U.S. DEPARTMENT OF ENERGY | Office of Science

BERAC Briefing on the

Basic Research Needs for Environmental Management Workshop

July 8–11, 2015

Michelle V. Buchanan
Associate Laboratory Director for Physical Sciences
Oak Ridge National Laboratory

October 28, 2015

Advanced Scientific Computing Research (ASCR)
Basic Energy Sciences (BES)
Biological and Environmental Research (BER)

Outline

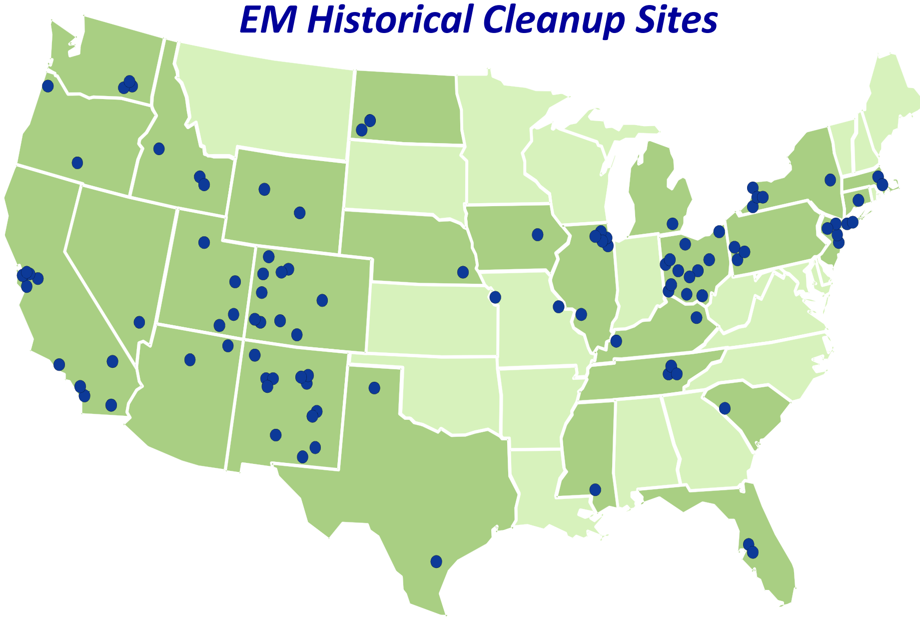
- **Workshop Motivation**
  - DOE Office of Environmental Management (EM) Mission and Challenges
  - Secretary of Energy Advisory Board (SEAB) Task Force Recommendations

- **Workshop Charge, Leadership, Structure**

- **Preliminary Workshop Output**
  - Grand Challenges
  - Priority Research Directions

