SAND2016-6240C

Used Fuel Disposition Campaign

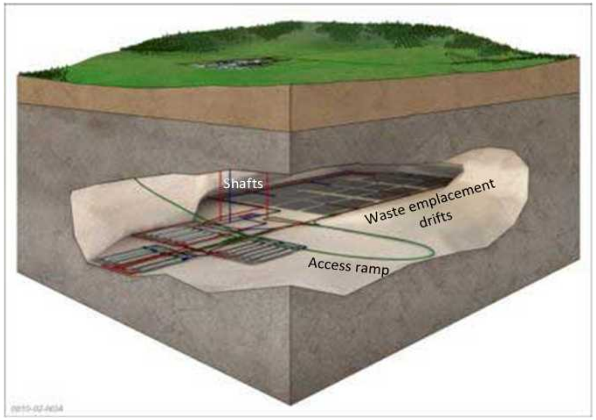
DR Crystalline Disposal R&D

Yifeng Wang
Sandia National Laboratories

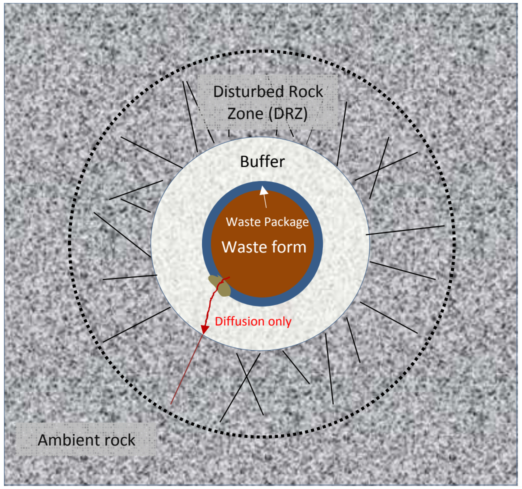
UFD Working Group Meeting
June 7-9, 2016

Crystalline Disposal R&D Work Packages

- **Objectives**
  - Advance our understanding of long-term disposal of used fuel in crystalline rocks;
  - Develop experimental and computational capabilities to evaluate various disposal concepts in such media.
- **Focus on two key components of deep geologic repository in crystalline rocks**
  - Better characterization and understanding of fractured media and fluid flow and transport in such media
  - Designing effective engineered barrier systems for waste isolation
- **Fully leverage international collaborations**
  - Korean Atomic Energy Research Institute
  - Äspö Hard Rock Laboratory (Sweden)
  - DECOVALEX (Bedrichov Tunnel Tests, Czech)
  - Colloid Formation & Migration Project (Switzerland)
  - Others



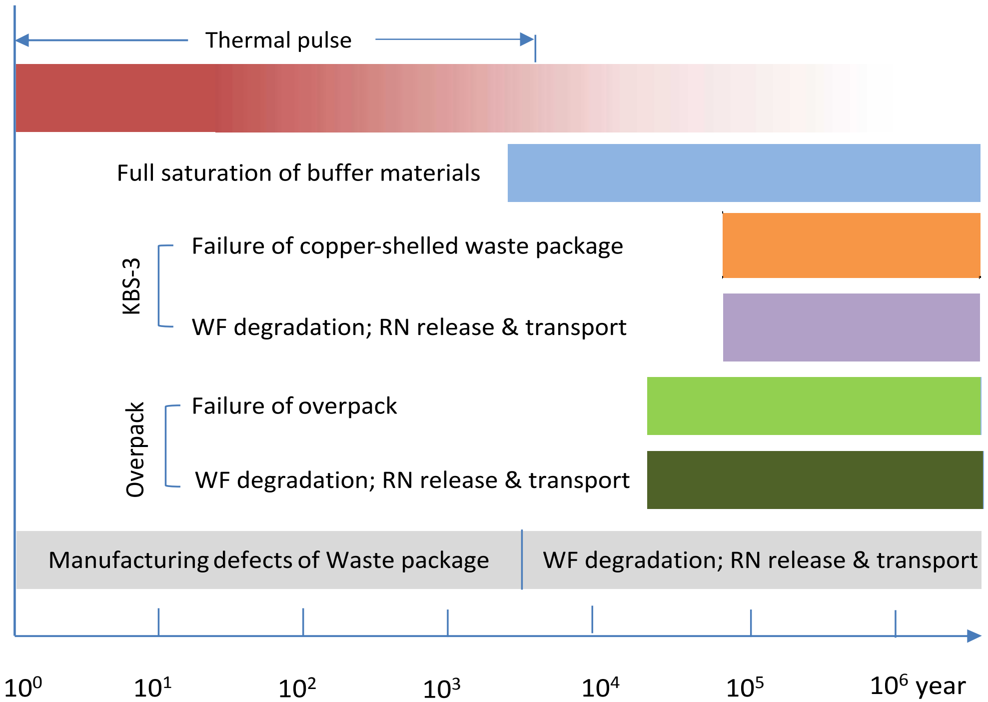
Modified from http://www.bbc.com/news/uk-england-cumbria-21253673

