The Science and Technology Program

Presented to:

Nuclear Waste Technical Review Board, Full Board Meeting

Presented by:

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Safety Case & Safety Assessment

- **The International Atomic Energy Agency (IAEA) 2006 standard for geological repositories defines safety assessment and safety case:**

*3.41. **Safety assessment** is the process of systematically analysing the hazards associated with the facility and the ability of the site and the design of the facility to provide for the safety functions and to meet technical requirements. . . .*

*3.40. . . . **The safety case** substantiates the safety, and contributes to confidence in the safety, of the geological disposal facility. The safety case is an essential input to all the important decisions concerning the facility. It includes the output of safety assessments . . . , together with additional information, including supporting evidence and reasoning on the robustness and reliability of the facility, its design, the design logic, and the quality of safety assessments and underlying assumptions. . . .*

Confidence Arguments in Light of Uncertainty

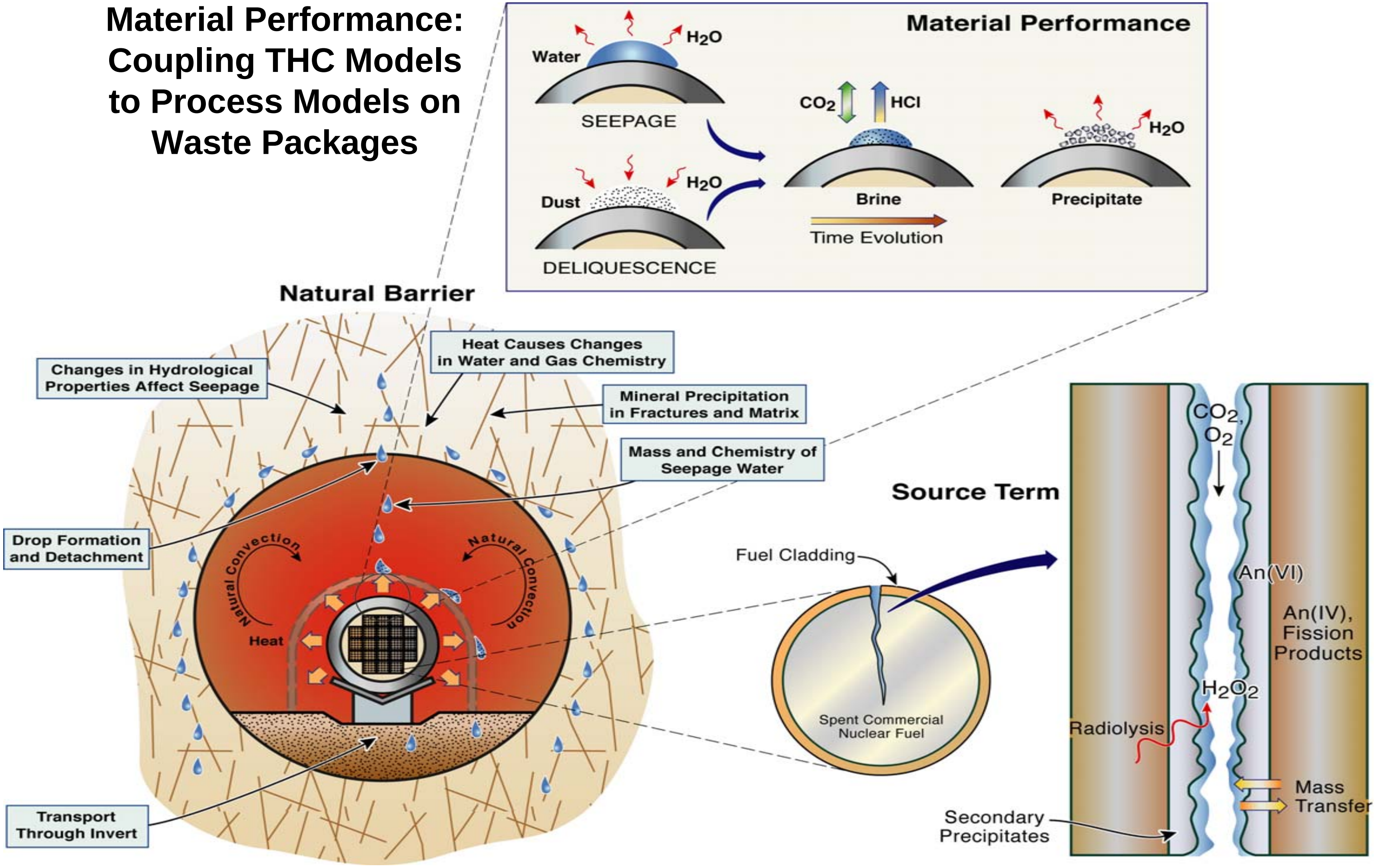
- By submitting a Safety Analysis Report (SAR), the DOE states it has confidence in system safety over its entire life-cycle
- Contributors to this confidence are:
  - Continued long-term testing, monitoring and regulatory defined performance confirmation studies will challenge as well as confirm the basis of the safety case
  - The current science and technology program and performance confirmation demonstrate DOE's long-term plan to continually enhance system safety and efficiency (part of a viable 'safety culture')

S&T Program Mission and Drivers

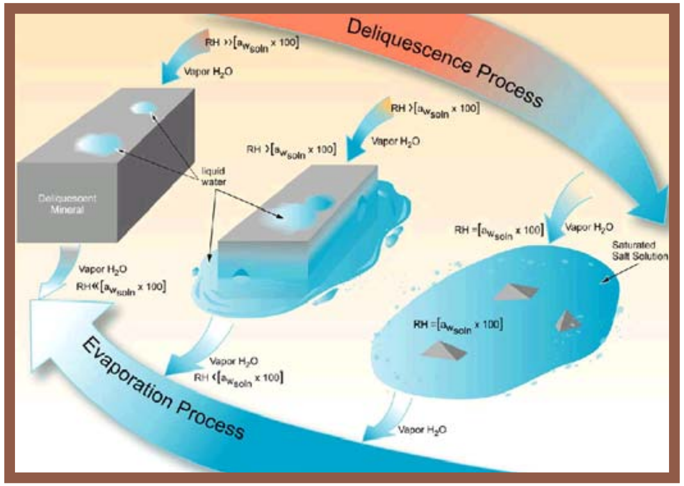
- **Mission**
  - **"Provide advanced science and technology to continually enhance our understanding of the repository system and to reduce the cost and schedule for the OCRWM mission."**
- **Vision**
  - **"OCRWM and the affected public will value the contributions that scientific and technological advances have made toward safer, more expeditious, and more cost-effective waste isolation."**
- **Current science program research areas**
  - **Materials Performance**
  - **Source Term**
  - **Natural Barriers**

Integrated Science Program

Material Performance: Coupling THC Models to Process Models on Waste Packages

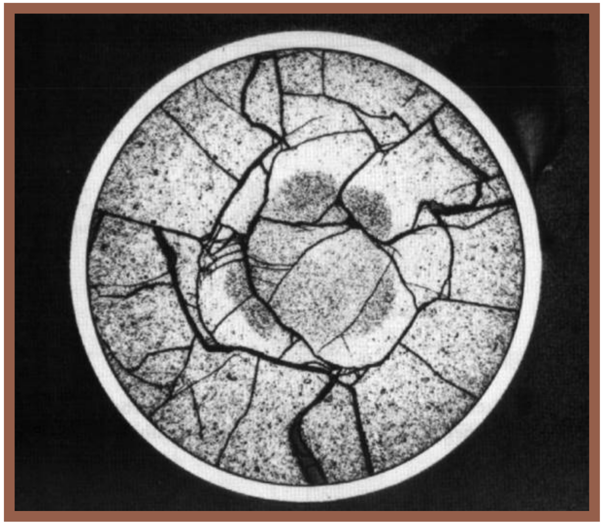


Materials Performance Research



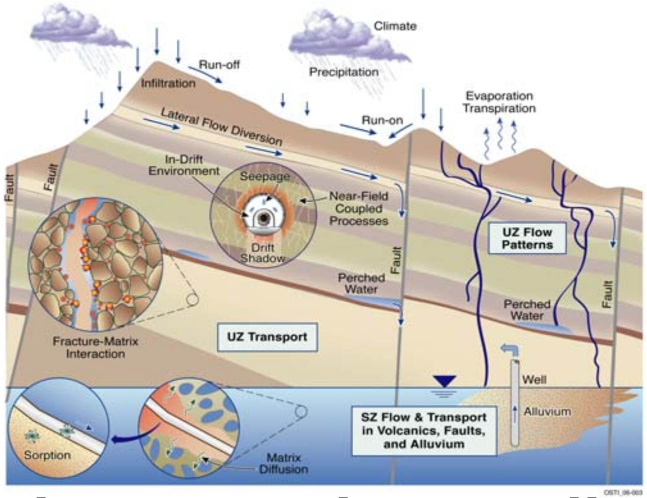
- **Objective - enhance the understanding of materials corrosion performance and explore technical enhancements**
- **Three major research areas**
  - **Corrosion processes on metal surfaces covered with particulates and deposits**
  - **Evolution of corrosion damage by localized corrosion**
  - **Evolution of the environment on metal surfaces**