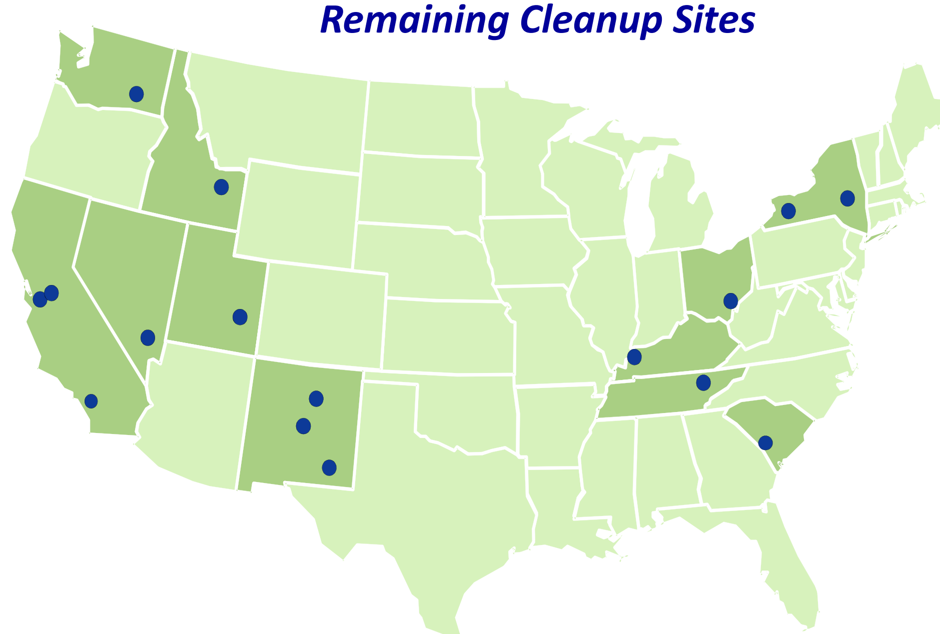
Addressing the Nuclear Weapons Legacy

EM Historical Cleanup Sites

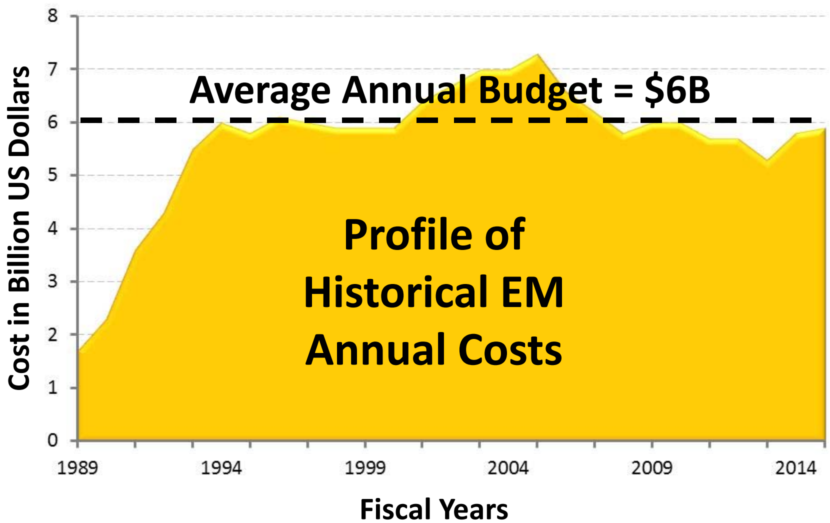


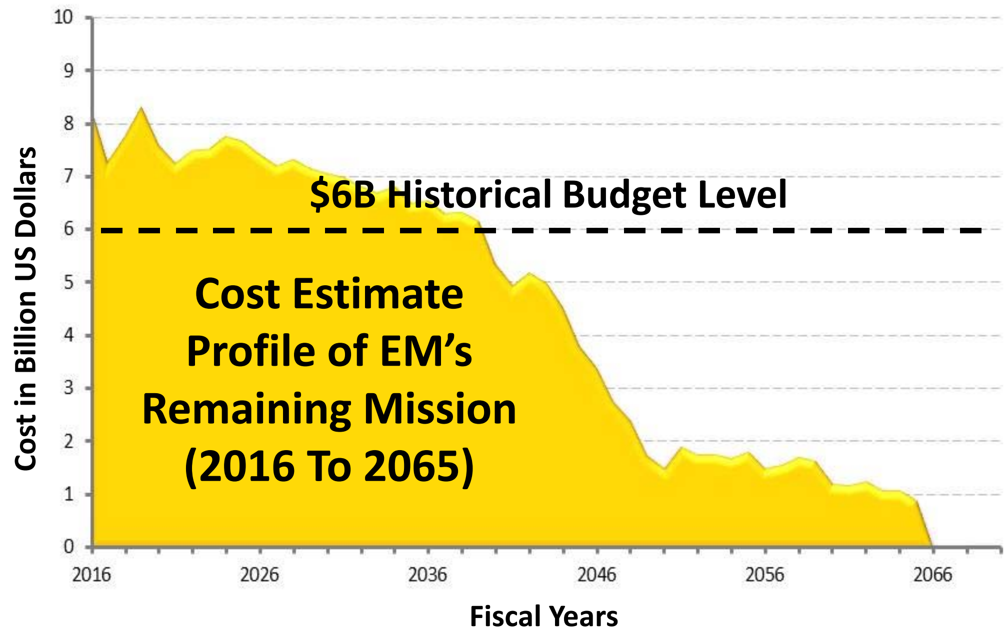
Since 1989, EM has completed its cleanup mission at 91 of the 107 major nuclear weapons and nuclear research sites.