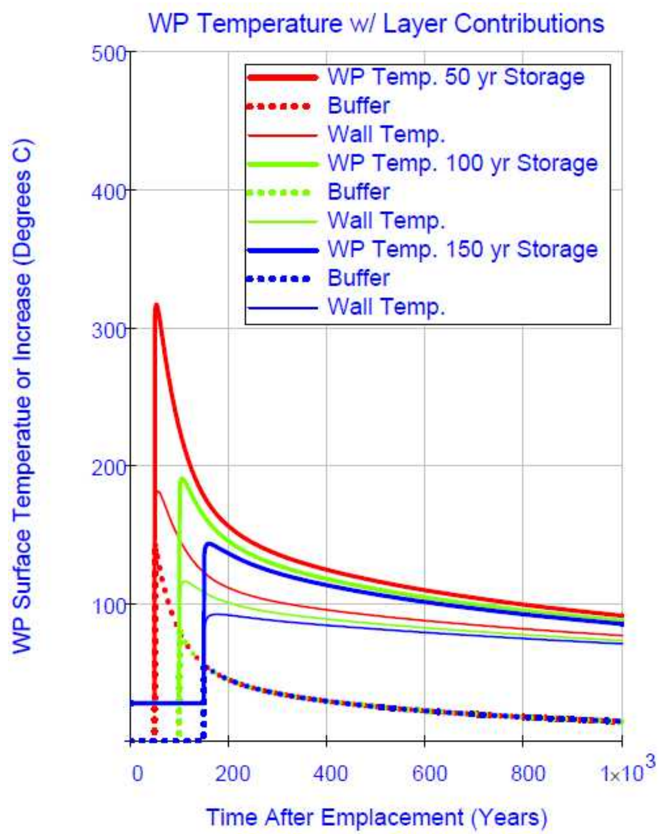


Institutions involved: ANL, LANL, LBNL, LLNL, SNL

Used
Fuel
Disposition

Relevant Physical & Chemical Conditions

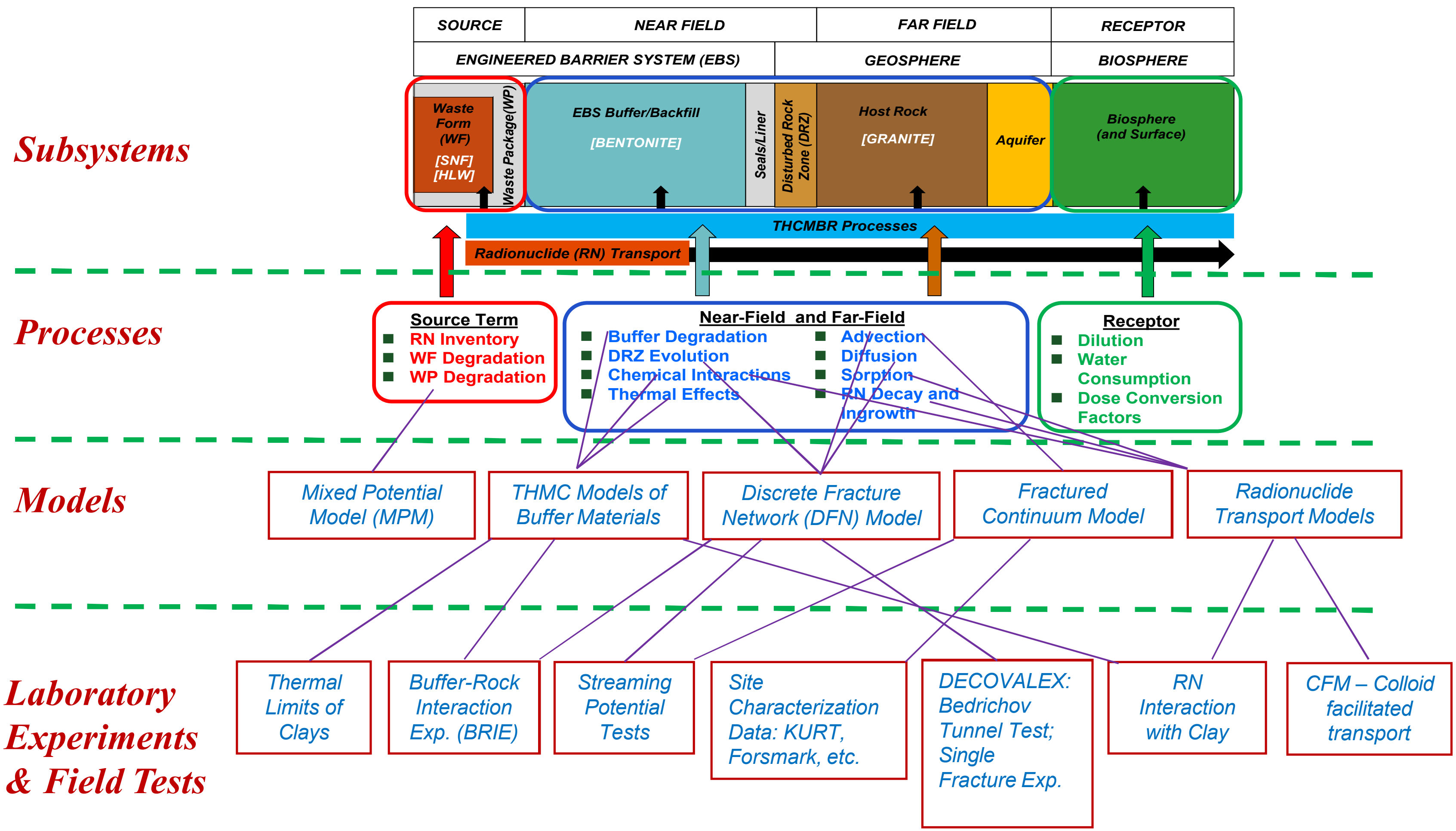




UOX fuel (40 GW-d/MT), 32-PWRs (Hardin & Voegele, 2013)

Used Fuel Disposition

Experimental & modeling activities for used fuel disposition in crystalline rocks



Integration & coordination among institutions

ANL
- *Mixed potential model*

PNNL
- *Radiolysis model*

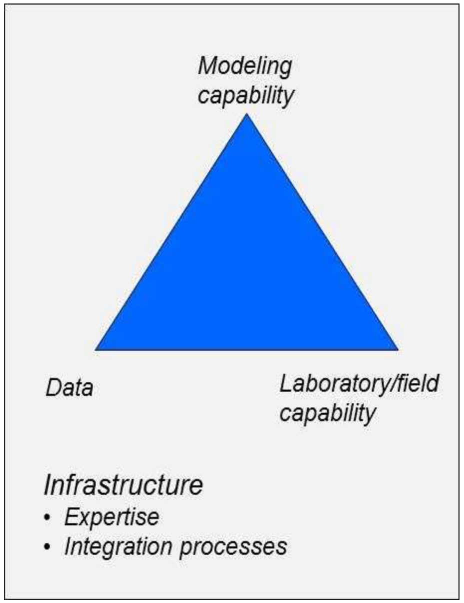
LLNL
- *Colloid stability*
- *Np diffusion in bentonite*
- *Analysis of CFM data from Grimsel*