Source Term Research



- **Objective – enhance the understanding of the release mechanisms of key radionuclides from spent nuclear fuel (SNF) and explore technical enhancements**
- **Four major research areas**
  - **SNF dissolution mechanisms and rates**
  - **Formation and properties of U^{6+} secondary phases**
  - **Waste form – waste package interactions**
  - **Integration of in-package chemical and physical processes**

Natural Barriers Research



- **Objective – enhance understanding of multiple barriers – natural and engineered, to isolate the waste in the proposed repository**
- **Five major research areas**
  - **Seepage in the near- and in-drift environment**
  - **Drift shadow – the area directly beneath where the waste package is emplaced**
  - **Unsaturated zone (UZ) and saturated zone (SZ) – nature of flow and transport in heterogeneous systems**
  - **Multi-scale/multi-physics coupled process modeling**

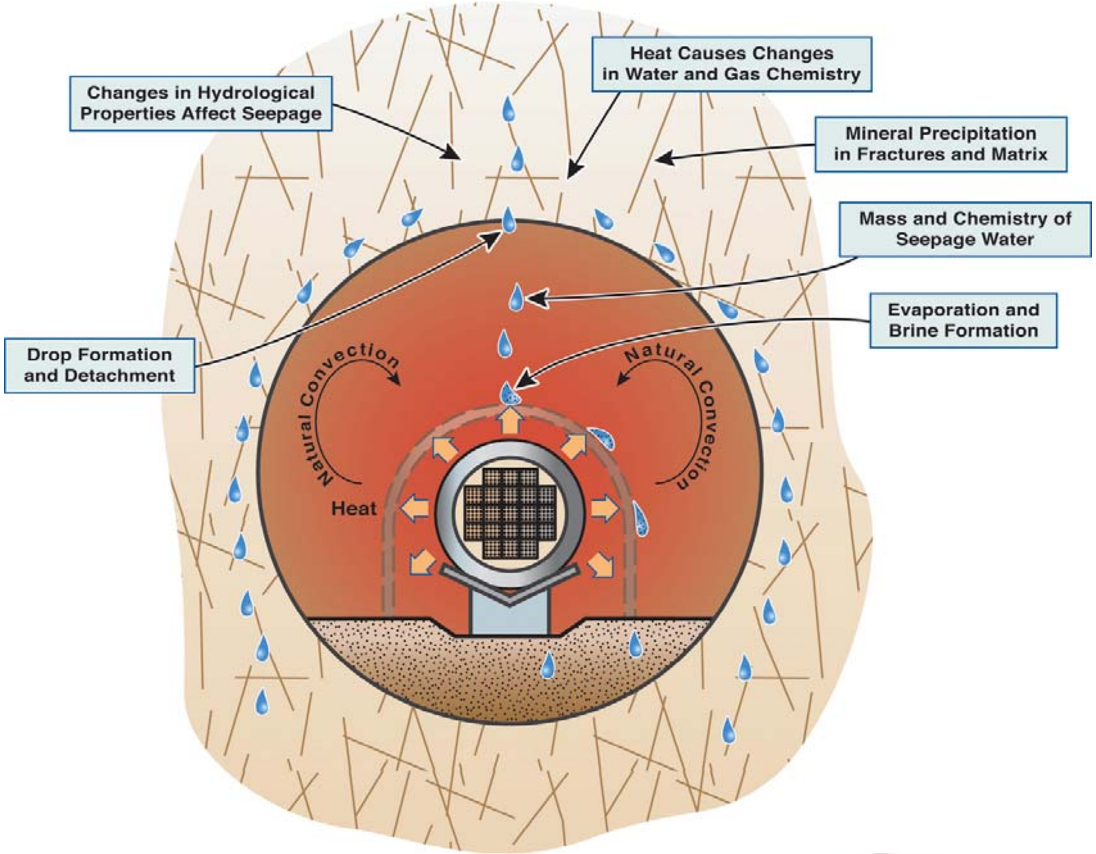
Some Results To Date

- The S&T Program has already demonstrated enhanced understanding of the natural and engineered systems, supporting the safety case for the proposed Yucca Mountain repository
- Integration of Source Term, Materials Performance, and Natural Barriers research in developing unified in-drift models, leading to enhanced understanding, greater transparency, and defensibility
- Potential stifling mechanisms for localized corrosion include limitations due to cathodic kinetics and loss of critical crevice chemistry
- Potential incorporation of radionuclides into secondary uranyl phases and waste package corrosion products (e.g., Fe oxyhydroxides) may limit source term
- Potential several orders-of-magnitude enhancement in matrix diffusion within both the UZ and SZ and potential one or more orders-of-magnitude increase in K_d values for several important radionuclides

An Integrated In-Drift/Near Field Flow and Transport Model with Reactive Chemistry

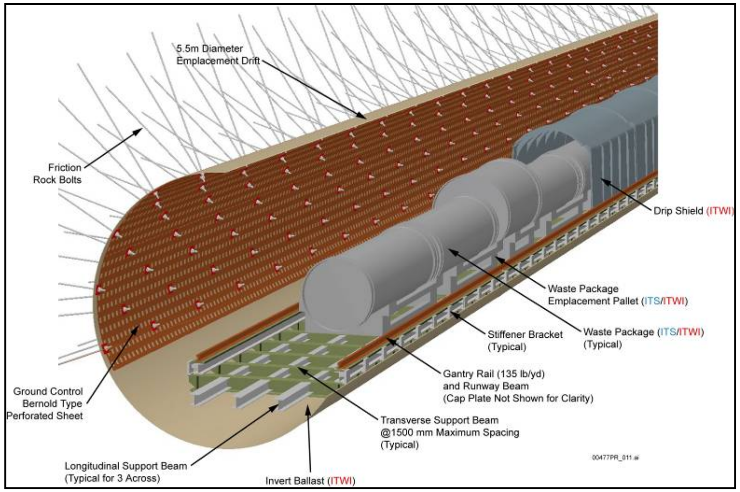
- **Integrated THC model combining heat, water and solute transport**
  - **Thermodynamics applicable to concentrated brines**
  - **Rigorous mass balance**
- **Evaluate water movement within drifts**
- **Incorporate and test additional chemical processes in TOUGHREACT**
- **Conduct THC simulations at multiple scales**

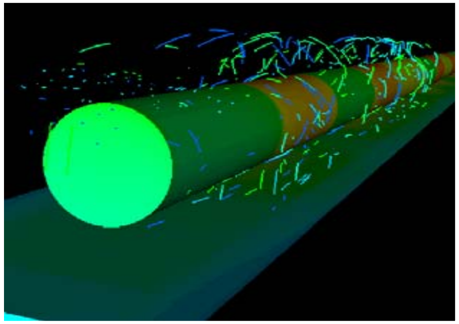
Integrate processes in in-drift environment with contributions from Source Term, Materials Performance, and Natural Barriers

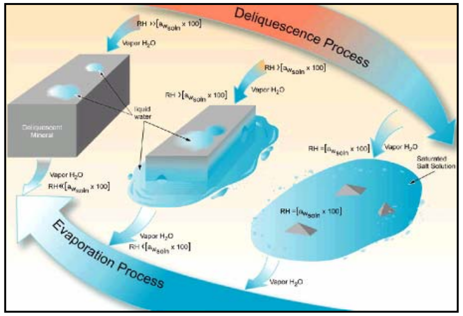


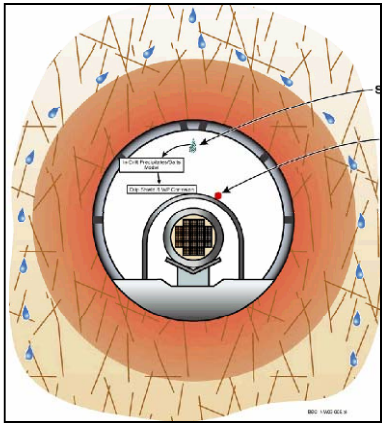
Materials Performance

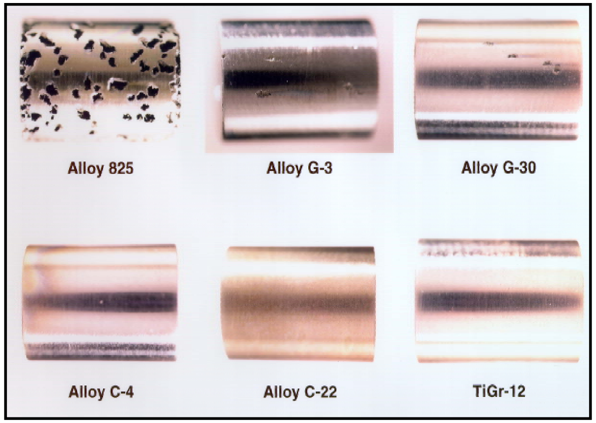
Technical basis: corrosion science, electrochemistry, materials science, physical chemistry, geochemistry