Remaining Cleanup Sites



EM Accomplishment and Challenge





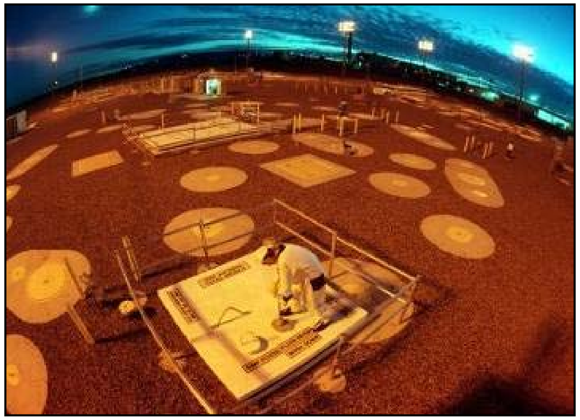
Past Investment

- $152 billion spent
- Completed cleanup at 91 of 107 major sites

Current Lifecycle Baseline

- To-Go Estimate
  - $235 billion
  - 2065 completion
- $28 billion gap

Significant Cleanup Challenges Remain



Safely storing highly radioactive liquid waste in over 220 underground tanks

Retrieving over 90 million gallons of liquid radioactive waste

Dispositioning radioactive, chemically hazardous waste

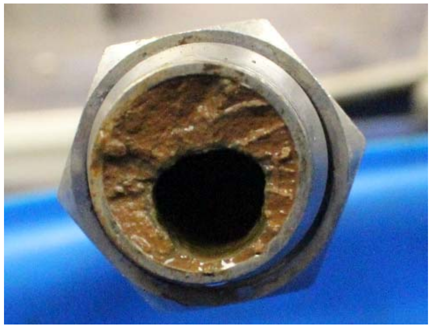
Remediating 93 square miles of contaminated groundwater

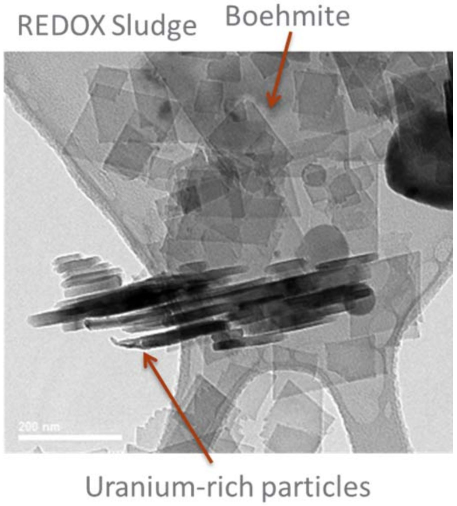
Decommissioning facilities and structures

Maintaining a stable and skilled workforce

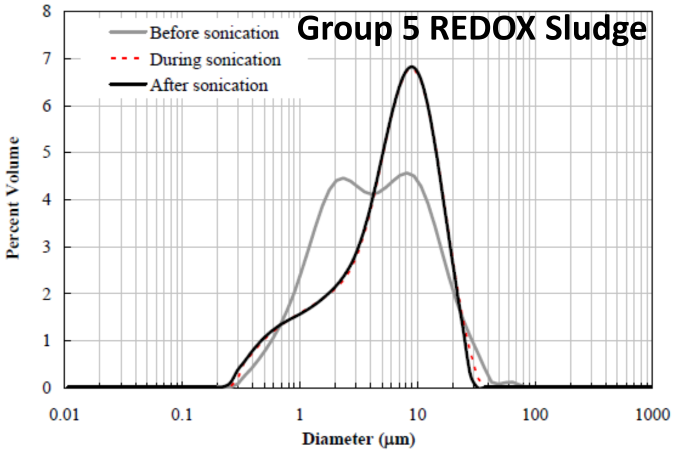
An Example: The Chemistry of High Level Radioactive Waste is Counterintuitive

