the corrosion rate can be predicted using Gibbs energy minimization method for molten salt systems.
- **Milestone (Task 3.3.1)**: Thermodynamic prediction of the corrosion resistance for container materials exposed to various molten salts at temperatures within the window of operation for HOT HTF systems. The predicted values will be in agreement with the experimentally determined values to within +/- 5%.
- **Milestone (Task 3.3.2)**: The changes in E_{corr} and I_{corr} compared with base cases will be evaluated when: corrosion inhibitors are added to the molten salt, reducing agents are added to the salt, or when coatings are applied to alloys.
- **Milestone (Task 3.3.3)**: Corrosion rates will be calculated for molten salt and container material systems based on thermodynamic principles. The corrosion rates will be calculated from thermodynamics and will be used to refine CFD modeling of corrosion in

static and flow systems. The predicted values will be in agreement with the experimentally determined values to within +/- 5%.

Task 3.4: Impurity Qualification Testing in Advanced HOT HTFs

Impurities and corrosion inhibiting additives will be added to baseline high-purity HOT molten salts in coupon immersion tests to determine the impact of impurities on material's corrosion behavior. As a minimum, six coupons of each type will be tested and the statistically relevant data (means, standard deviations, upper and lower bound values) will be reported. Experiments under this task will investigate the long-term stability of corrosion inhibitors undergoing thermal cycling and experiencing thermal gradients. High-purity molten salt will be used to isolate the effect of impurities and prevent coupling with thermal cycling and thermal gradients in the corrosion rate. Industry experiences and codes and standards requirements indicate that materials with maximum corrosion rates below 3 mpy are recommended and materials with corrosion rates above 20 mpy are not recommended. For our qualification testing, our target maximum allowable corrosion rate will be set at ≤ 3 mpy.

- Subtask 3.4.1: Impurity long-term qualification testing for HOT HTFs performed under isothermal and thermal cycling conditions. For qualification testing, a target maximum allowable corrosion rate will be set at ≤ 3 mpy.
- Subtask 3.4.2: Physics-probabilistic-based model for predicting service lifetime considering the effects of temperature cycling and presence of impurities. The epistemic uncertainties of the Arrhenius parameters (pre-exponential factor and the activation energy) will be propagated in the predictive model using Monte Carlo sampling (MCS) or the Latin Hypercube sampling (LHS) techniques. As a result, the predicted corrosion rate will be generated as a probability distribution (in the form of a probability density function as well as cumulative function) with a mean and a standard deviation. The prediction will be at 95% confidence. The mean, upper bound and lower bound values of the corrosion rate will be compared with the experimentally measured value at a given time (t).
- Subtask 3.4.3: Identification of degradation mechanisms and mitigation methods. Examples of the proposed risk mitigation methods that will be investigated include: the addition of corrosion inhibitors and the use of protective surface coating on the containment material.
- **Milestone (Task 3.4)**: By the end of this reporting period, the following milestones will be delivered: 1) Results of tests performed to characterize the impact of impurities on corrosion rates in the selected containment materials [Task 3.4.1]. 2) Physics-probabilistic models to predict weight loss by corrosion. The model parameters will be estimated empirically based on the tests performed under Task 3.4.1. Also, model predictions will account for the parameters' uncertainty [Task 3.4.2]. 3) Demonstration of effectiveness of proposed risk mitigation methods for the identified materials degradation/corrosion mechanisms [Task 3.4.3]. The maximum allowable corrosion rate will be ≤ 3 mpy.

<u>Final Project Technical Report:</u>

The final deliverables at the end of this project will be documented in a final technical report that documents all the milestones listed under the three Budgetary Periods 1 to 3.

Changes to the target numerical values for any milestone, including those indicated to be adjusted based upon modeling outputs or other learning throughout the course of the phase, must receive DOE concurrence in order to be altered to a value other than what is listed in this document. Without DOE concurrence, the original target value remains the milestone and therefore the go/no-go criteria by which the project will be evaluated for continuation.

