U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Fuel Cycle Research & Development

NEAMS Nuclear Waste Management Integrated Performance and Safety Codes

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NEAMS PI Meeting

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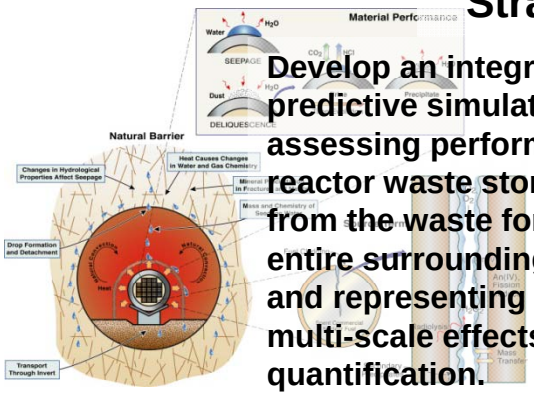
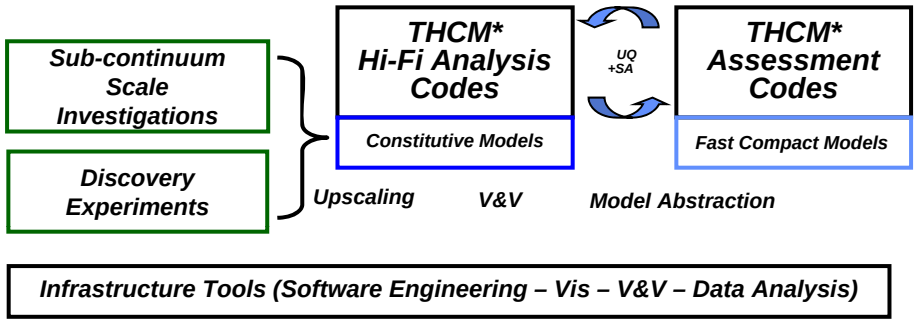
Nuclear Waste Management Integrated Performance and Safety Code

Strategic Vision



Develop an integrated, science-based predictive simulation package for assessing performance of potential nuclear reactor waste storage or disposal options, from the waste form itself through the entire surrounding engineered environment and representing the range of important multi-scale effects, with uncertainty quantification.

Approach



** THCM: Thermal/Hydrological/Chemical/Mechanical*

Milestones

- **Years 0-3:**
  - **IPSC Design Specifications**
  - **PIRT/FEPs & V&V Plan**
  - **THCM Architecture and Prototype**
  - **High priority sub-continuum studies**
  - **Generation of constitutive models**
  - **Initial Demonstrations of Capabilities to Waste Issues**
- **Years 4-10**
  - **High-fidelity continuum models and fast meta-models**
  - **Initial release of THCM and Assessment Codes**
  - **Full application to WF/repository environment**

Risks & Issues

- **Success depends on support from other NEAMS Strategies (FMM, VU, CT & ECT)**
- **Need to coordinate modeling activities with Fuel Cycle Technologies Campaigns (Separations/Waste Forms and Used Fuel Disposition) and with ASCEM in DOE/EM**
- **Availability of appropriate experimental data**
- **Lack of existing integrated performance codes in this area**
- **Current plans are predicated on a much larger NEAMS program**

NEAMS NWM IPSC - Objectives

- **Short-Tem Programmatic Objective**
  - Coordinate with and support both the Waste Forms Campaign and the Used Fuel Disposition Campaign in Office of Fuel Cycle Technologies
    - *IPSC System Requirements*
    - *R&D Priorities*
  - Coordinate with the ASCEM development efforts in DOE/EM
- **Long-Term Technical Objectives:**
  - Develop an integrated suite of advanced modeling capabilities for simulation of the long-term performance of waste management systems
    - *Engineered environment of a radioactive waste storage or disposal system*
    - *Geosphere and biosphere*
    - *Multiscale effects*
    - *Uncertainty quantification*
  - Simulate radionuclide movement to a specified receptor for a range of system designs (WFs, WPs, buffer/backfill, host rock) and conditions