High level radioactive waste characteristics are often not acceptable for pumping materials from tanks, causing significant operational risks





- Slurry yield stress often does not scale with colloidal size distributions
- Sonication of waste slurries can sometimes make colloids larger
- Dilution of waste slurries can sometimes cause precipitation
- Finely divided materials are often more refractory than larger crystalline solids



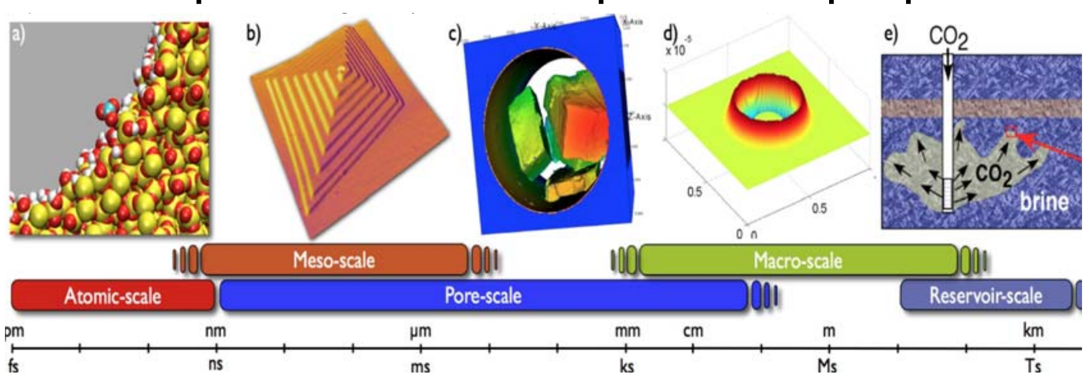
SEAB Task Force Report on Technology Development for Environmental Management (Dec. 2014)

Task Force's primary recommendations:

- Incremental technology development (EM)
- High-impact technology development (EM)
- EM university program (EM)
- Fundamental Research Program (SC)

Fundamental Research program should:

- Develop new knowledge and capabilities that bear on the EM challenges
- Be managed by the Office of Science in close coordination with EM
- Have a budget of ~$25M/year
- Commence with a workshop involving all potential participants to develop a strategic research plan to inform requests for proposals

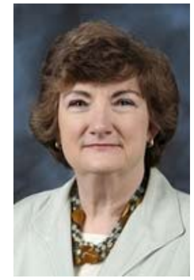


Basic Research Needs for Environmental Management Workshop

Co-sponsored by ASCR, BER, BES; July 8–11, 2015

Workshop Chair: Sue Clark (PNNL/WSU)
Associate Chairs: Michelle Buchanan (ORNL)
Bill Wilmarth (SRNL)

SC Technical Lead: Andy Schwartz (BES)


CHARGE: To conduct a thorough assessment of the scientific issues associated with the environmental management stewardship responsibility of DOE, and to identify scientific challenges, fundamental research opportunities, and priority research directions in the following areas:

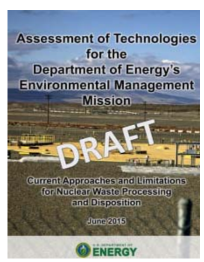
1. Waste stream characterization, transformation, and separations
2. Waste form
3. Contaminant fate and transport in geological environments

Breakout Sessions and Chairs:

1. *Waste Stream Characterization, Transformation, and Separations*: Jen Braley (CSM), Mark Antonio (ANL)
2. *Waste Form*: Jerry Frankel (OSU), Jim Marra (SRNL)
3. *Contaminant Fate and Transport in Geological Environments*: David Cole (OSU), Susan Hubbard (LBNL)
4. *Crosscutting Research*: Aurora Clark (WSU) & Todd Allen (INL)

Factual Document:

"Assessment of Technologies for the DOE EM Mission"



Pre-Workshop Webinars:

EM Overview: June 25, 2015
SC Overview: June 30, 2015

Plenary Session Speakers:

- Pat Dehmer, DOE-SC
- Monica Regalbuto, DOE-EM
- Richard Meserve, Covington & Burling LLP
- Andrew Felmy, PNNL
- Bill Weber, UTK
- Carl Steefel, LBNL

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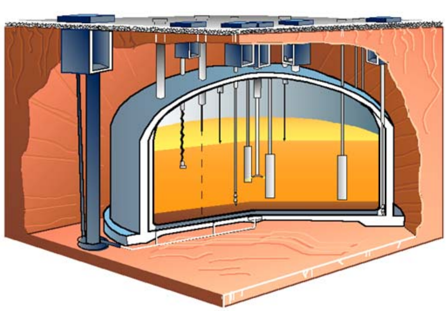
Grand Challenge 1: *Interrogation of inaccessible environments over extremes of time and space*

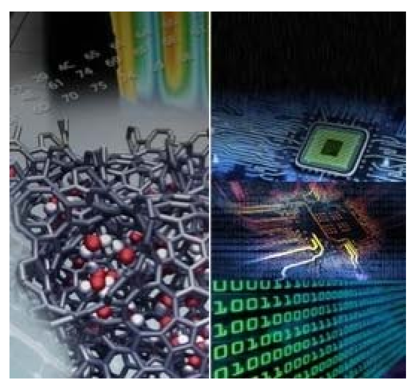
Current efforts are stymied by limited ability to safely and confidently assess existing containment structures, waste forms, and environmental contamination

- Inaccessible environments due to extremes such as radiation and geologic isolation may become accessible by innovations that combine advances in imaging capabilities, remote and in-situ sensing, and data analytics, from fractions of a second to millennia, from atoms to kilometers
- Coupling advances in characterization and sensing with high quality analytics can enable understanding and control of composition, structure, reactivity, and transport to support decision making processes