As a result of the go/no-go, stage-gate, or continuation reviews, DOE may, at its sole discretion, make any of the following determinations: (1) continue to fund the project, depending on the availability of appropriations; (2) recommend specific direction or redirection of work under the project; (3) place a hold on the project pending further supporting data, funding, or to evaluate other projects concurrently; or (4) stop funding the project due to noncompliance, insufficient progress, inadequate business plan, schedule slip, change in strategic direction, or other factors.

Patents and Publications: File patents for relevant intellectual property. Results of research published in high-visibility, high-impact, peer-reviewed journal(s). All publications resulting from the funded research are required to include an acknowledgement that the work was supported by the U.S. Department of Energy, SunShot Initiative, under the specific award number.

References

1. Olson, L.C., et al., Journal of Fluorine Chemistry, 2009. **130**(1): p. 67-73.
2. Williams, D.F., *Assessment of Candidate Molten Salt Coolants for the NGNP/NHI Heat-Transfer Loop*, D.o. Energy, Editor. 2006. p. 44.
3. MacPherson, ORNL-2626, 1958.
4. Williams, D.F., L. Toth, and K. Clarno, *Assessment of Molten Salt Coolants for the Advanced High-Temperature Reactor*, D.o. Energy, Editor. 2006.

Attachment 2

Contract Work Authorization

No. HQ1001-0-SR

Project Title: Energy Employees Occupational Illness Compensation Program (EEOICPA)

Project Number: 2013-HS-2001036

WORK AUTHORIZATION

U.S. DEPARTMENT OF ENERGY
Management and Operating (M & O) Contract Work Authorization

1. INITIATOR(s): Pat Worthington (Name & Signature) — HS-10 (Organization Code) — 301-903-5926 (Phone)

2. PROJECT TITLE: Energy Employees Occupational Illness Compensation Program (EEOICPA) AC:

3. RESPONSIBLE PROGRAM SECRETARIAL OFFICE: Office of Health, Safety, and Security

4. RESPONSIBLE FIELD OFFICE: Savannah River

5. M & O CONTRACTOR NAME: Savannah River / 410225 / 410225 (SR - SRO)

6. WORK AUTHORIZATION NO: HQ1001 - 0 - SR

7. FUNDS HEREBY AUTHORIZED (WHOLE DOLLARS)

TOTAL BUDGET AUTHORITY: $125,000.00

TOTAL BUDGET OUTLAY: $125,000.00

B & R	Program	ORG	Transaction Type	Rev.	Date	Budget Authority	Budget Outlay
HQ1001000	3184701	HS-10	Fund Project from B&R	0	10/1/2012	$125,000.00	$125,000.00

8. PERFORMANCE PERIOD COVERED BY FUNDS: FROM: 10/1/2012 TO: 9/30/2013

9. WORK START DATE: 10/1/2012

10. EXPECTED COMPLETION DATE: TBD

11. FUTURE FUNDING PLANNED: To Be Determined

12. WORK AUTHORIZED:
See attached Statement of Work.

	NAME AND SIGNATURE	DATE
13. WORK AUTHORIZATION OFFICIAL:	[signature] Stephen Kirchhoff	9/28/12
14. OPERATIONS OFFICE OFFICIAL:	[signature]	10/24/12
15. M & O CONTRACTOR OFFICIAL:	[signature]	10/12/12
HEADQUARTERS BUDGET POINT OF CONTACT:	[signature] Debra James, 301-903-3465	9-24-12
FIELD/CONTRACTOR POINT OF CONTACT:	[signature]	10/24/12

9/21/2012 3:31:07 PM

WAS Project No.: 2013-HS-2001036

Laboratory/Contractor: The Savannah River Site (CID#: 410225)

Laboratory/Contractor Contact: Regina Price Phone: 803-952-6288

HS Program Contact: Greg Lewis Org: HS-14 Phone: 202-586-2784

OVERALL PROJECT GOAL/OBJECTIVE:

The Energy Employees Occupational Illness Compensation Program Act of 2000 (EEOICPA) establishes a program to provide compensation to current and former employees of the Department of Energy (DOE), its contractors and subcontractors, companies that provided beryllium to DOE, and atomic weapons employers (AWE's). Under EEOICPA, DOE is required to verify employment histories, provide medical records, and provide radiation dose records and other information pertinent to National Institute for Occupational Safety and Health (NIOSH) radiation dose reconstruction and Department of Labor (DOL) Subtitle B and Subtitle E case preparation for anyone who applies for compensation under EEOICPA.