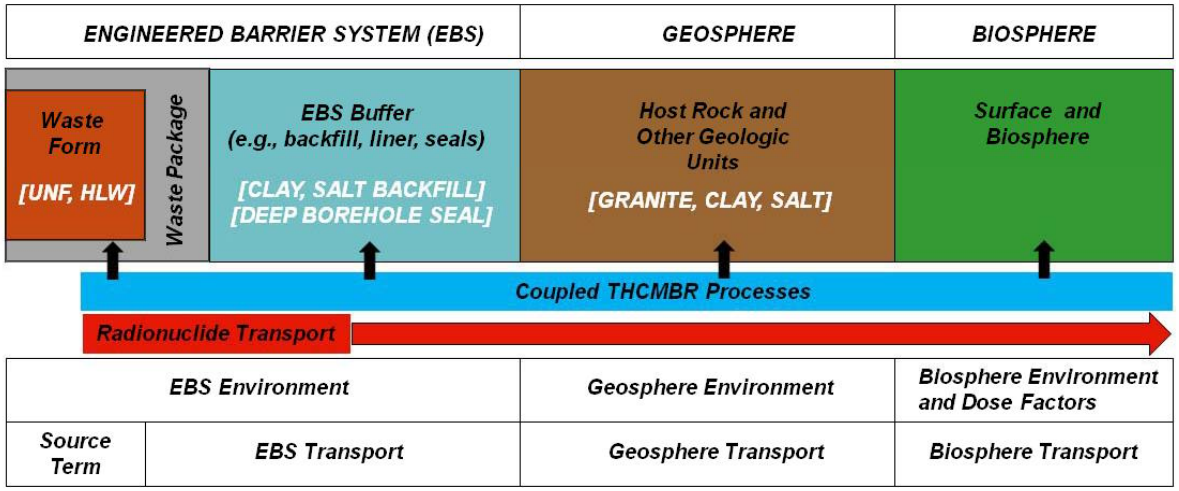
NEAMS NWM IPSC – FY10 Tasks

- **Specifications for Challenge Problems**
- **Verification and Validation (V&V) Plan**
- **THCM* Code Capability**
  - Gap Analysis
  - Sub-continuum Glass Corrosion Model Development
- **Frameworks and SQE Tools**
  - Gap Analysis

Thermal/Hydrological/Chemical/Mechanical

NEAMS NWM IPSC – Task 1 Develop Challenge Problems

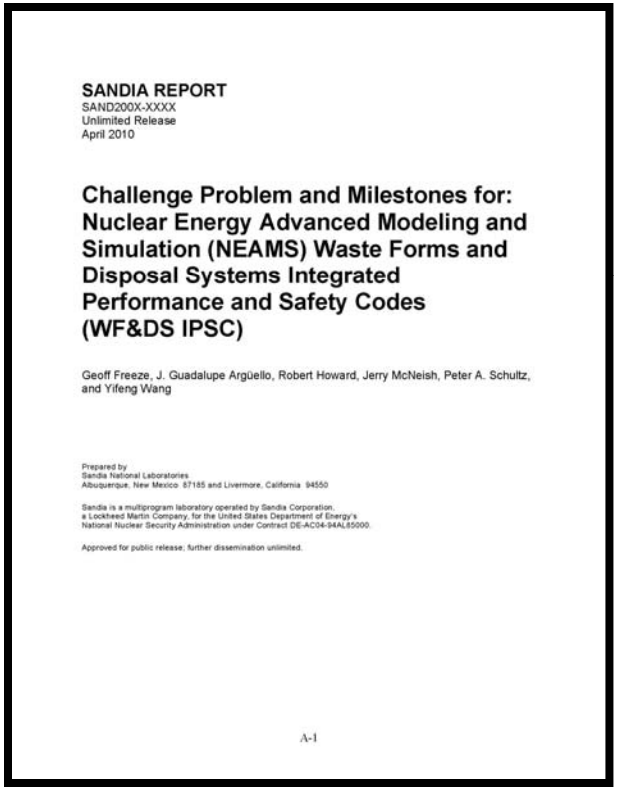
- **Identified one overarching challenge problem**
  - Simulate radionuclide mobilization and transport from the waste form, through the EBS, Geosphere, and Biosphere to a human receptor
    - *Traceable to FEPs / PIRTs and use cases*
    - *Represent long time-scales and associated large uncertainties*
    - *Implement multiple model fidelities (Hi-Fi THCM, PA)*
    - *Implement robust THCM coupling*
    - *Applicable to full range of potential disposal options (concepts, WF types, EBS designs, geologic settings)*