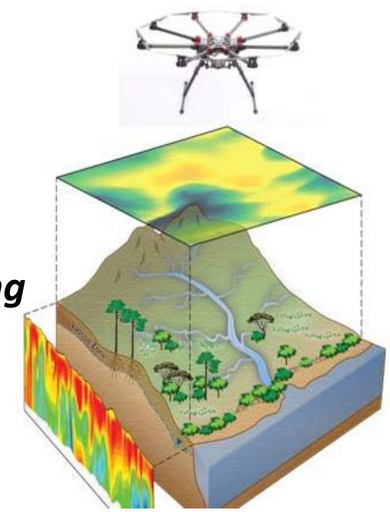


Interrogation of HL Waste Tanks

Data Analytics



Field Scale Remote Sensing

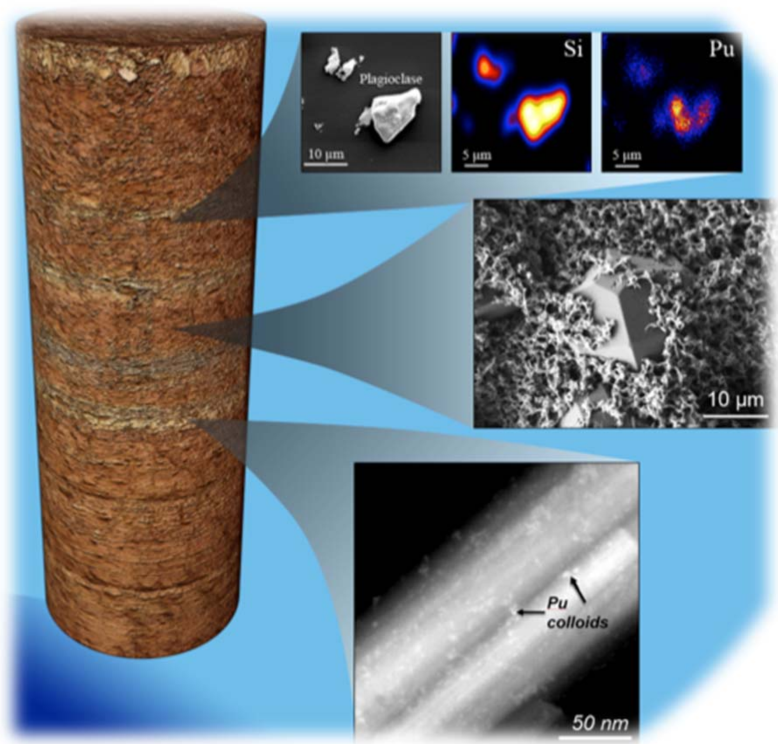


Grand Challenge 2: *Understanding and exploiting interfacial phenomena in extreme environments*

Unprecedented extremes in complexity, harshness, space, and time impede progress toward radioactive waste processing, disposal, and environmental remediation

- **Elucidate how interfacial phenomena in highly heterogeneous environments dictate system properties and functionality**
  - Will enable improved engineering of processing strategies, waste form designs, and subsurface containment and cleanup
- **Understand interfacial phenomena in extreme environments**
  - Will lead to new separations methods, new materials for waste forms, and new control of subsurface contamination

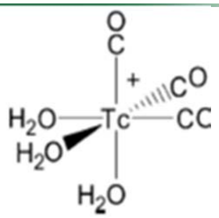
Radionuclide Partitioning at Interfaces



Priority Research Directions (DRAFT)

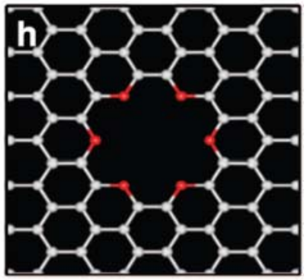
1. High dimensional interrogation of inaccessible environments with diverse data
2. Predicting and controlling chemical and physical processes far from equilibrium
3. Understanding critical physicochemical interfacial reactions across scales
4. Long term evolution of non-equilibrium structures
5. Harnessing physical and chemical mechanisms to revolutionize separations
6. Mechanisms of materials degradation in harsh environments
7. Mastering hierarchical structures to tailor waste forms
8. Scale-aware prediction of terrestrial system behavior and response to perturbations

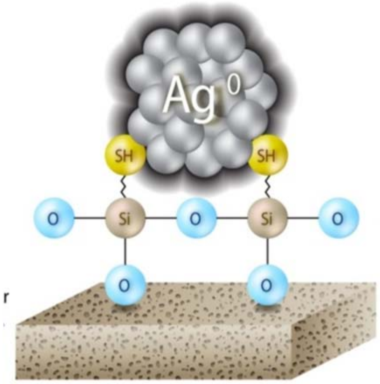
Microtomography at the ALS



Unexpected redox forms

New separations materials based on graphene





Nano-tailored waste forms

Why Now?

- **Over the past decade, incredible strides have been made in nanoscale materials science and, computing, imaging, biogeochemical system science, and data analytics, creating opportunities to:**
  - Pursue complexity and heterogeneity
  - Span unprecedented scales of time and space
  - Access and assess the inaccessible
- **The time is ripe to apply these advances to develop foundational knowledge of complex, coupled radiological and chemical systems**
- **DOE user facilities, such as light and neutron sources, nanoscience centers, high performance computing, and other state-of-the-art facilities, are available to enable research success**