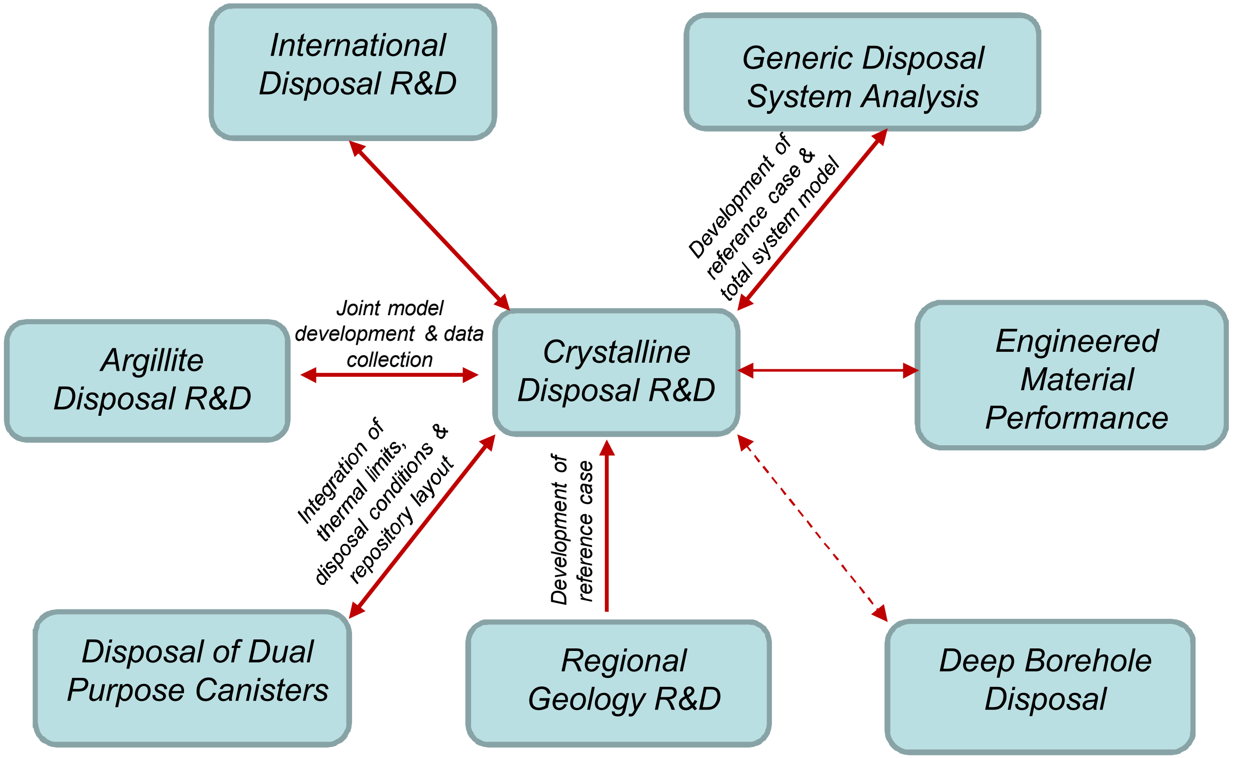
SNL
- *Technical integration & coordination*
- *Thermal limit of buffer materials*
- *Iodide diffusion & sorption in compacted clays*
- *Fracture continuum model (FCM)*
- *DECOVALEX (Czech - Bedrichov, fracture closure/opennng)*
- *KURT*

LBNL
- *U diffusion in compacted bentonite*

LANL
- *Discrete fracture network (DFN) model*
- *Colloid transport*
- *Grimsel (CFM)*
- *SKB BRIE*

Integration & coordination





Institutions involved: ANL, LANL, LBNL, LLNL, SNL

Used Fuel Disposition

FY16 Work

- **Objectives**
  - Advance our understanding of long-term disposal of used fuel in crystalline rocks;
  - Develop experimental and computational capabilities to evaluate various disposal concepts in such media.
- **Focus on two key components of deep geologic repository in crystalline rocks**
  - Better characterization and understanding of fractured media and fluid flow and transport in such media
  - Designing effective engineered barrier systems for waste isolation
- **Fully leverage international collaborations**
  - Korean Atomic Energy Research Institute
  - Äspö Hard Rock Laboratory (Sweden)
  - Bedrichov Tunnel Tests (Czech)
  - Colloid Formation & Migration Project (Switzerland)
  - Others
- **Model development & integration**
  - Integration with GDSA: PA model for crystalline media
  - Wrapping up some activities (e.g. colloid formation & transport)
  - Model demonstration with actual data