NEAMS NWM IPSC – Task 1 Develop Challenge Problems

- **Identified 5 challenge problem milestones**
  - Early challenge milestones focus on isolated domains, processes, THCM couplings, model fidelities, and/or disposal options
  - Subsequent challenge milestones build on prior challenge milestones, combining domains, processes, couplings, etc.
- **Challenge problem milestones will be refined over time**

Challenge problem and milestones documented in Level 3 Milestone Report delivered April 30, 2010



SANDIA REPORT
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April 2010

Challenge Problem and Milestones for: Nuclear Energy Advanced Modeling and Simulation (NEAMS) Waste Forms and Disposal Systems Integrated Performance and Safety Codes (WF&DS IPSC)

Geoff Freeze, J. Guadalupe Argüello, Robert Howard, Jerry McNeish, Peter A. Schultz, and Yifeng Wang

Prepared by
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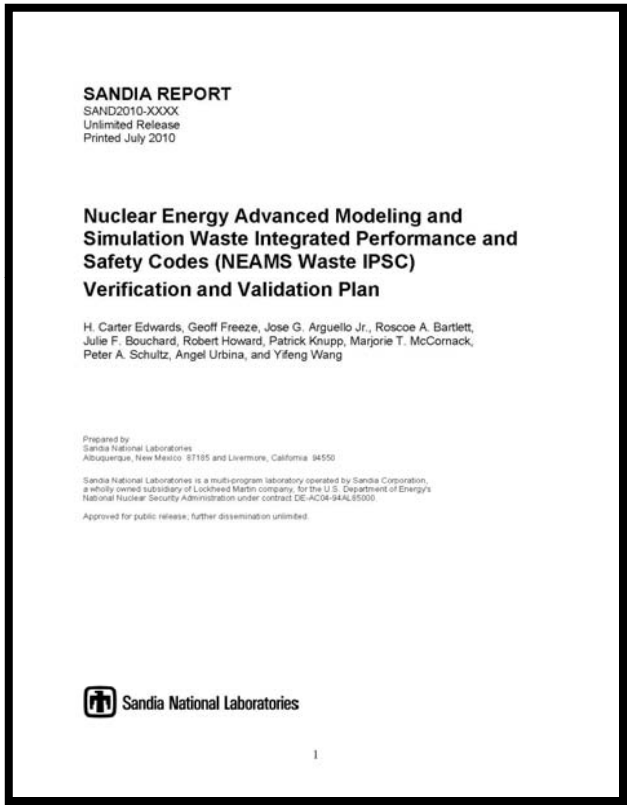
NEAMS NWM IPSC – Task 2 Verification & Validation Plan

- **Collaboration with NEAMS VU element**
- **Incorporated a broad collection of resources & experiences**
  - NRC, DOE, YMP, WIPP, ASC
- **Comprehensive plan for NWM modeling and simulation capabilities**
  - Scope is larger than V&V for a single code or capability
- **Assess whether a code or capability is "fit for intended use"**
  - Establish metrics for the degree or level of confidence
  - Each code or capability can have a different level of confidence
- **Required level of confidence depends upon <u>impact</u> and <u>uncertainty</u>**
  - Impact on waste form & system performance
  - Impact takes into account uncertainty bounds
  - High impact requires high confidence, low impact requires less confidence
  - Prioritize V&V tasks by comparing assessed level to required level

NEAMS NWM IPSC – Task 2 Verification & Validation Plan

- **V&V metrics for assessing confidence level**
  - Foundation: SNL's Predictive Capability Maturity Model (PCMM)
  - R&D: "Rolling up" metrics for coupled multiphysics / multiscale simulations?
- **Assess the level of confidence throughout code capability lifecycle**
  - "Born assessed"
- **Managing V&V evidence and metrics**
  - Collected and evolved throughout lifecycle of codes and capabilities
  - Some codes / capabilities developed, others acquired
  - Traceability of evidence, metrics, and assessments
  - Traceability of "rolled up" metrics for coupled simulations



