U.S. DEPARTMENT OF ENERGY

Nuclear Energy

Environmental Management

Summary of Programs and Collaborations

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PNNL-SA-126100

NWTRB Questions Addressed

May 15, 2017 pre-meeting briefing questions for DOE:

- Provide an overview of the compositions and projected quantities of existing and future HLW glass at the West Valley Demonstration Project, Savannah River Site, and the Hanford Site (including "German" glass logs).
  - How is the variability in DOE HLW glass composition taken account of in DOE's glass corrosion models?
  - How well are the glass corrosion model parameters supported by experimental data?
- What is the status of DOE R&D activities to understand and model the long-term performance of borosilicate HLW glass?
  - Which R&D activities are run or managed by the different DOE offices and programs [DOE-NE (including NEUP), DOE-EM, DOE Office of Science (if any)] and how are these activities integrated? What are the accomplishments?
  - A detailed plan for joint DOE-NE and DOE-EM R&D activities on glass corrosion initially was developed in 2011 (Ryan et al. 2011)1 that included experiments and modeling. What are the status and results of the tasks described in the plan?
  - How are the results of international R&D activities integrated with the results of DOE R&D?
- From DOE's perspective, what are the remaining technical uncertainties and gaps in data and understanding of the long-term performance of HLW glass? How is DOE addressing these uncertainties and gaps?
- How is DOE integrating process-level models of HLW glass corrosion and radionuclide release into generic repository performance assessments?
  - How is the DOE approach to HLW glass performance modeling different from that for the low-activity waste (LAW) glass to be disposed of at the Hanford Site Integrated Disposal Facility?
  - What lessons learned from LAW glass corrosion experiments and modeling can be applied to HLW glass?
- What is the technical basis for extrapolating the results of short-term, small-scale tests on glass corrosion to long-term glass waste form performance in a repository?

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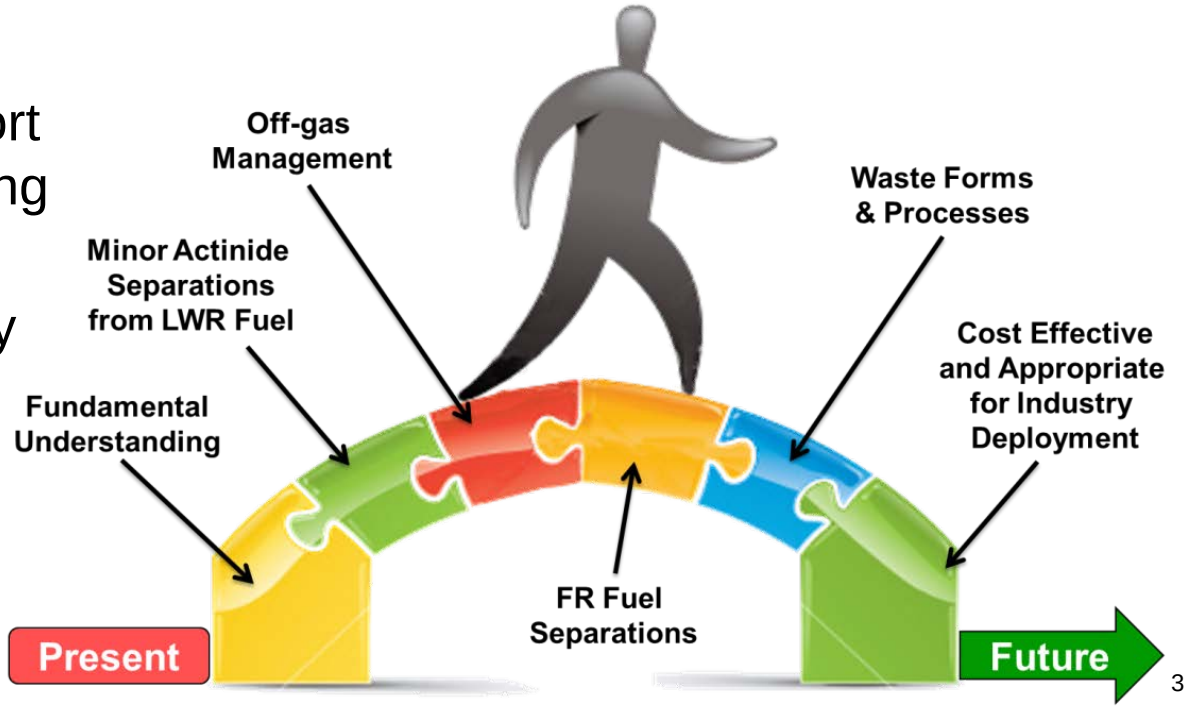
Department of Energy Programs Related to Glass Corrosion