FUNDING FOR THE FOLLOWING ACTIVITIES:

The funding provided through this financial plan is to be used to conduct the following work tasks to implement EEOICPA, including claims under both Subtitle B and Subtitle E of the EEOICPA. These tasks include:

1) Perform the work necessary to complete Employment Verifications requested by DOL for the EEOICPA Subtitle B program.

- Work with corporate entities or unions to verify employment of former site workers.
- Complete all necessary claims forms associated with the request.
- Research and retrieve records needed to complete claims forms.
- Complete declassification, as needed, of records required for the processing of claims forms.

2) Perform the work necessary to provide radiation dose records requested by NIOSH as part of the EEOICPA Subtitle B program.

- Complete and sign off on all necessary claims forms associated with the request.
- Research and retrieve records needed to complete claims forms.
- Complete declassification, as needed, of records required for the processing of claims forms.

3) Perform the work necessary to complete Document Acquisition Request (DAR) requested by DOL as part of the EEOICPA Subtitle E program.

- Complete and sign off on all necessary claims forms associated with the request.
- Research and retrieve records needed to complete claims forms.

- Complete declassification, as needed, of records required for the processing of claims forms.

4) Perform other necessary EEOICPA related records work as needed.

5) Maintain local records to track the activities conducted under EEOICPA.

FY 2013 DELIVERABLES:	DATES:
Provide monthly reports that include the number of records requests received, number completed and cost per request for each of the three types of requests. This report should be sent to: • HS-14 (Greg Lewis), • HS-10 Budget Contact (Jeanette Yarrington) • HS-81 Budget Contact (Debra James).	15^{th} of the following month

FY 2013 FUNDING FOR OCTOBER FINANCIAL PLAN:
$125,000

*The FY 2013 Annual Financial Plan (AFP) amount of $500,000 is the amount allocated for a full year of EEOICPA activity. Your site should only obligate $125,000 that is indicated in this Work Authorization. If your site has already obligated the full AFP amount and a contractor or contractors have exhausted funds, please contact the EEOICPA Program Manager (Gregory Lewis 202-586-2784) and the HS-10 Budget Contact (Jeanette Yarrington 301-903-7030) immediately.

Attachment 3

Contract Work Authorization

No. SR071801

Project Title: Center for Sustainable Groundwater and Soil Solutions, Attenuation-Based Remedies for the Subsurface Applied Field Research Initiative (ABRS AFRI)

U. S. DEPARTMENT OF ENERGY
CONTRACT WORK AUTHORIZATION

1a. Project Title
Center for Sustainable Groundwater and Soil Solutions: Attenuation-Based Remedies for the Subsurface Applied Field Research Initiative (ABRS AFRI)

1b. Work Proposal Number
DE-AC09-08SR22470 - SR071801

2. Headquarters Program Point of Contact
Name: Mark Gilbertson | Organization Code: EM-10, Office of Site Restoration | Phone: 202-586-5042 | E-mail: mark.gilbertson@em.doe.gov

3. Headquarters Budget Point of Contact
Name: Jeffrey McMillan | Organization Code: EM-61, Office of Budget | Telephone: 301-903-7701 | E-mail: jeffrey.mcmillan@em.doe.gov

4. Responsible Program
Office of Environmental Management

5. Responsible Secretarial Officer
Tracy P. Mustin
Phone: 202-586-7709
Routing: EM-1

6. Responsible Field Organization
U.S. Department of Energy, Savannah River Operations

7a. Site and Facility Management Contractor
Savannah River Nuclear Solutions, LLC

7b. Contractor Point of Contact
Name: John W. Temple | Telephone No. (803) 952- 7210

8. Work Authorization Number
DE-AC09-08SR22470 - SR071801

9. Revision Number
0

10. Funds Authorized ($ in thousands)(See NOTE below)
NOTE: Funding obligated under most current contract modification and related approved financial plan executed under contract clauses B-4, Obligation of Funds, and I.53, DEAR 970.5232-4 Obligation of Funds (Dec 2000) applies.