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Nuclear Energy Advanced Modeling and Simulation Waste Integrated Performance and Safety Codes (NEAMS Waste IPSC)
Verification and Validation Plan

H. Carter Edwards, Geoff Freeze, Jose G. Arguello Jr., Roscoe A. Bartlett, Julie F. Bouchard, Robert Howard, Patrick Knupp, Marjorie T. McCornack, Peter A. Schultz, Angel Urbina, and Yifeng Wang

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V&V Plan Level 2 Milestone Report delivered July 31, 2010

NEAMS NWM IPSC – Task 3
THCM Code Capability:
Source term: glass degradation

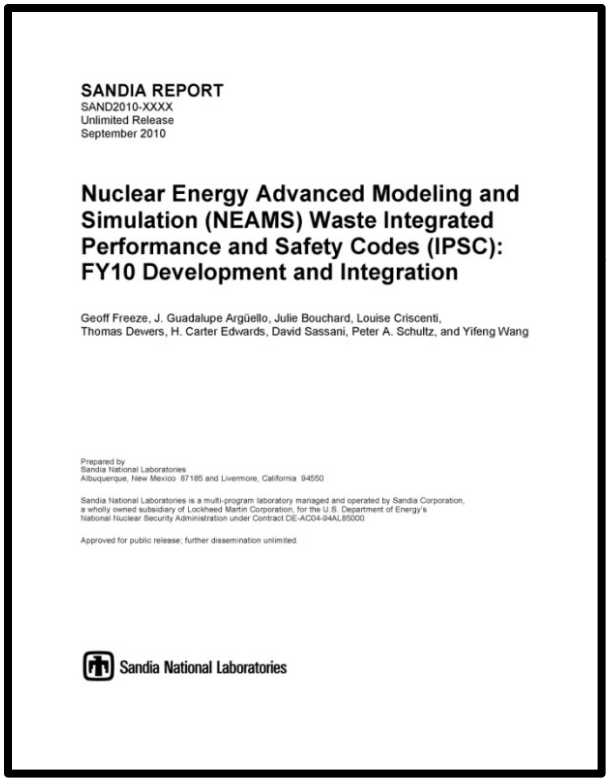
- **Target challenge problem: corrosion of borosilicate glass**
  - multi-lab (LBNL, ANL, SNL, …) coordinated effort for narrow target problem
- **Complex process determines long term glass degradation**
  - multilayer corrosion: PRI, hydration, leaching, secondary phases
  - interaction with near field via diffusion, sorption
- **Objective: from first-principles to constitutive models & parameters**
  - model development on well-characterized systems (orthoclase/feldspar)
  - continuum formulations on complex systems (Roman glass)

NEAMS NWM IPSC – Task 3 THCM Code Development: Gap Analysis

- Identified required phenomena and couplings through specification of challenge problems/milestones, PIRT/FEPs, and use cases
- Initiated identification of codes and gaps with respect to phenomena, couplings, V&V
- Upscaling from finer scale phenomena will be required for adequacy of constitutive models
- Existing codes/models may be sufficient for some uncoupled or partly coupled processes
- Robust THCM couplings and V&V will need to be developed (SIERRA may provide a useful framework)

NEAMS NWM IPSC – Task 4 Frameworks and SQE Tools: Gap Analysis

- **Survey existing frameworks and tools to leverage**
  - Use existing capabilities that fit the needs
  - E.g., FCR&D, ASC, international programs, NEAMS– ECT, ASCEM
- **Collaborate with existing programs with similar needs**
  - Try to become a "customer" for frameworks and tools under development
  - E.g., SNL's SIERRA mechanics, SNL' Analysis Data Management



SANDIA REPORT
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September 2010

Nuclear Energy Advanced Modeling and Simulation (NEAMS) Waste Integrated Performance and Safety Codes (IPSC): FY10 Development and Integration

Geoff Freeze, J. Guadalupe Argüello, Julie Bouchard, Louise Criscenti, Thomas Dewers, H. Carter Edwards, David Sassani, Peter A. Schultz, and Yifeng Wang

Prepared by
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Progress on Tasks 3 & 4 (gap analysis, code/model development) documented in Level 3 Milestone Report delivered September 30, 2010