- DOE-NE scope includes: "…to conduct research and development to help develop sustainable fuel cycles, as described in the Nuclear Energy Research and Development Roadmap. Sustainable fuel cycle options are those that improve uranium resource utilization, maximize energy generation, minimize waste generation, improve safety, and limit proliferation risk."
  - National laboratory support for improved understanding of WF performance
  - Nuclear Energy University Programs (NEUP) related to glass corrosion



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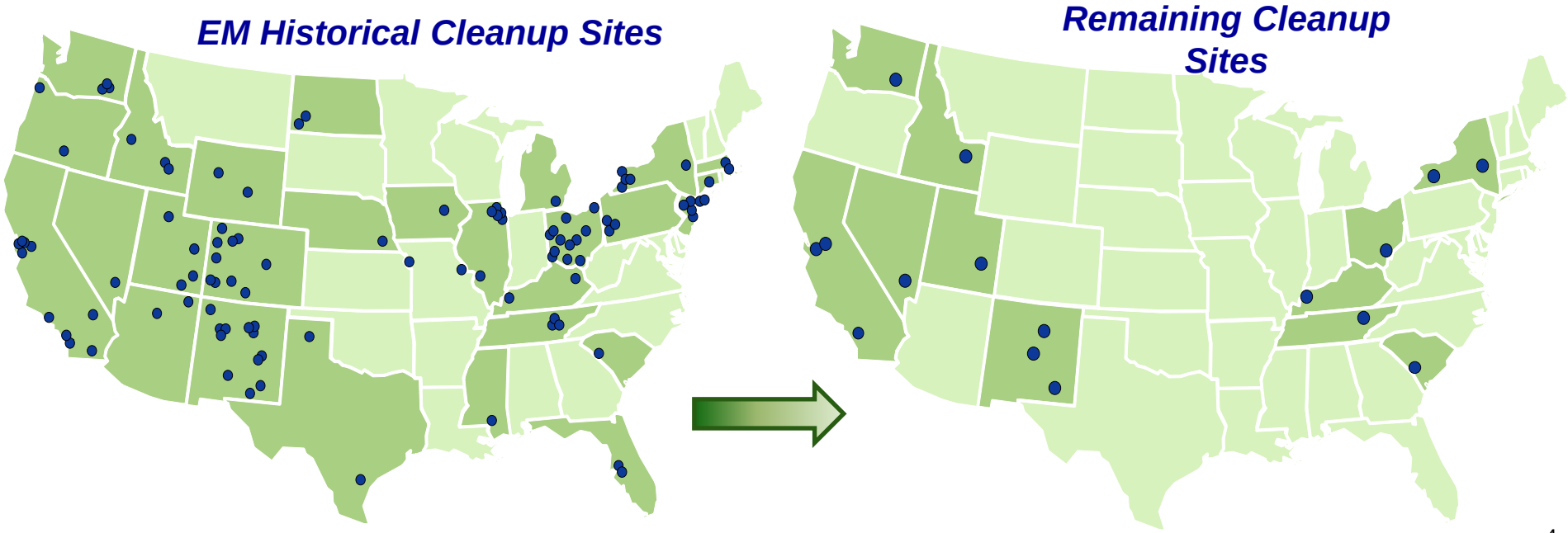
Department of Energy Programs Related to Glass Corrosion

- DOE-EM scope includes: "… to complete the safe cleanup of the environmental legacy brought about from five decades of nuclear weapons development and government-sponsored nuclear energy research."
  - EM HQ program to reduce conservatism glass corrosion models
  - ORP/WRPS program to populate rate model data for LAW glasses