Budget and Reporting Code:	Previous:	Change:	Current:
See Table in Statement of Work	$0	~~$0~~ 140,000	$ 140,000.00

11. Performance Period Covered by Funds		12. Work Start Date	13. Expected Completion Date
EY4049110	To: September 30, 2013	From: Oct. 1, 2012	To: Sept. 30, 2013

14. Statement of Work (Includes attachments)
NEEDS STATEMENT:
The objective of the Attenuation-Based Remedies for the Subsurface Applied Field Research Initiative (ABRS AFRI) at the Savannah River Site is to develop and bring to maturity science based approaches and associated tools to clean up sites contaminated with combinations of metals, radionuclides, and recalcitrant organic compounds. Without these approaches and tools many contaminated sites in the DOE complex will be unable to achieve acceptable end-states.

	Fund	Year	Reporting Entity	Program	B&R	Project	PBS	Amount ($k)
	01250	2013	410003	1110676	EY4049110	0003925	SRO71801	$ 140,000.00

15. DOE Budget Official
Name (typed): Harold K. Nielsen | Signature: Harold K. Nielsen | Date: 10/22/12

16. Contractor's Authorized Representative
Name (typed): John Temple | Signature: [signature] | Date: 10/24/12

17. DOE Contracting Officer (or delegated representative)
Name (typed): Jim Lovett | Signature: James Lovett | Date: 10/25/12

Technical Task Plan

NEEDS STATEMENT:

The objective of the Attenuation-Based Remedies for the Subsurface Applied Field Research Initiative (ABRS AFRI) at the Savannah River Site is to develop and bring to maturity science based approaches and associated tools to clean up sites contaminated with combinations of metals, radionuclides, and recalcitrant organic compounds. Without these approaches and tools many contaminated sites in the DOE complex will be unable to achieve acceptable end-states.

BACKGROUND AND PURPOSE:

Groundwater contamination plumes with toxic metals and/or radionuclides are present at the majority of DOE complex facilities. These plumes have reached up to a mile in length at some sites and discharge to surface water exposure points (e.g., Hanford, Savannah River Site and Oak Ridge). Remediation of these groundwater units to negotiated end-states is required to meet federal and state regulations. The F-Area groundwater contaminant plume at the Savannah River Site is the primary filed research site of the ABRS AFRI. Contaminants being addressed at this site are uranium, strontium-90, iodine-129, and tritium. SRNL and SRS are designated as the lead for the EM-12 funded ABRS AFRI because:

- SRNL and the Savannah River Nuclear Solutions Area Completion Projects have a decades long history of working together to develop and deploy innovative technical approaches to achieving desired end-states at contaminated sites
- SRNL was a key collaborator in development of the in situ remediation at the F-Area plume that allowed the abandonment of the pump-and-treat system, moving the site closer to end-state goals in a more cost effective and efficient way
- The desired end-state at F-Area will be met in phases that are specified in the SRS RCRA Permit (2009) that also encourages continued development and deployment of innovative technologies to achieve the end-state
- Successful applied research conducted at this AFRI will provide the means of achieving the end-state specified in the RCRA permit, as well as being widely applicable across the DOE complex

Applied science at the ABRS AFRI is directed at five program areas – Understanding the System, Sampling and Characterization Approaches and Tools, Decision-Making Tools, Enhanced Attenuation Technologies, and Long-Term Monitoring Strategies and Tools.

Advancements achieved at the ABRS AFRI work in conjunction with those achievements realized at the Hanford and Oak Ridge AFRIs as well as the Advanced Simulation Capability for Environmental Management (ASCEM) Initiative to make up the applied science portfolio established within the EM-12 Soil and Groundwater Remediation Program. Specifically, the data-rich and mature nature of the SRS F-Area site provides a great opportunity for testing ASCEM developed concepts.