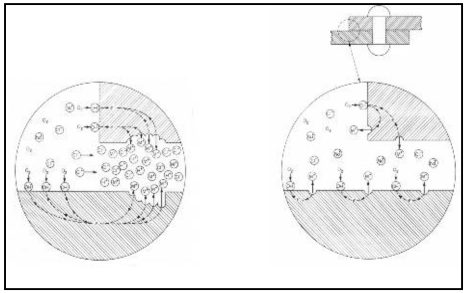




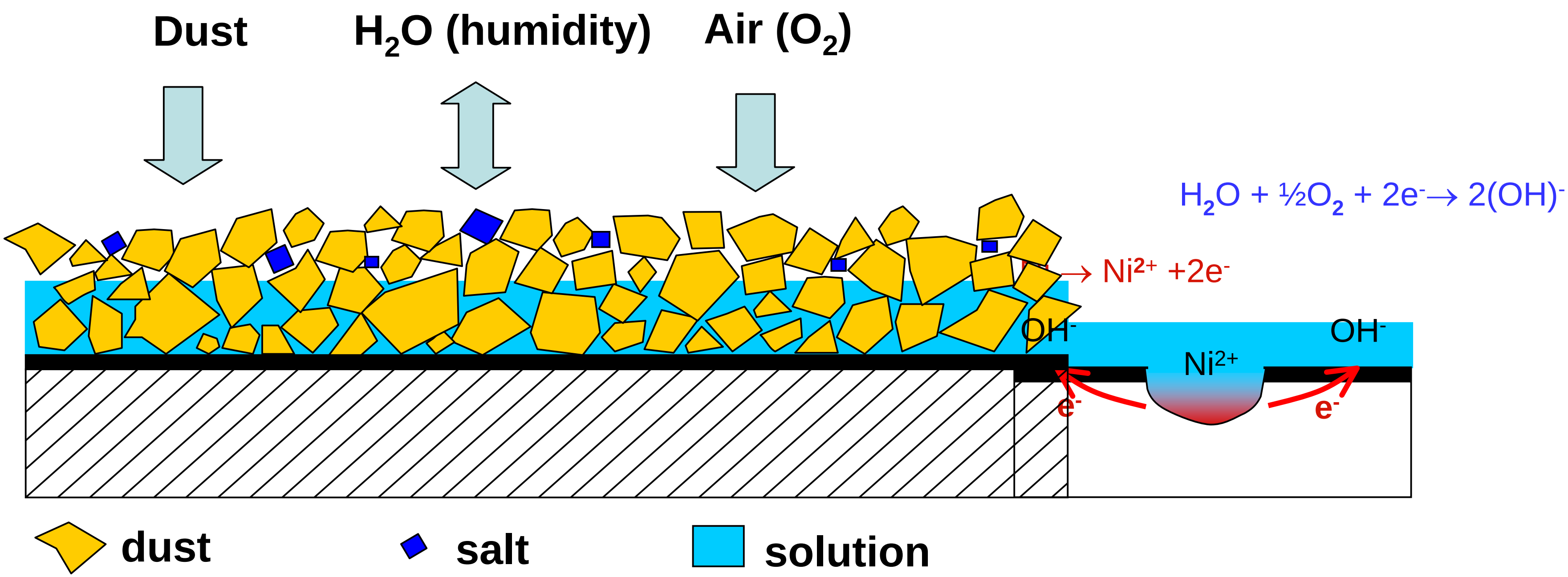








Corrosion in Thin Layers of Particulate



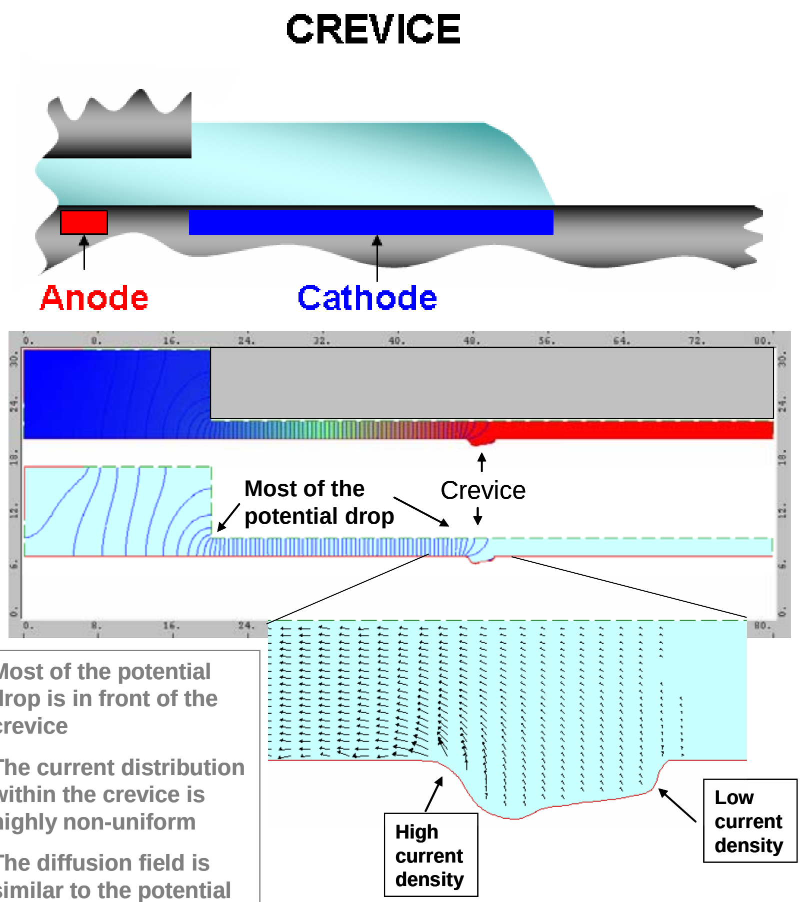
- Dust deposited
- Degree of wetness
- Soluble salts
- Gas composition and property, T, RH
- Particulate layer properties, such as conductivity, temperature, pH, degree of wetness etc.
- Localized environment on the surface
- Anode: $Ni \rightarrow Ni^{2} + 2e^{-}$
- Cathode: $H_2O + ½O_2 + 2e^{-} \rightarrow 2(OH)^{-}$

Localized Corrosion Can be Stifled by Limits on the Cathodic Processes

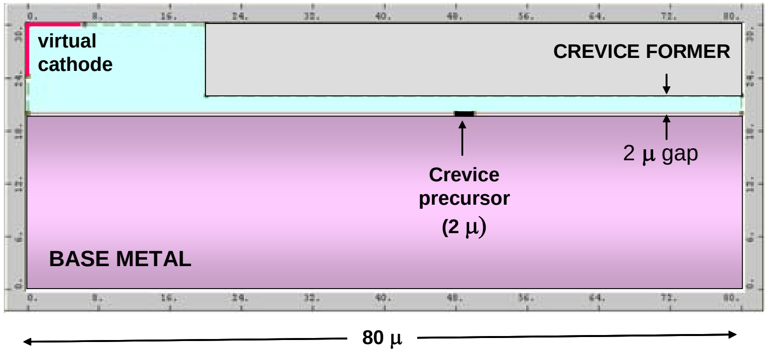
- In the proposed repository waste packages will never be fully immersed in solution
- Moisture and particulates may be present on surfaces
- Corrosion behavior in moist particulate can differ from full immersion
  - Limited size of corrosion site
  - Limited cathodic area to support localized corrosion
  - Limited cathodic kinetics could stifle corrosion

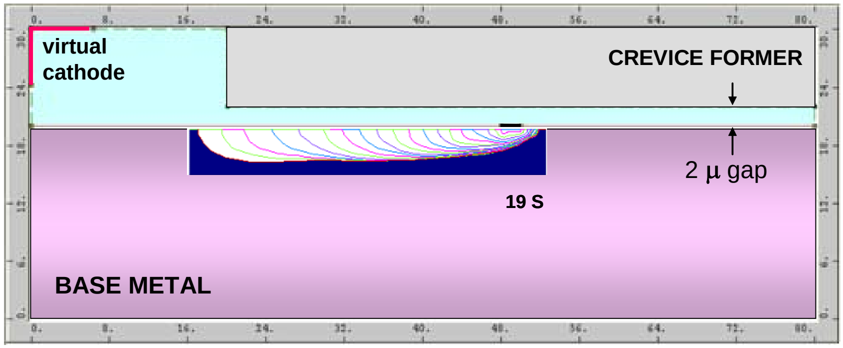
Model of Profile of Damage from Crevice Corrosion