Used Fuel Disposal in Crystalline Rocks: Status and FY14 Progress

Fuel Cycle Research & Development

Prepared for
U.S. Department of Energy
Used Fuel Disposition
Y. Wang, E. Matteo
Sandia National Laboratories
J. Rutqvist, J. Davis, L. Zheng, J. Houseworth, J. Birkholzer
Lawrence Berkeley National Laboratory
T. Dittrich, C. W. Gable, S. Karra, N. Makedonska, S. Chu, D. Harp, S. L. Painter, P. Reimus, F. Perry
Los Alamos National Laboratory
P. Zhao, J. Begg, M. Zavarin, S. J. Tumey, Z. Dai, A. B. Kersting
Lawrence Livermore National Laboratory
J. Jerden, K. Frey, J. M. Copple, W. Ebert
Argonne national laboratory
September 26, 2014
FCRD-UFD-2014-000060

APPENDIX A

RESEARCH & DEVELOPMENT (R&D) PLAN FOR USED FUEL DISPOSAL IN CRYSTALLINE ROCKS

Note: This R&D plan is a revision of an early developed R&D plan for natural system evaluation and tool development (Wang, 2013). In this revision, the newly added research topics are indicated in red. The topics that are no longer applicable to crystalline rocks are indicated in gray.

A1.0 Objectives

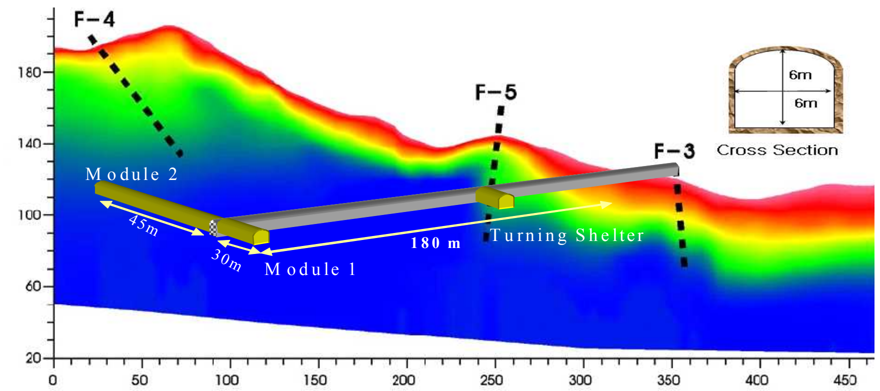
The U.S. Department of Energy Office of Nuclear Energy, Office of Fuel Cycle Technology established the Used Fuel Disposition Campaign (UFDC) in fiscal year 2010 (FY10) to conduct the research and development (R&D) activities related to storage, transportation and disposal of used nuclear fuel and high level nuclear waste. The Mission of the UFDC is

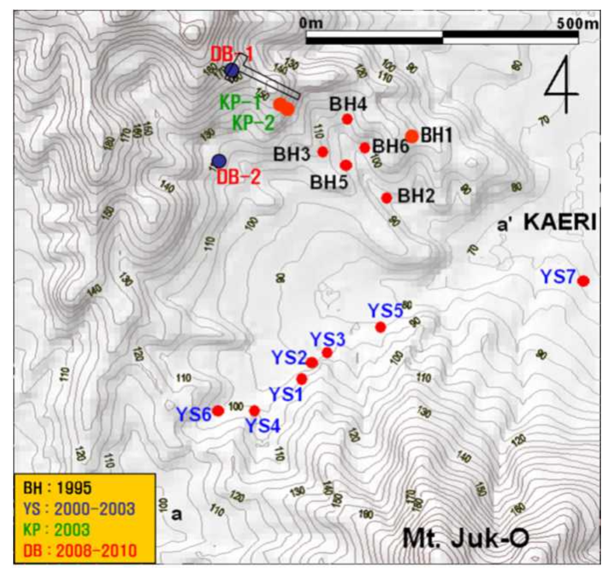
> *To identify alternatives and conduct scientific research and technology development to enable storage, transportation and disposal of used nuclear fuel and wastes generated by existing and future nuclear fuel cycles.*