ABRS AFRI GOALS

As stated in the ABRS AFRI Strategic Plan, the initiatives goals are:

- Develop tools and approaches for attenuation-based remedies and integrate them into the regulatory framework established by the US EPA and ITRC.
- Develop characterization and monitoring tools that focus on the geochemical properties that control contaminant fate and transport, facilitate evaluation on the field-scale, and are inexpensive and easy to use.
- Develop approaches that will optimize the number of locations and the number of samples and measurements required to achieve an acceptable level of uncertainty in decision making.
- Develop remediation technologies that will effectively and efficiently attenuate contaminants and result in their long-term stabilization.
- Through a collaboration of applied and basic research provide the technically defensible underpinnings for approaches, tools and technologies to implement attenuation-based remedies leading to completion of remediation activities for contamination of groundwater by metals and radionuclides.
- Transfer the ABRS AFRI products to site owners, regulators and other members of the communities of practice to foster usage by the DOE community, as well as the national community.

AFRI COLLABORATORS

DOE Office of Science funded Sustainable Systems Scientific Focus Area at LBNL is the main collaborator providing funding independent of this AFRI. Other collaborators include:

Interstate Technology & Regulatory Council
North Carolina State University
GSI Environmental, LLC
Oregon State University
Sandia National Laboratory
Pacific Northwest National Laboratory
Technical Assistance Collaborators TBD

2013 TECHNICAL APPROACH

R&D Area1: UnderstandingtheSystem (200K)

Task 1.1: Phase II of Understanding Aquifer Heterogeneity with the Reactive Facies Approach

Phase I of Understanding Heterogeneity with the Reactive Facies Approach focused on the upper aquifer at the F-Area Applied Field Research Site. Reactive facies proved to be a valuable construct for understanding geochemical heterogeneity in this relatively simple system. The lower aquifer is more complex and the degree of heterogeneity more representative of aquifers across the DOE complex. Phase I was completed in collaboration with the Science Focus Area (SFA) Plume Challenge at LBNL. Phase II began in FY11 but was interrupted by a funding hiatus in FY12. The activities of Phase II will be resumed in collaboration with LBNL to develop the concept of reactive facies into a more general approach to aquifer heterogeneity that can be applied across the DOE complex. The general approach to aquifer heterogeneity, based on reactive facies, will ultimately transfer to ASCEM allowing inclusion of a powerful means of accounting for subsurface heterogeneity in modeling.

Sub-tasks

1.1.1 Sampling and analysis of existing lower aquifer cores by high vertical resolution x-ray fluorescence and acid-base titrations; providing samples to LBNL for mineralogical and surface chemistry analysis

1.1.2 Continued analysis of sample textures by optical microscopic image analysis

1.1.3 Borehole flow-meter tests at two wells to obtain a vertical profile of aquifer flow properties

R&DArea2: Characterization (100K)

Task 2.1: Supporting the development of Risk based end states: Indicators of systemic changes that predict likely changes to mobility of stabilized contaminants (100K). Seeplines are the endpoint of the kinetic source term for metals and radionuclides. They become part of the source term because the relative abundance of organic matter and sudden changes in "master variable" gradients cause sorption or precipitation of contaminants. Even after eliminating contaminant flux into these zones they may continue to release contaminants to the associated stream. Understanding the factors that control this release is critical to establishing a path toward an acceptable end state, developing a timeline to reach that end state, and providing a basis for long-term monitoring. Consistent with the ABRS AFRI Strategic Plan, this task will provide baseline data for understanding the processes controlling contaminant release from seeplines and hyporheic zones and the effects of boundary conditions, such as fluctuations in water table, on these processes. The seepline at the F-Area Field Research Site will be the focus of these initial studies. These studies will advance the capability of ASCEM products to incorporate the dynamic processes occurring at seeplines and hyporheic zones. This task will leverage support from the SRNS Environmental Compliance & Area Completion Projects division. The results of this activity will support end state monitoring initiatives at SRS as well as the Oak Ridge and Hanford sites, as well as other sites within in larger DOE complex.