For this case: crevice gap opens, critical crevice chemistry is lost, and corrosion stops (stifles)



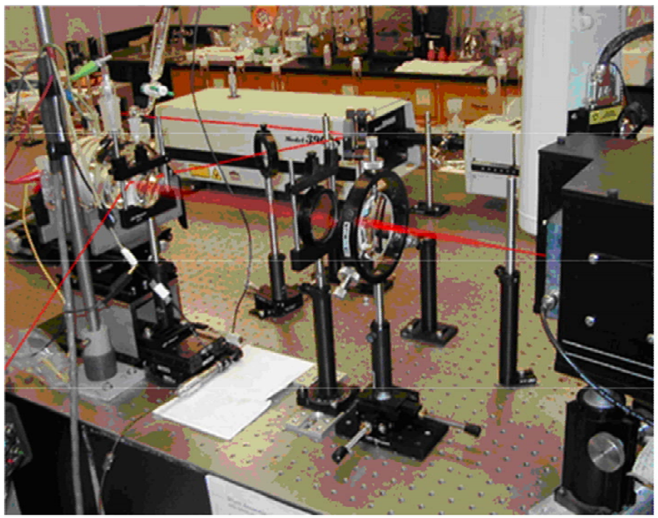
- Most of the potential drop is in front of the crevice
- The current distribution within the crevice is highly non-uniform
- The diffusion field is similar to the potential field



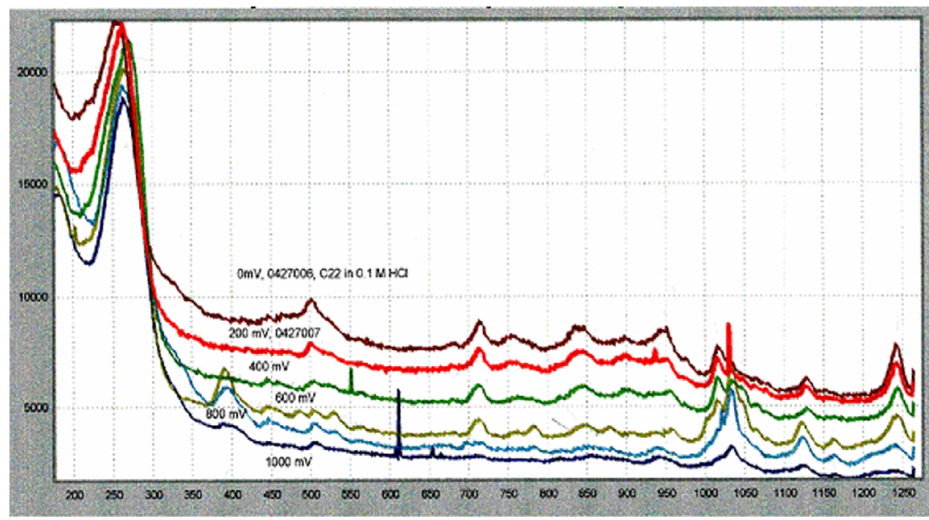


Effect of Environmental Variables on the Structure and Composition of Passive Films

- **In-situ surface analysis and characterization**
- **To determine structure, composition, electrochemical and electronic properties of passive films on Ni-Cr-Mo alloys in hot, chloride solutions**



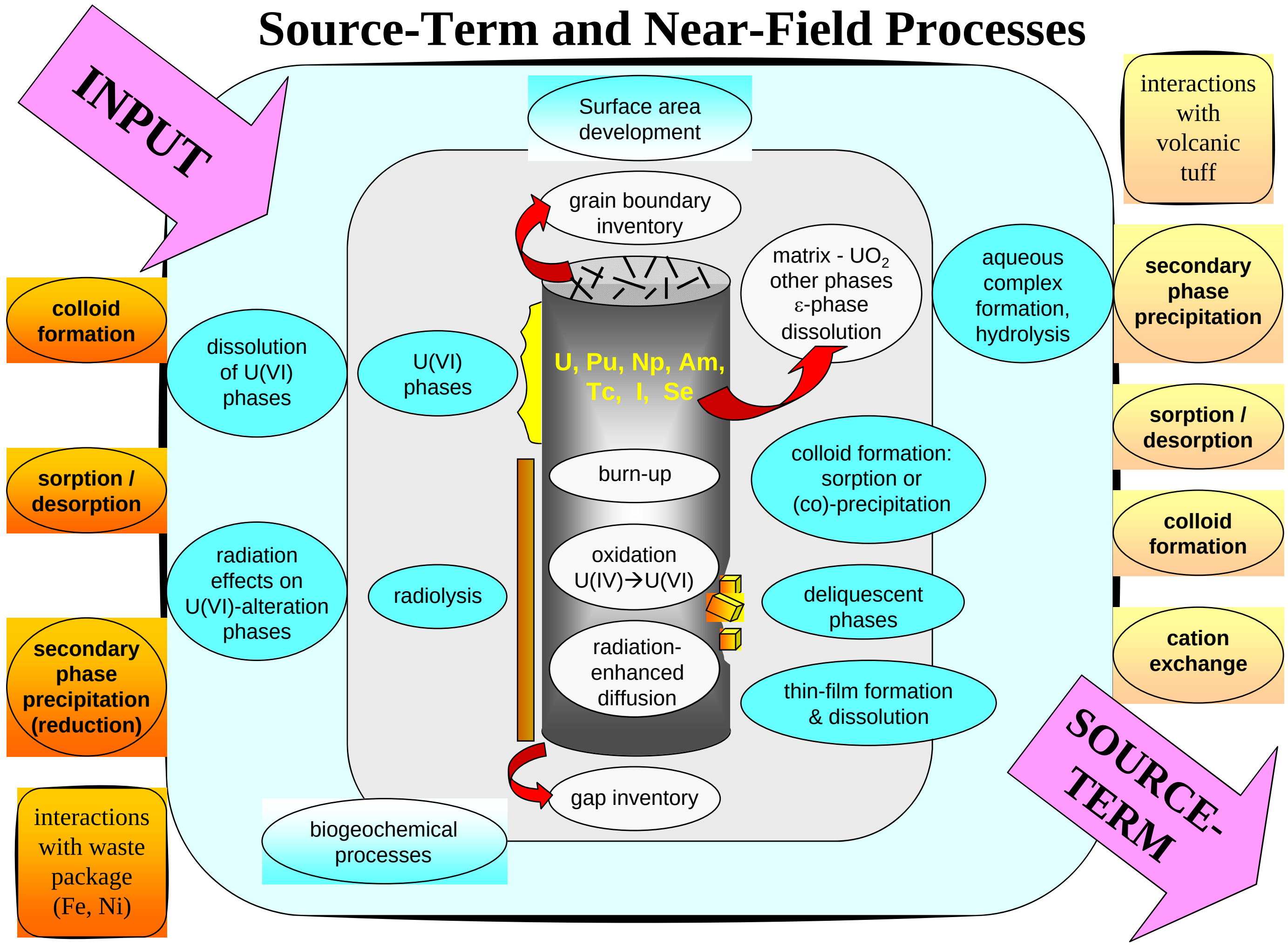
Surface Enhanced Raman Spectroscopy (SERS) – The electrochemical cell containing the sample under investigation (e.g. Alloy 22) by SERS.



SERS of passive film formed on Alloy 22 in 0.1M HCl at potentials of 0V, 0.2V ,0.4V, 0.6V, 0.8V, 1.0V vs.. SCE.