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FY11 Work Packages

- **THCM Modeling & Simulation Capabilities (SNL)**
  - Implementation of initial capabilities for challenge problem simulation
    - *Chemical equilibrium*
    - *Glass form dissolution and metal waste package degradation*
    - *Thermal/fluid transport in the engineered barrier system (EBS)*
  - Gap analysis refinement
  - M2 Milestone: Simulation of Challenge Problem #1
- **Sub-continuum modeling (SNL, LBNL, ANL)**
  - Validated, mechanistically-derived constitutive models for waste form degradation
  - Emphasis on glass corrosion, with up-scaling from atomistic to continuum models for dissolution of orthoclase and generalization to amorphous glass
  - M2 Milestone: Guidelines and requirements for V&V and UQ for principal classes of sub-continuum modeling methods
  - M2 Milestone: Millimeter scale continuum model for borosilicate glass dissolution
- **IPSC Infrastructure and Frameworks (SNL)**
  - Deployment of prototype work-flow environment to support challenge problem milestones
  - Evaluate frameworks in an operational setting
  - Implement and evaluate V&V and UQ processes
  - VV-UQ evidence information management
  - M2 Milestone: Evaluation of frameworks and implemented VV-UQ processes

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Late-Breaking News!

- **September 10 – Initial Telecon with ASCEM**
  - Summarized objectives, scope, structure, and status of each program
- **October 15 – First formal discussions with ASCEM**
  - NEAMS – Randy Summers (SNL, Program Element Lead), Carter Edwards and Geoff Freeze (SNL, Technical PIs), Dan Funk (DOE)
  - ASCEM – Paul Dixon (LANL Program Manager), Juan Meza (LBNL, Technical PI), Mark Williamson (DOE)
  - Identified specific areas for coordination and collaboration
  - Established plans for an initial joint workshop
- **February 17-18, 2011 – Joint NEAMS-ASCEM Workshop**
  - Location: Somewhere in New Mexico (Buffalo Thunder??)
  - Goal: Coordination of FY12 work packages
  - Needed Participation from NEAMS
    - *Waste IPSC*
    - *VU*
    - *ECT*
    - *FMM*

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Technical Presentations

- **Thermal-Hydrologic-Chemical-Mechanical (THCM) Modeling and Simulation**
  - Geoff Freeze (SNL)
  - Lupe Arguello (SNL)
  - Yifeng Wang (SNL)
- **Sub-continuum Modeling for Waste Forms**
  - Peter Schultz (SNL)
  - Carl Steefel (LBNL)
  - Peter Zapol (ANL)
- **Verification & Validation Plan and Frameworks & Infrastructures Gap Analysis**
  - Carter Edwards (SNL)

BACKUP SLIDES

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Modeling & Simulation Requirements Separations & Waste Campaign

- **Structure and chemistry of radionuclide-bearing phases and corrosion products**
- **Corrosion and alteration of extremely durable materials**
- **Prediction of thermo-chemical parameters for long-term behavior of waste forms in the environment, including the thermodynamics of surface and interface reactions.**
- **Atomic-scale behavior of solid-liquid-vapor interfaces, particularly the long-term corrosion behavior of waste forms**
- **Effect of radiation and radiolysis on the properties of materials and their long-term behavior in the disposal environment**
- **An integration of all data and understanding within the IPSC**

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Modeling & Simulation Requirements Used Fuel Disposition (UFD) Campaign

- **Waste Disposal**
  - **Includes M&S requirements for waste forms/near-field environment**
  - **Additional M&S requirements for the far-field environment (region between near-field and point at which human exposure may occur)**
    - *Identification of M&S needs will be a focus of UFD campaign in FY10 to support planning for FY11 and to include far-field capabilities necessary for an integrated approach to disposal and storage concepts.*
- **Long-Term Waste Storage**
  - **Clad mechanical properties characterization – high burn-up, embrittlement, etc.**
  - **Clad integrity characterization, for example increased pin hole defects with increasing burn-up and longer-term storage**
  - **Fuel characterization - condition of oxides with high burn-up (e.g., cracking), fuel/clad gap, rim layer effects, etc.**
  - **FMM requirements may be driven by both Fuels and NWM IPSCs**