Sub-task

2.1.1 Establish correlations between variation in master variables and contaminant attenuation/release in reactive facies at the seepline

R&DArea3: EnhancedAttenuation (300K)

Task 3.1: Enhanced Attenuation of Uranium and ^{129}I by Humic Acid

Uranium and ^{129}I are primary contaminants of concern at the F-Area Applied Field Research Site. Both are also of concern at Hanford and uranium is a concern across the DOE complex. Bench-scale studies by Lawrence Berkeley National Laboratory showed that humic acid strongly binds uranium at mildly acidic pH and potentially binds ^{129}I. This suggests humic acid would be an ideal enhanced attenuation amendment for use for hot-spot treatment at the F-Area Applied Field Research site where both contaminants are present in acidic groundwater. It would also be applicable to a wide variety of other DOE sites. Field tests and optimization of this technology are required to move it from basic science to deployment.

Sub-tasks

3.1.1 Column studies to optimize use of humic acid at the F-Area Field Research Site

3.1.2 Field test of humic acid technology for uranium and ^{129}I remediation at the F-Area Field Research Site using single well push-pull type tests deployed by direct push methods

Task 3.2: Monitoring of the Biostimulation Site for Remediation of Uranium

In 2010 Arcadis began a small pilot demonstration of uranium and other radionuclide removal from groundwater at the F-Area Applied Field Research site. The project funded by DOE-EM involved injection of molasses into the subsurface to create a zone of reducing conditions designed to force precipitation of uranium and ^{99}Tc by converting them to their less soluble reduced forms. Funding to Arcadis from DOE-EM ended in FY2012. The purpose of the test was to evaluate whether immobilization of uranium and ^{99}Tc by creation of a zone of reduced iron minerals is sustainable for long periods in an oxygenated aquifer. The period of funding to Arcadis was long enough to demonstrate that reducing conditions were created by the molasses injection. It was not long enough to determine whether the reducing zone will remain or will quickly become re-oxidized accompanied by remobilization of uranium and ^{99}Tc. Additional monitoring of the reduced zone is important to ensure the goals of the initial funding are realized.

Sub-tasks

3.2.1 Sampling and analysis of groundwater from monitoring wells at the injection site

3.2.2 Push-pull tests to interrogate the reduced zone for mineralogy and stability of uranium and ^{99}Tc

Task 4: Management of the Technical Assistance Program

For over two decades, SRNL has managed a dynamic and efficient national program sponsored by DOE Office of Environmental Management that provides teams of technical experts with a broad experience base to recommend strategies to address DOE's challenging environmental problems when standard approaches haven't worked. The Technical Assistance program is managed through the Center for Sustainable Soil and Groundwater Solutions at SRNL. The Technical Assistance program organizes and manages small teams of nationally recognized experts in support of both DOE's smaller sites, such as Paducah, Portsmouth, Pinellas, Ashtabula, Fernald, Mound, and Kansas City Plant, and larger sites such as Oak Ridge, Los Alamos, Lawrence Livermore and Savannah River. Typically these teams visit the sites for a week to work with site problem holders to develop efficient and effective solutions to address their complex/difficult technical issues. This task provides funding for administration of the technical assistance program including helping site problem holders to develop technical needs statements, selection of the technical experts, contracting of non-SRNL participants, management of the team meeting, and preparation of the technical assistance team report.

Attachment 4

Contract Work Authorization

No. HO091101

Project Title: Advanced Simulation Capability for Environmental Management

U. S. DEPARTMENT OF ENERGY
CONTRACT WORK AUTHORIZATION

1a. Project Title	1b. Work Proposal Number
Advanced Simulation Capability for Environmental Management	DE-AC09-08SR22470 - HO091101

2. Headquarters Program Point of Contact

Name: Justin Marble	Organization Code: EM-12. Soil and Groundwater Remediation	Phone: 301-903-7210 E-mail: justin.marble@em.doe.gov

3. Headquarters Budget Point of Contact

Name: Tracey Whipp	Organization Code: EM-61. Office of Budget	Telephone No. 301-903-7157