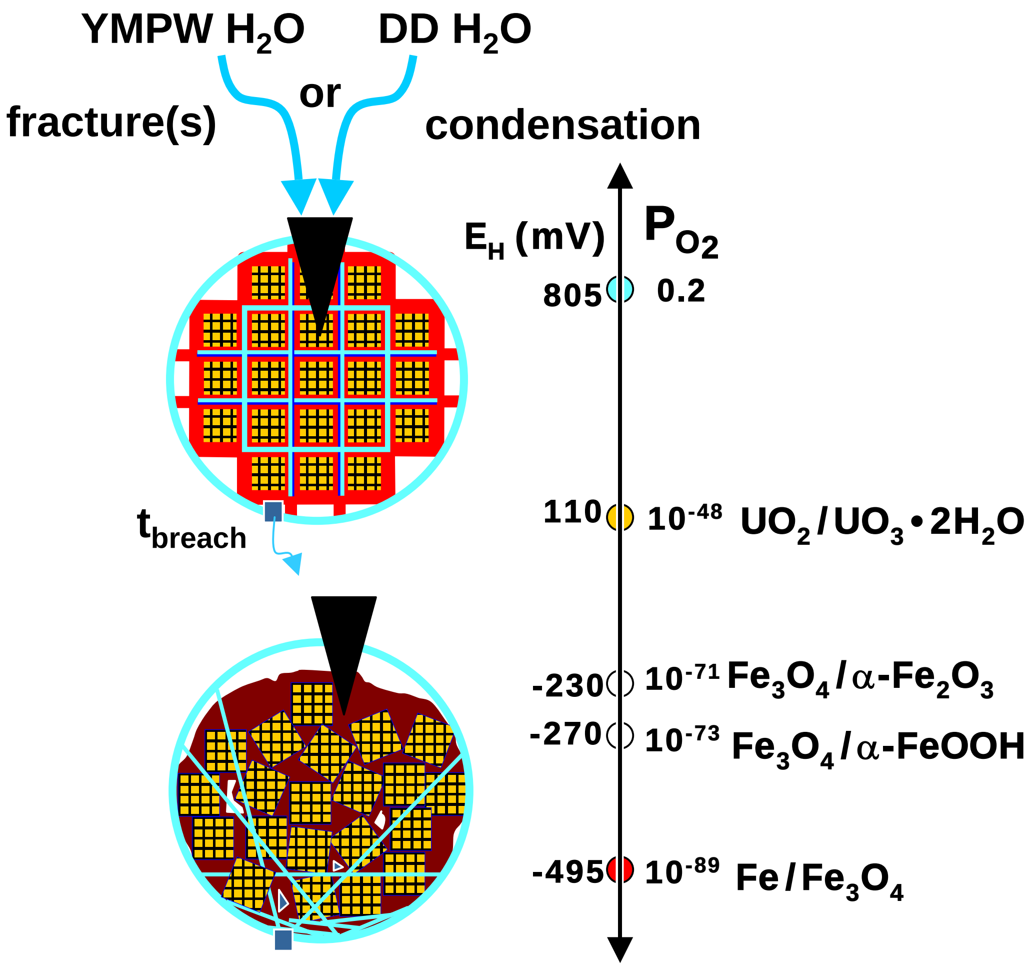
Thanks to Thomas M. Devine, University of California - Berkeley

Source Term



Source-Term and Near-Field Processes
INPUT
SOURCE-TERM
interactions with volcanic tuff
secondary phase precipitation
sorption / desorption
colloid formation
cation exchange
colloid formation
sorption / desorption
secondary phase precipitation (reduction)
interactions with waste package (Fe, Ni)
Surface area development
grain boundary inventory
matrix - UO_2 other phases ε-phase dissolution
aqueous complex formation, hydrolysis
dissolution of U(VI) phases
U(VI) phases
U, Pu, Np, Am, Tc, I, Se
burn-up
colloid formation: sorption or (co)-precipitation
radiation effects on U(VI)-alteration phases
radiolysis
oxidation U(IV)→U(VI)
deliquescent phases
radiation-enhanced diffusion
thin-film formation & dissolution
gap inventory
biogeochemical processes

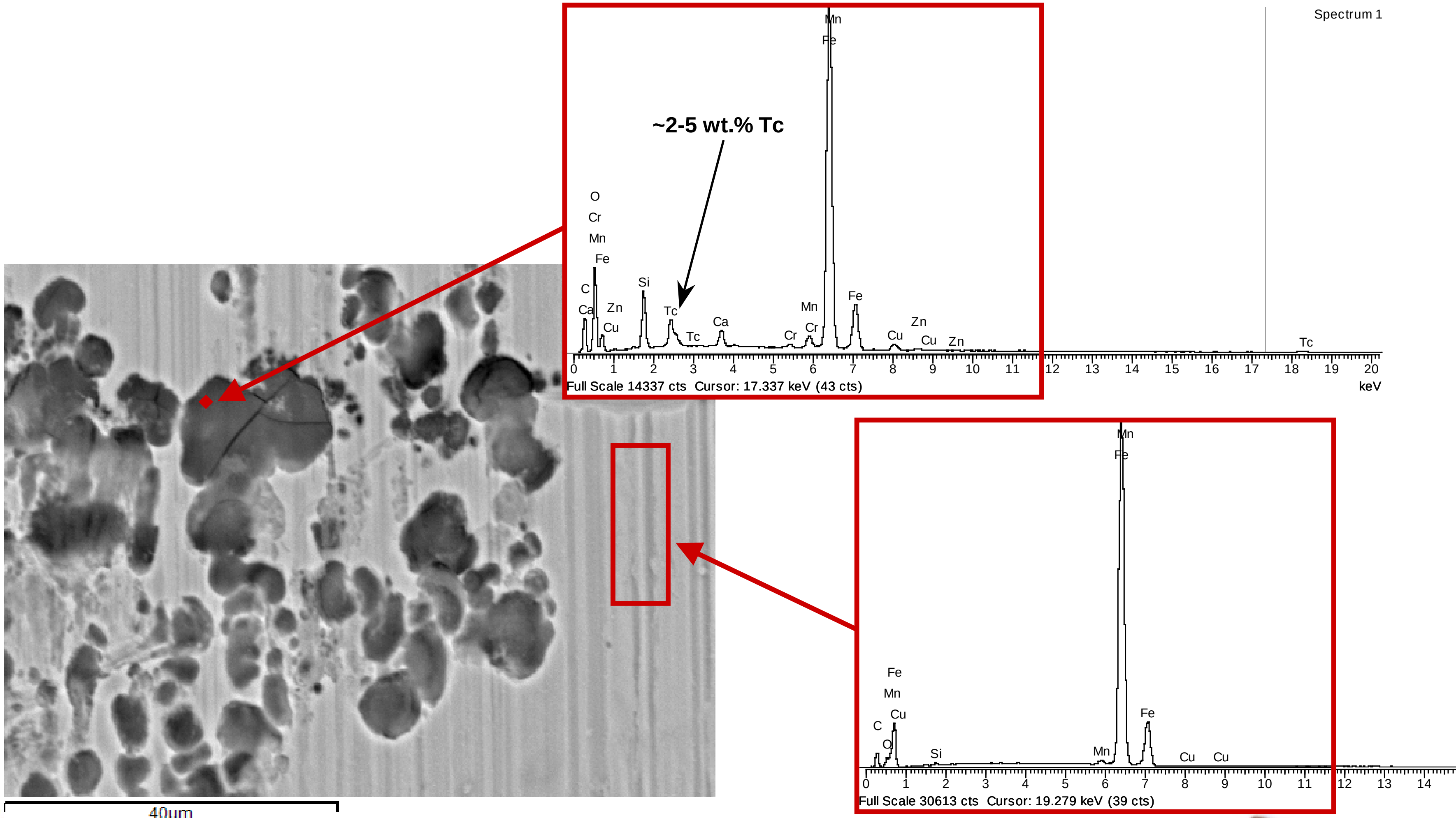
In Situ Redox State - The Approach



$t > t_{breach}$ + 100 years

Technetium Uptake by Iron-Based Materials

SEM/EDS Showing Uptake of Tc by Corrosion Product on A-516 Carbon Steel Coupon Reacted in 0.1-mmol/L Tc Spiked YMPW after 175 Days