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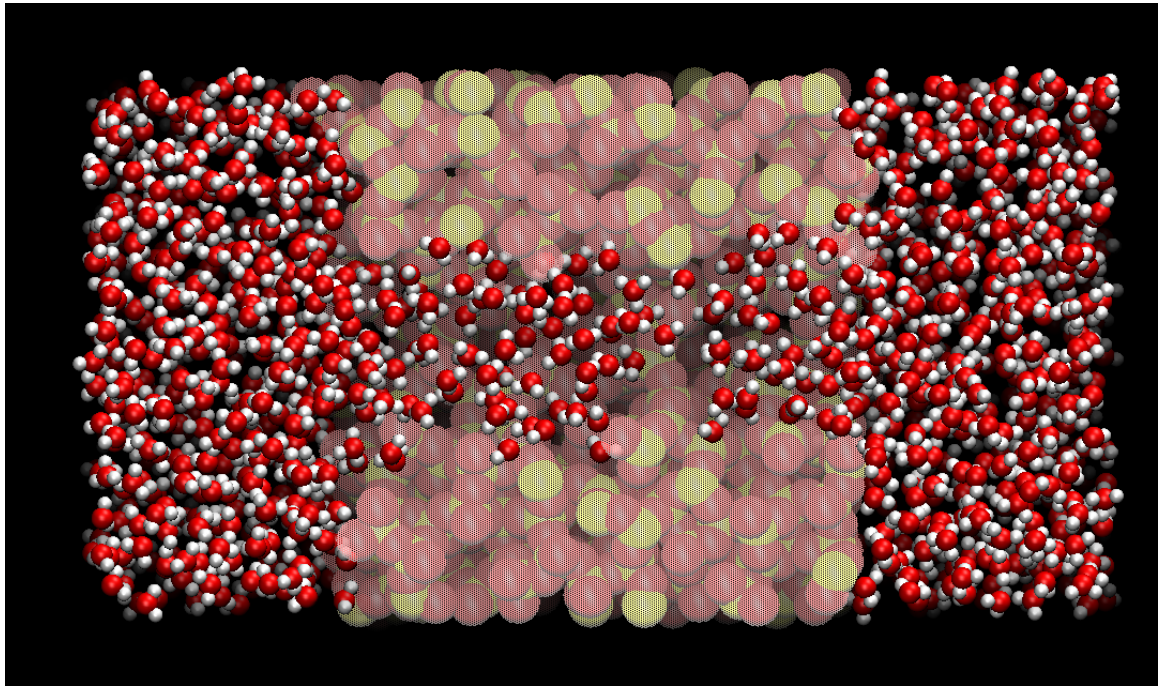
Department of Energy Programs Related to Glass Corrosion

- DOE-SC scope includes: "…is the delivery of scientific discoveries and major scientific tools to transform our understanding of nature and to advance the energy, economic, and national security of the United States."
  - EFRC program to improve understanding of waste forms degradation



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FY2013 Scope By Program

DOE-EM	DOE-NE
• Initial ALTGlass database (Jantzen-SRNL) • Evaluate VSI technique for forward rate measurement (Icenhower-LBNL) • kMC modeling of gel layer formation (Kerisit-PNNL) • Shape influence on dissolution (Ryan-PNNL) • Critical evaluation of state of the art in glass corrosion (Vienna-PNNL) *2 Papers / 2 Reports*	• Advanced Characterization: isotope tracing, ancient glass, ISG (Ryan-PNNL) • Inverse Modeling (Wiliford-PNNL) • Stephane Gin support (Ryan-PNNL) • Secondary phase model (Ebert-ANL) • kMC model development (Kerisit-PNNL) • Multi-scale model tool development (Rieke-PNNL) • 1st principles modeling (Zapol-ANL) • Initial 'Super-Flow' development (Strachan-PNNL) • International program on glass corrosion (co-chair with CEA) (Ryan-PNNL) *5 Papers / 2 Reports*

* Does not include efforts on LAW glasses

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FY2014 Scope By Program

DOE-EM	DOE-NE
• Complete APT testing of CEA 26y glass sample (Ryan-PNNL) • Development of superflow test (dissolution rate) (Neeway-PNNL) • Update ALTGlass and analyze for relationships with Stage III (Jantzen-SRNL) *1 Papers / 1 Reports*	• Isotope Tracer Technique for IEX (Ryan-PNNL) • Synthesis of an artificial PRI (Neeway-PNNL) • Study coupling of glass dissolution and secondary phases for stage III triggers (Ebert-ANL) • Alteration product precipitation kinetic modeling using TST (Strachan-PNNL) • Multi-scale model tool development (Rieke-PNNL) • Investigate iron impacts on corrosion (Neeway-PNNL) • Apply 1st principles modeling to simulated glass structure (Zapol-ANL) • Mechanistic model development (Ryan-PNNL) *5 Papers / 3 Reports*

* Does not include efforts on LAW glasses

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FY2015 Scope By Program

DOE-EM	DOE-NE
• Investigate high alkaline earth glass corrosion with UK (Vienna-PNNL) • ALTGlass update (Jantzen-SRNL) • Gel composition evaluation (Jantzen-SRNL) • kMC of interdiffusion in glass (Kerisit-PNNL) *3 Papers / 1 Report*	• Ion exchange parameterization (Neeway-PNNL) • Iron impacts on glass corrosion (Neeway-PNNL) • Mechanistic model development (Ryan-PNNL) • CNWG Support (Ryan-PNNL) • Reaction Interface Studies (Ryan-PNNL) • Experimental effort on Stage III and model development to incorporate Stage III in glass source term model (Ebert-ANL) • Report on aspects and issues for incorporating glass model in PA (Rieke-PNNL) • 1st principles modeling to examine energy barriers for ion exchange and dealkalization reactions in glass (Zapol-ANL) • Modeling Tool Demonstration: Evaluation of Existing Models (Rieke-PNNL) *6 Papers / 8 Reports*