4. Responsible Program	5. Responsible Secretarial Officer
Office of Environmental Management	Tracy P. Mustin Phone: 202-586-7709 Routing: EM-1

6. Responsible Field Organization

U.S. Department of Energy, Savannah River Operations

7a. Site and Facility Management Contractor	7b. Contractor Point of Contact
Savannah River Nuclear Solutions, LLC	Name: John W. Temple Telephone No. (803) 952- 7210

8. Work Authorization Number	9. Revision Number
DE-AC09-08SR22470 - HO091101	0

10. Funds Authorized (S in thousands)(See NOTE below)

NOTE: Funding obligated under most current contract modification and related approved financial plan executed under contract clauses B-4, Obligation of Funds, and I.53, DEAR 970.5232-4 Obligation of Funds (Dec 2000) applies.

Budget and Reporting Code:	Previous:	Change:	Current:
EY4049110	S0	~~S0~~ $59,000.00	S 59,000.00

11. Performance Period Covered by Funds		12. Work Start Date	13. Expected Completion Date
From: October 1, 2012	To: September 30, 2013	From: Oct. 1, 2012	To: Sept. 30, 2013

14. Statement of Work (Includes attachments)

NEEDS STATEMENT:

The United States Department of Energy (DOE), Office of Environmental Management (EM), in collaboration with other DOE offices, is leading a multi-institution, multi-disciplinary team of geoscientists, material scientists, and computational scientists from Los Alamos, Lawrence Berkeley, Pacific Northwest, Oak Ridge, and Savannah River National Laboratories with support from Argonne, Lawrence Livermore, and Idaho National Laboratories to develop a modeling initiative for Advanced Simulation Capability for Environmental Management (ASCEM). ASCEM is a state-of-the-art scientific toolset and approach for understanding and predicting contaminant fate and transport in natural and engineered systems. This modular and open source high performance computing (HPC) tool will facilitate graded and integrated approaches to modeling and site characterization that enable more robust and standardized assessments of performance and risk for EM disposal operations, cleanup and closure activities. The ASCEM Multi-Laboratory program is aimed at addressing critical EM program needs to provide the capability to better understand and quantify subsurface flow and contaminant transport behavior in complex geological systems and the long-term performance of engineered components including cementitious materials in nuclear waste disposal facilities, in order to reduce uncertainties and risks associated with DOE EM's disposal, environmental cleanup and closure programs.

	Fund	Year	Reporting Entity	Program	B&R	Project	PBS	Amount (Sk)
	01250	2013	410003	1110676	EY4049110	0004017	HQ091101	S 59,000.00

15. DOE Budget Official

Name (typed):	Signature:	Date:
Harold K. Nielsen	Harold K. Nielsen	10/23/12

16. Contractor's Authorized Representative

Name (typed):	Signature:	Date:
John Temple	Lloyd C Cheney for JWT	10/24/12

U. S. DEPARTMENT OF ENERGY
CONTRACT WORK AUTHORIZATION

1a. Project Title	1b. Work Proposal Number
Advanced Simulation Capability for Environmental Management	DE-AC09-08SR22470 - HO091101