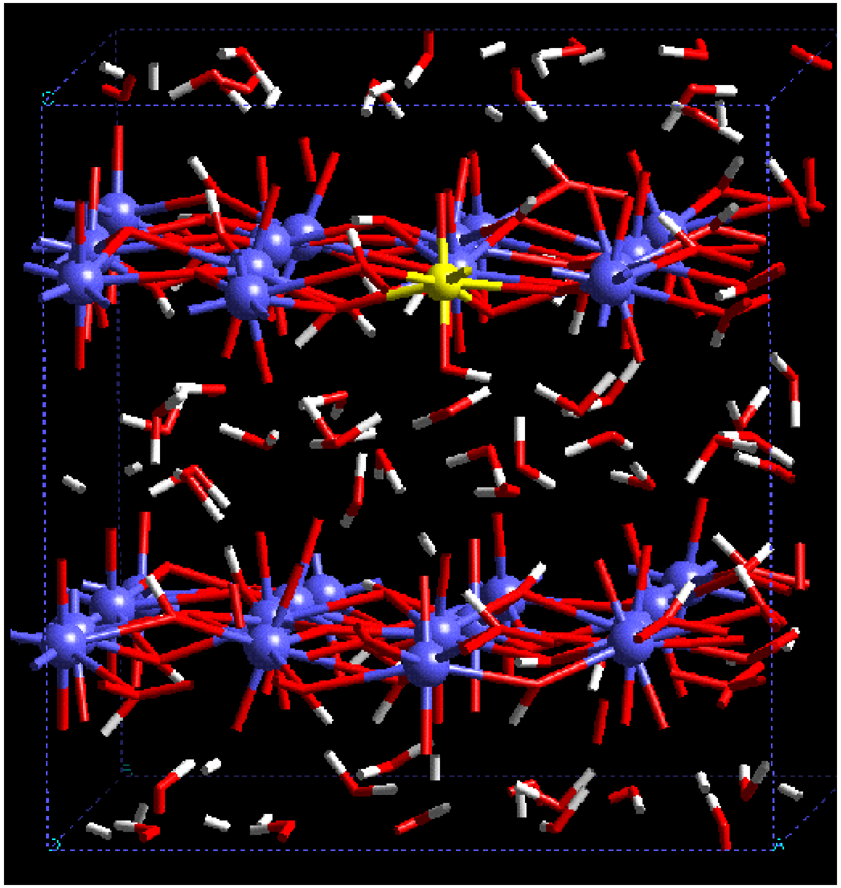


Fate of Neptunium in a Geologic Repository

Incorporation and stability of neptunium in uranium alteration phases

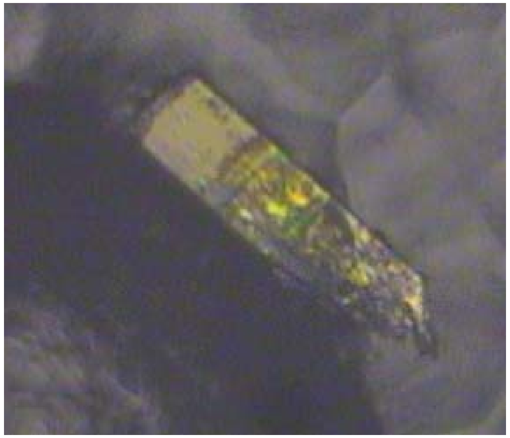
Schematic of NpO_2^+ (plus H^+) substituting for UO_2^{2+} in a schoepite unit cell

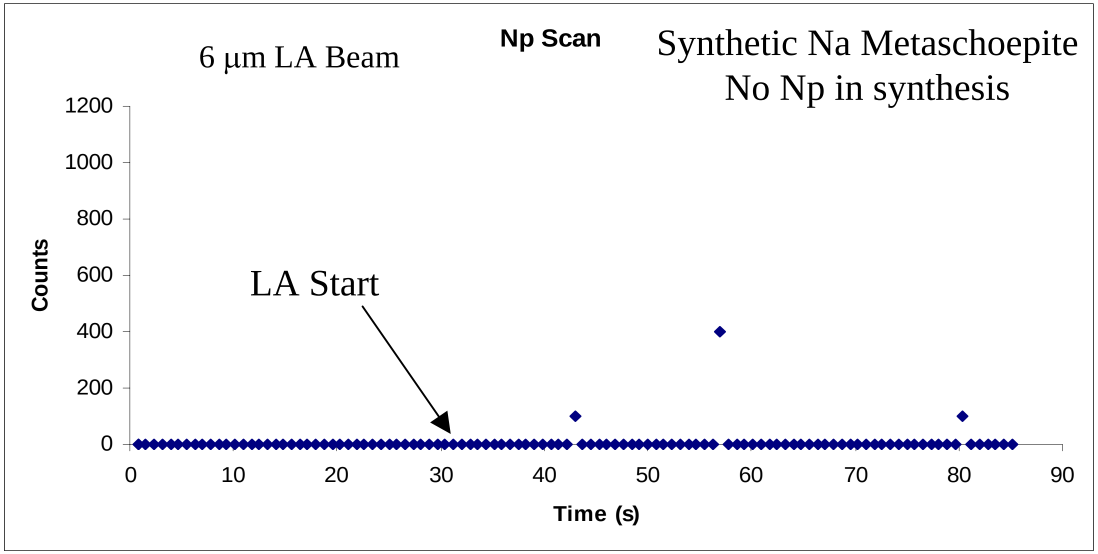
- Yellow = Np^{5+}
- Blue = U^{6+}
- Red = O
- White = H



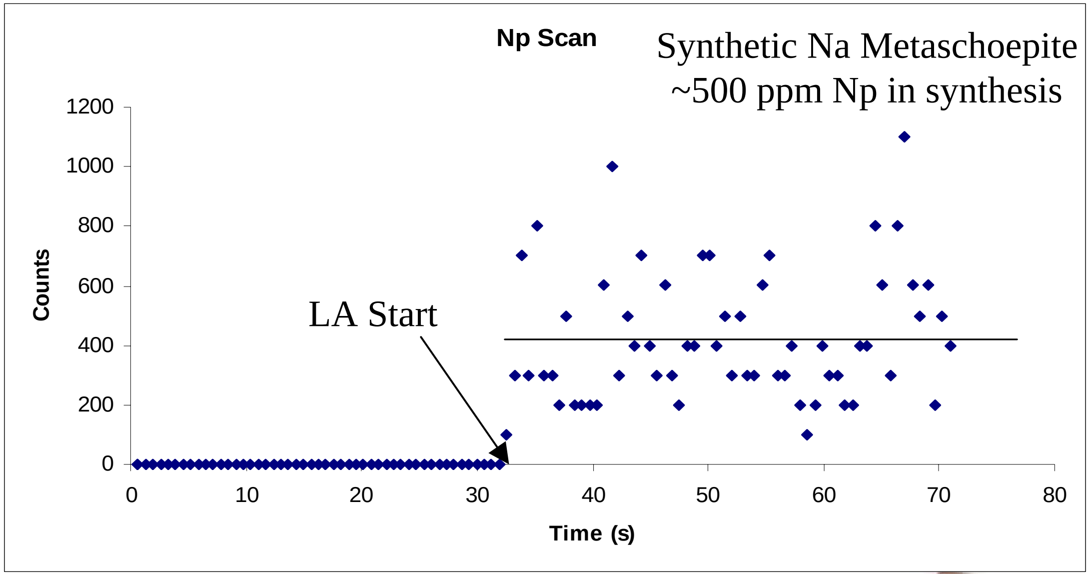
- **Incorporation energy**
- **Solid solution calculations – limits of Np incorporation**
- **Np^{5+} interactions with Fe-oxides**