* Does not include efforts on LAW glasses

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FY2016 Scope By Program

DOE-EM	DOE-NE
• In-situ monitoring of corrosion using Raman spectroscopy (Ryan-PNNL) • Ion-exchange data in ancient glass (Ryan-PNNL) • Hydrogel correlation to state III initiation (Jantzen-SRNL) • Ancient glass use (Ryan-PNNL) *2 Papers / 1 Reports*	• Evaluate gel structure and composition with reaction progress (Ryan-PNNL) • Morphological evolution model development (Ryan-PNNL) • Modeling tool application and improvements (Rieke-PNNL) • Glass model incorporation into generic repository performance code (Rieke-PNNL) • Stage III model testing (Ebert-ANL) *3 Papers / 6 Reports*

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FY2017 Scope By Program

DOE-EM	DOE-NE
• In-situ monitoring of corrosion using Raman spectroscopy to evaluate Stage III initiation (Ryan-PNNL) • Update III in ALTGlass Database (Jantzen-SRNL) *3 Papers / 0 Reports*	• Impacts of seeding on stage 3 corrosion (Ryan-PNNL) • Gel structure, formation, and sol-gel proxies (Ryan-PNNL) • SPFT data of ISG and NE glasses (Neeway-PNNL) • Modeling Tool Coupling to Fate and Transport Code (Rieke-PNNL) • Stage III modeling of Mg impact on corrosion using joint CNWG data (Ryan-PNNL) • International efforts to create a consensus mechanistic rate model (Ryan-PNNL) *2 Papers / 1 Reports*

* Does not include efforts on LAW glasses

NEUP Scopes

- 2010-2014, Exploration and Modeling of Structural Changes in Waste Glass under Corrosion, Pantano-PSU (*2 papers, 1 report*)
- 2012-2016, Surface Layer-Bulk Glass Interface Evolution with Aqueous Corrosion, Mellott-AU (*3 papers, 1 report*)
- 2012-2015, Coupling of nuclear waste form corrosion and radionuclide transport in presence of relevant repository sediments, Wall-WSU (*3 papers, 1 report*)
- 2013-2016, Molecular dynamics-based simulations of bulk/interfacial structures and diffusion behaviors in nuclear waste glasses, Du-UNT (*8 papers, 0 reports, 1 book chapter*)
- 2013-2016, Glass Composition and Solution Speciation Effects on Stage III Dissolution, Pantano-PSU (*2 papers, 0 report*)
- IRP 2016-2019, Understanding of Fundamental Science Governing the Development and Performance of Nuclear Waste Glasses, Goel-Rutgers

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DOE-BES, EFRC Scope

- 2016-2020, Center for Performance and Design of Nuclear Waste Forms and Containers, Frankel-OSU

- Understand the fundamental mechanisms of waste form performance, and apply that understanding to develop tools for design of waste forms with improved performance.

https://efrc.osu.edu

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International Collaborations

U.S. National Laboratories

Pacific Northwest NATIONAL LABORATORY

SRNL SAVANNAH RIVER NATIONAL LABORATORY

Argonne NATIONAL LABORATORY

Sandia National Laboratories

International Laboratories

cea

amec

Subatech

National Nuclear Laboratory

IAEA

JAEA

SCK•CEN STUDIECENTRUM VOOR KERNENERGIE CENTRE D'ETUDE DE L'ENERGIE NUCLEAIRE

Universities

PENNSTATE

九州大学 KYUSHU UNIVERSITY

Alfred University

UNT

universitätbonn

The University Of Sheffield.