17. DOE Contracting Officer (or delegated representative)

Name (typed):	Signature:	Date:
Jim Lovett	[signature]	10/25/12

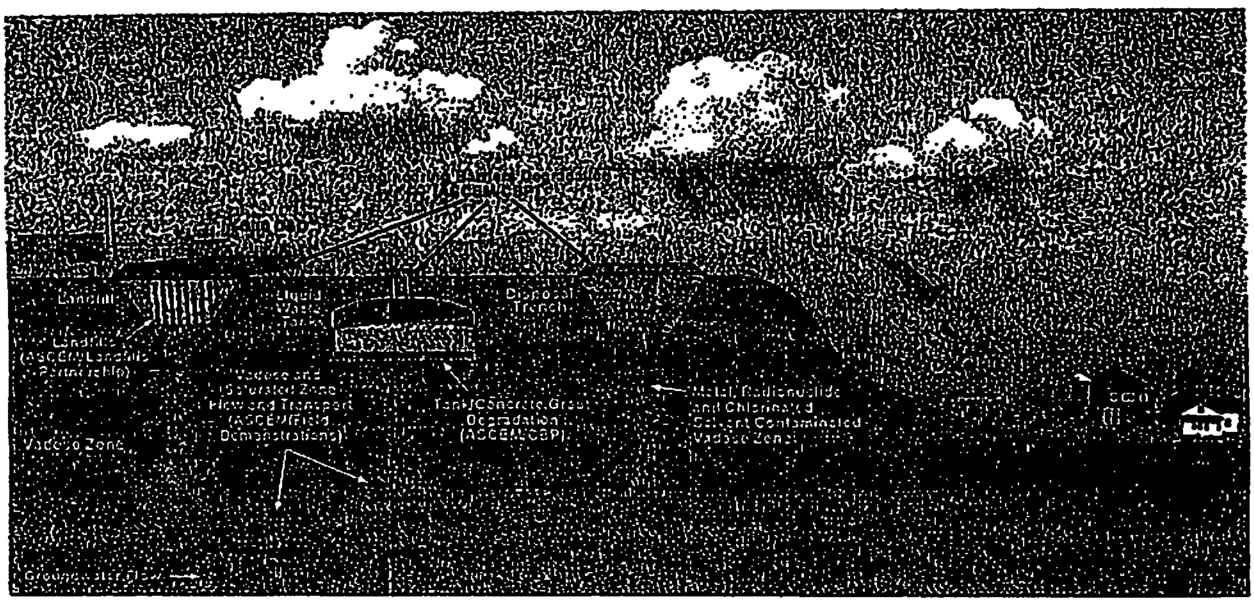
Technical Task Plan ASCEM WBS 1-1

NEEDS STATEMENT:

The United States Department of Energy (DOE), Office of Environmental Management (EM), in collaboration with other DOE offices, is leading a multi-institution, multi-disciplinary team of geoscientists, material scientists, and computational scientists from Los Alamos, Lawrence Berkeley, Pacific Northwest, Oak Ridge, and Savannah River National Laboratories with support from Argonne, Lawrence Livermore, and Idaho National Laboratories to develop a modeling initiative for Advanced Simulation Capability for Environmental Management (ASCEM). ASCEM is a state-of-the-art scientific toolset and approach for understanding and predicting contaminant fate and transport in natural and engineered systems. This modular and open source high performance computing (HPC) tool will facilitate graded and integrated approaches to modeling and site characterization that enable more robust and standardized assessments of performance and risk for EM disposal operations, cleanup and closure activities. The ASCEM Multi-Laboratory program is aimed at addressing critical EM program needs to provide the capability to better understand and quantify subsurface flow and contaminant transport behavior in complex geological systems and the long-term performance of engineered components including cementitious materials in nuclear waste disposal facilities, in order to reduce uncertainties and risks associated with DOE EM's disposal, environmental cleanup and closure programs.

BACKGROUND AND PURPOSE:

EM-30's Office of Technology and Innovation Development (OTID) mission is to develop technologies that advance the safe and timely cleanup of legacy wastes and facilities from defense nuclear applications. This is the largest cleanup program in the world [1]. Although EM has made great progress toward this goal during the past twenty years, the remaining clean-up challenges are far more complex than those previously addressed. The role of the ASCEM initiative is to develop a transformational modeling approach and toolset to help EM better meet these challenges through improving its long-term risk and performance modeling capabilities and by characterizing and reducing the uncertainty associated with the resulting predictions for the types of EM clean-up sites illustrated in the figure below.



In a review of the EM technology roadmap, the National Research Council (NRC) of the National Academies provided advice to DOE-EM for addressing principal science and technology gaps. The NRC identified the principal technology gaps in the groundwater and soil remediation program and the major recommendation was on the development and use of advanced computational models to better understand subsurface flow and contaminant transport behavior in complex geological systems, and the long-term performance of engineered components and barriers, including cementitious materials in nuclear waste disposal facilities.