Na-Substituted Metaschoepite

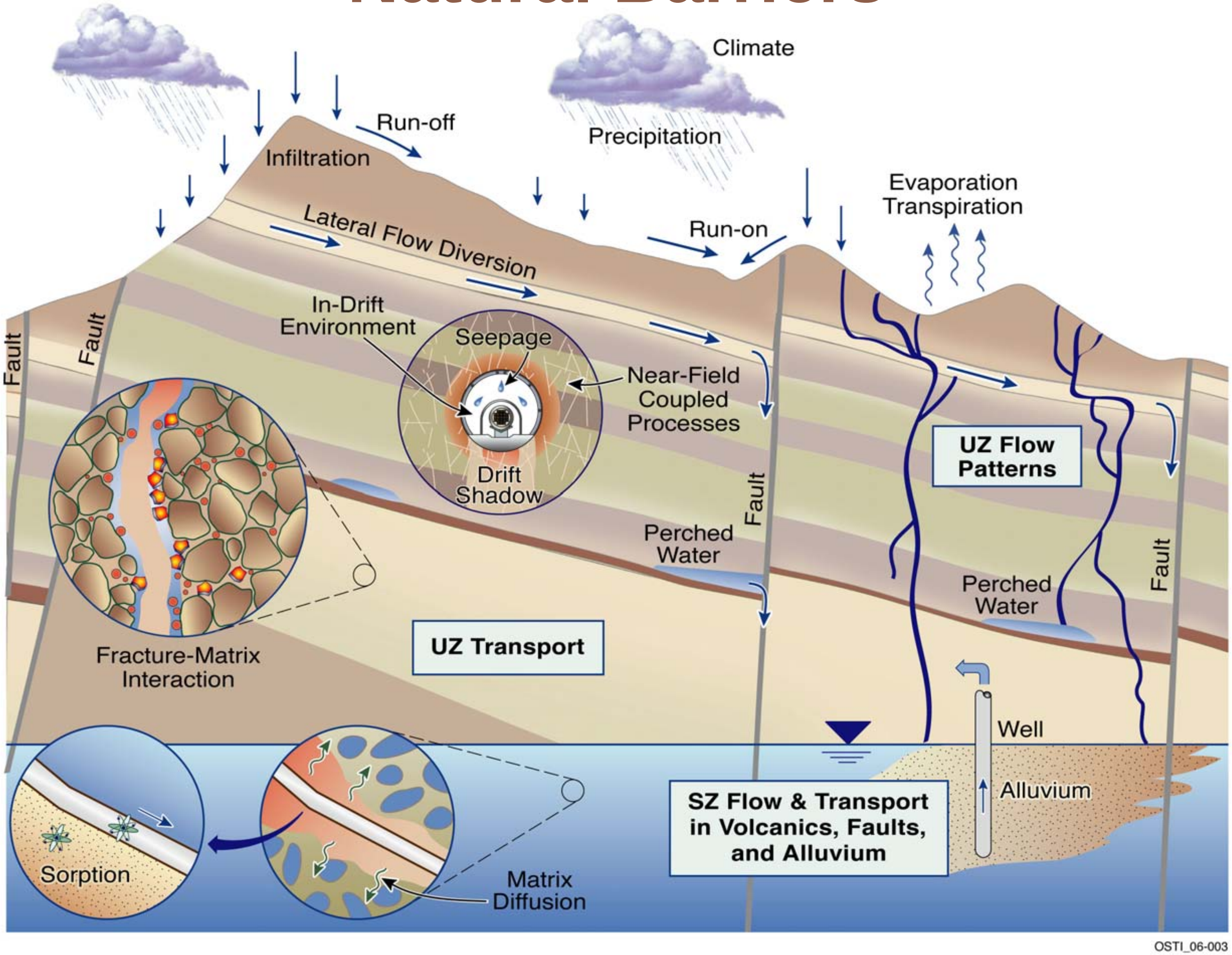




6 µm laser



Natural Barriers

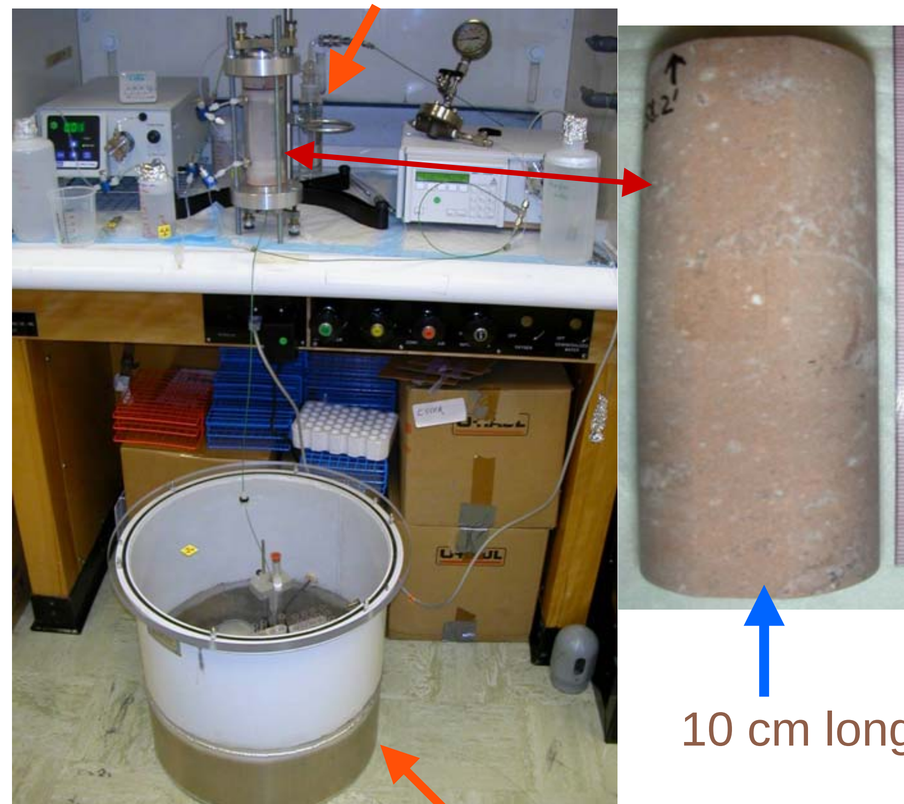


Pore Connectivity, Episodic Flow, and Unsaturated Diffusion in Fractured Tuff

- Experimental and modeling research components
  - Sample acquisition and processing
  - Gas diffusion
  - Water imbibition and tracer transport
  - Episodic fracture flow and tracer transport
  - Synchrotron microtomography
  - Pore-scale network modeling
- Ambitious, integrated, and rigorous tests designed and implemented, large amount of data currently under analysis
- Interacting imbibition-diffusive-sorption processes leading to radionuclide retardation under fracture-dominated flow

Episodic Transport in Fractured Core
Multiple tracers: H-3, Br, I, Re, NP-237, U-235, Sr, Se, Cs-133, Sm-147, Pu-242