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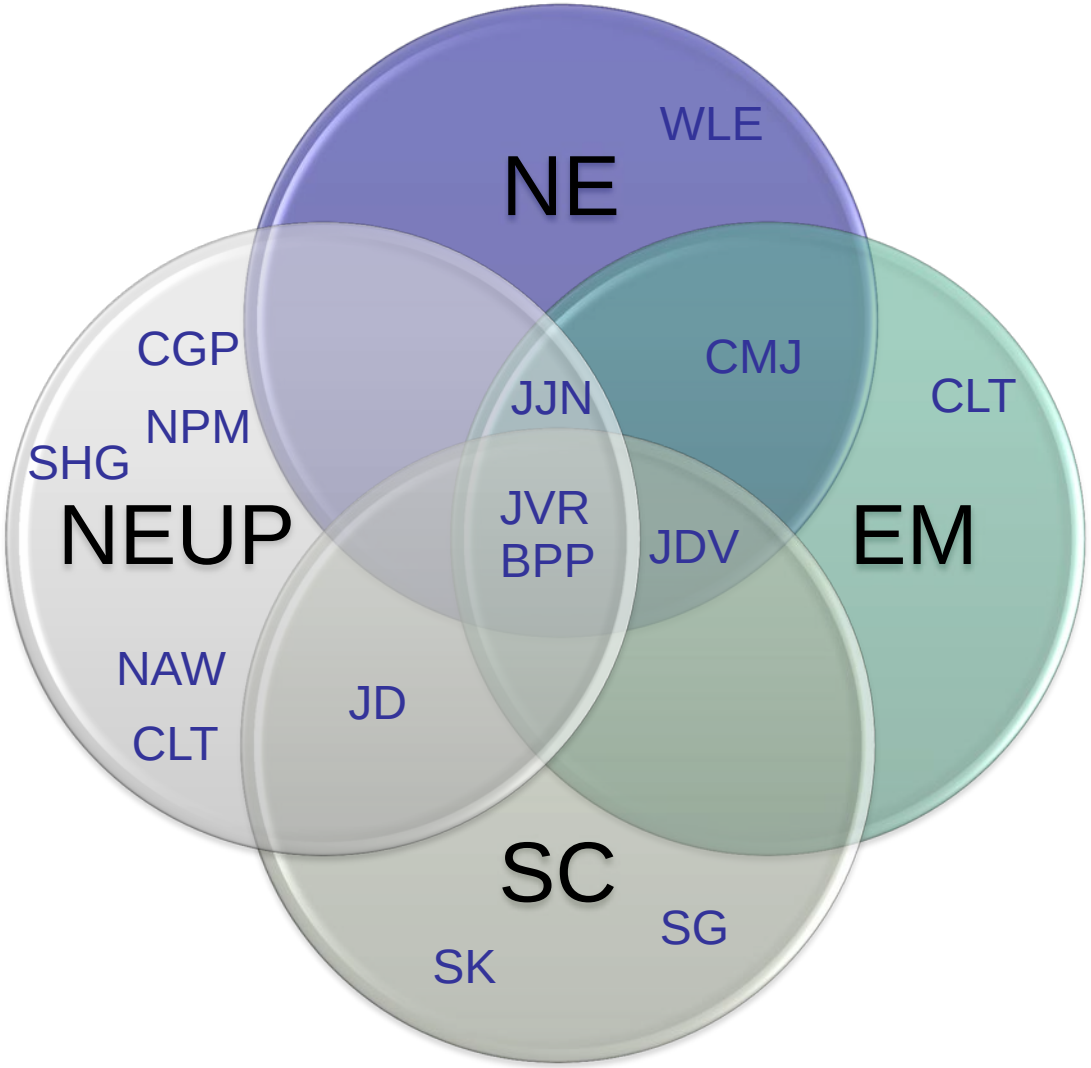
Collaborations Supporting Glass Corrosion



BPP – Benjamin Parruzot (PNNL)
CGP – Carlo Pantano (PSU)
CLT – Cory Trivelpiece (SRNL)
CMJ – Carol Jantzen (SRNL)
JD – Jincheng Du (UNT)
JDV – John Vienna (PNNL)
JJN – Jim Neeway (PNNL)
JVR – Joe Ryan (PNNL)
NAW – Nathalie Wall (WSU)
NPM – Nathan Mellott (MSU)
SG – Stephane Gin (CEA)
SHG – Steve Garofalini (Rutgers)
SK – Seong Kim (PSU)
WLE – Bill Ebert (ANL)

* Not including LAW

Collaborations

- Annual face-to-face meetings with international community on glass corrosion (typically in May alongside GOMD conference)
  - Discuss priorities, present results (unpublished and published), decide on collaborative tests and modeling efforts, discuss interpretations
- Regular bilateral meetings with different nations (France, UK, Japan)
  - Discuss bilateral collaborative efforts
- Staff exchanges
  - PNNL – CEA, KU – PNNL, WSU – PNNL, WSU – CEA, PNNL – PSU, UNT – PNNL
  - Joint research
- Frequent webinars
  - Present results, discuss interpretations, discuss plans for future research
- International team include testing on common glass
  - International Simple Glass (ISG) contains SiO_2, B_2O_3, Al_2O_3, Na_2O, CaO, and ZrO_2 in ratios representing a typical high-level waste glass