RH (>98%) bubbler



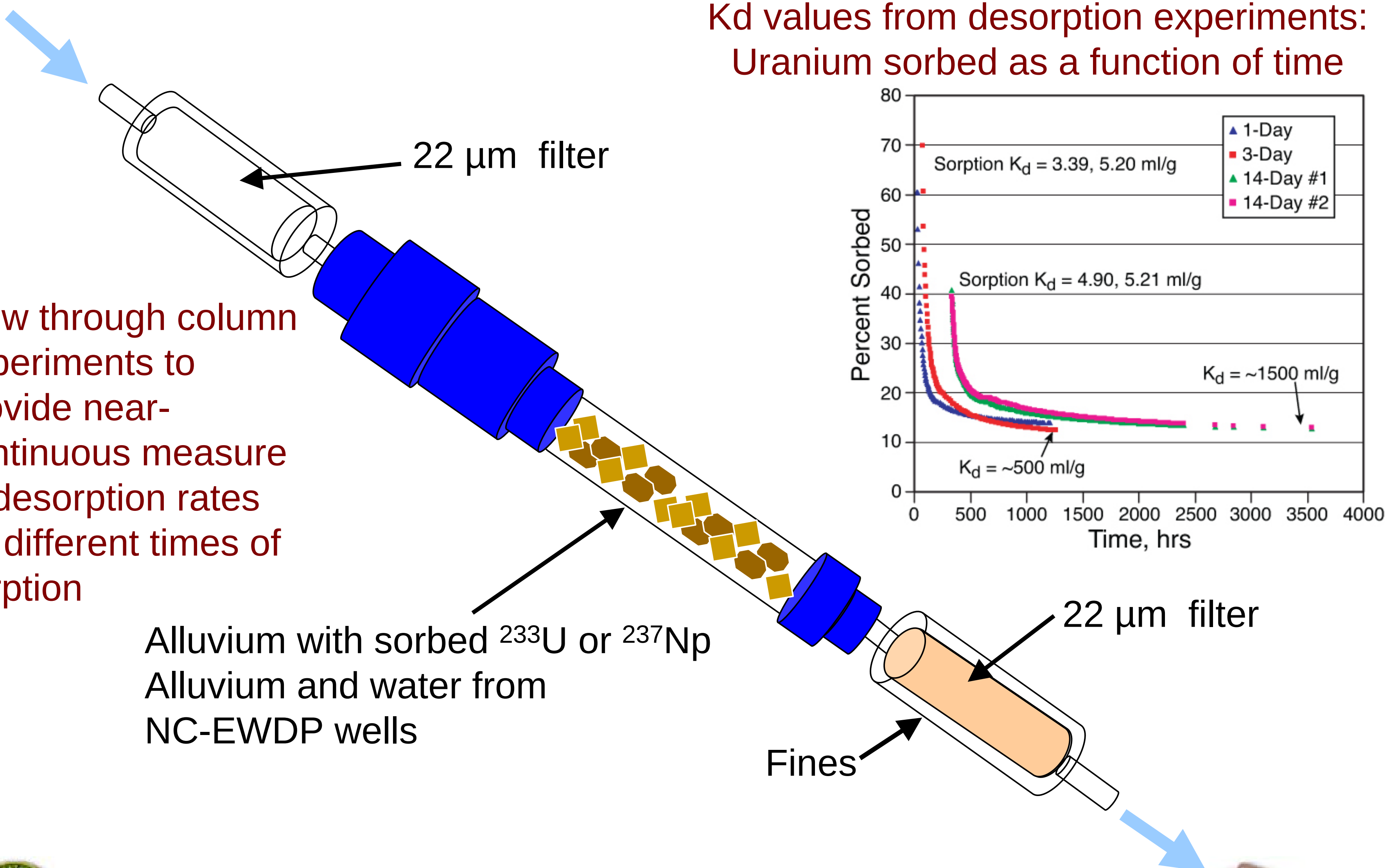
10 cm long

Fraction collector inside a high RH chamber

Improved Characterization of Radionuclide Retardation in Volcanics and Alluvium

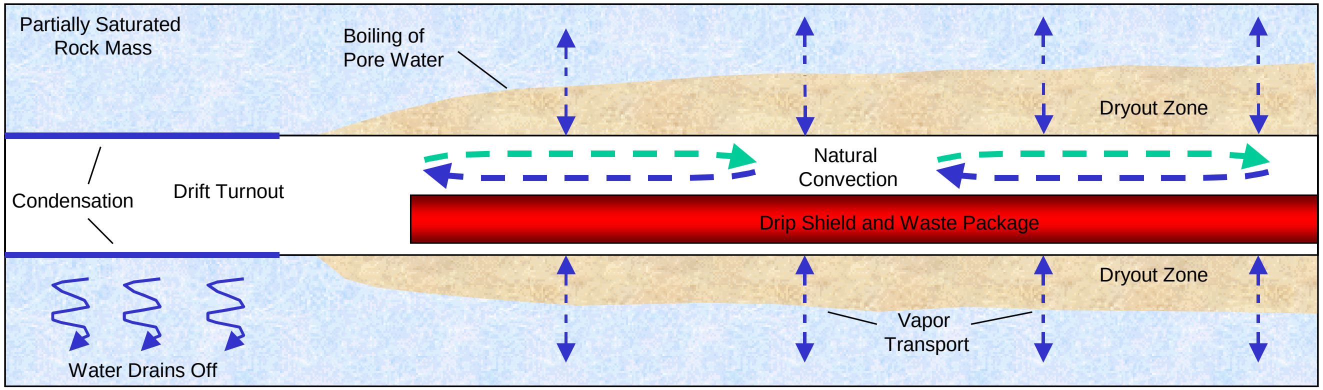
Kd values from desorption experiments: Uranium sorbed as a function of time

Flow through column experiments to provide near-continuous measure of desorption rates for different times of sorption

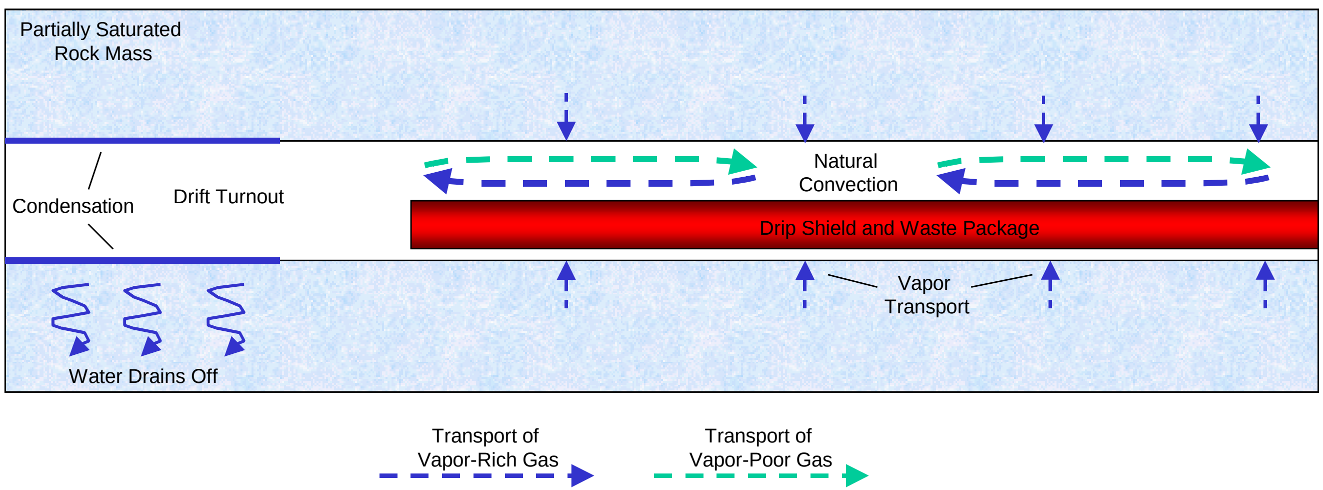


Coupled In-drift, Near-Field, and Mountain-Scale Fluid and Heat Flow Processes

(a) Boiling Phase: Heated Drift Section Above Boiling Temperature



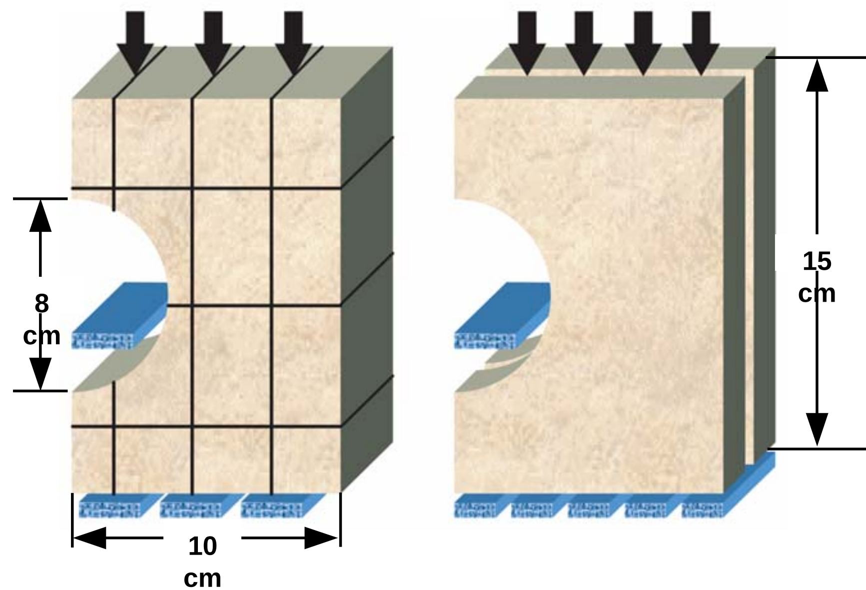
(b) Sub-Boiling Phase: Heated Drift Section Below Boiling Temperature

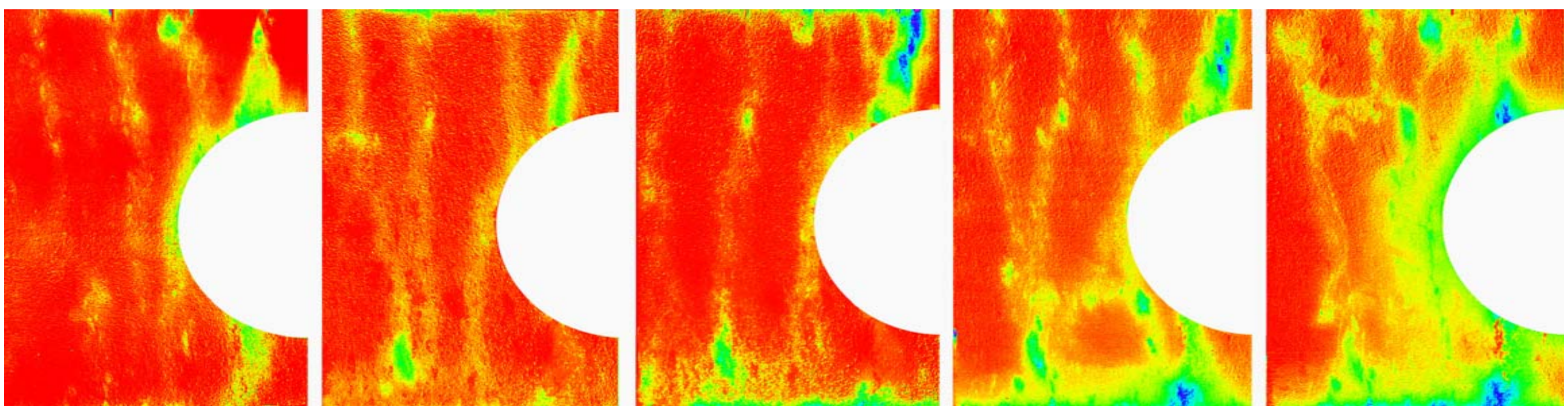


Natural ventilation and convection can greatly reduce seepage into drift

Testing the Concept of Drift Shadow with X-Ray Absorption Imaging Experiments

- Design for multi- and in-plane fracture system
- Tracer being diverted around the drift
- Tracer shedding off the drift and not under the drift
- Capillary fringe at the bottom of the test cell for tests with higher flow rates (experimental design needs to be improved)





0.01 ml/min #4 | 0.05 ml/min #2 | 0.09 ml/min #1 | 0.13 ml/min #3 | 0.24 ml/min #6

Summary

- Our investment in S&T is generating additional insight into the potential performance of the proposed repository's natural and engineered systems and source term
- The diversity and quality of program participants brings new ideas and approaches to the forefront
- The integration with the technical basis for the SAR will be managed to result in enhanced understanding, confidence in system safety over its entire life-cycle, and support of the safety case