Used Fuel Disposition

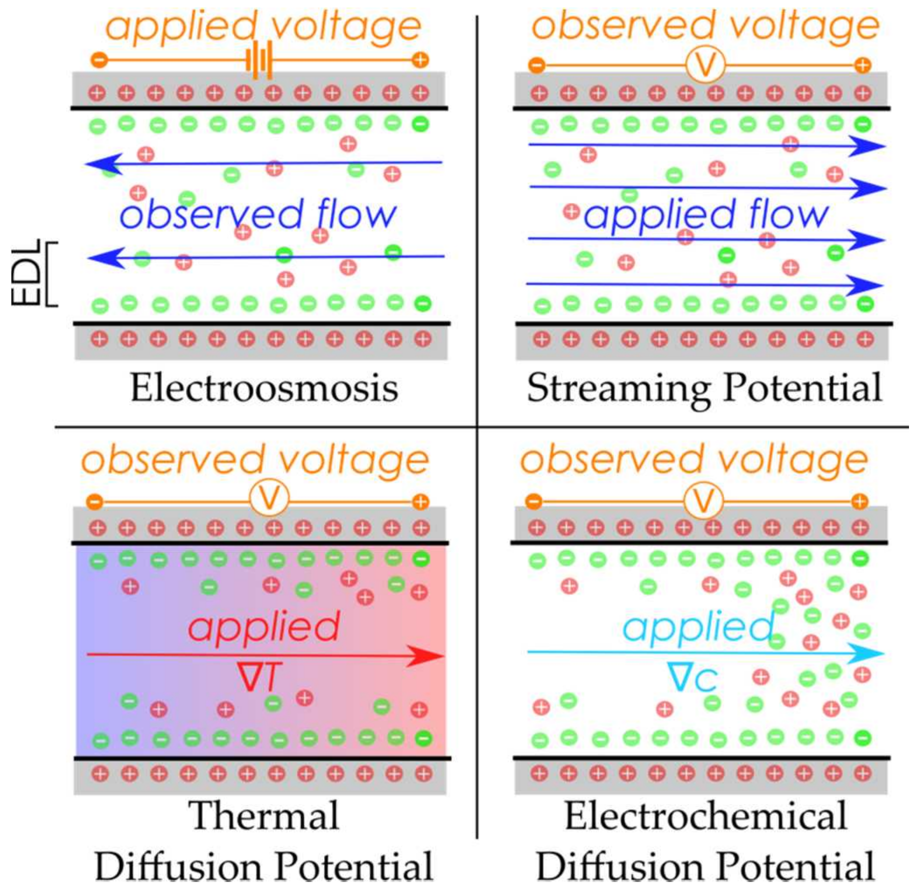
KAERI Underground Research Tunnel (KURT)

- **SNL and KAERI have developed a multi-year plan for joint field testing and modeling crystalline disposal media.**
- **Work currently planned includes three tasks:**
  - Streaming potential (SP) testing
  - Sharing KURT site characterization data
  - Technique development for in-situ borehole characterization.
- **Status updates**
  - Site characterization data received
  - Plan for the development and demonstration of in-situ borehole measurements developed
  - Report on material specifications for Ca-bentonite (e.g. swelling pressure) received
  - Received the data set of SP test
  - New contract on borehole trace testing placed (joint with Depp Borehole WP)





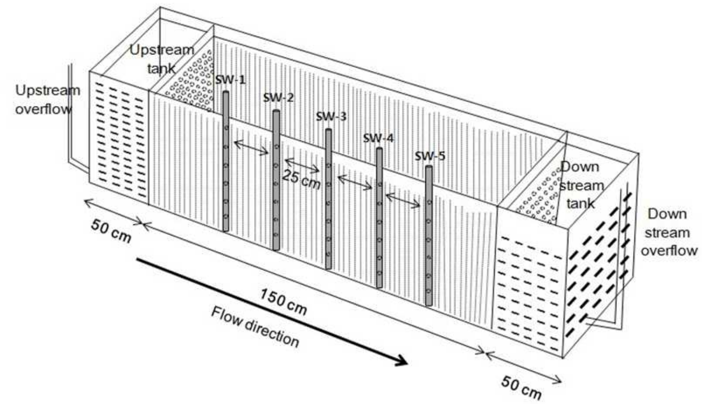
Streaming potential test: the Concept

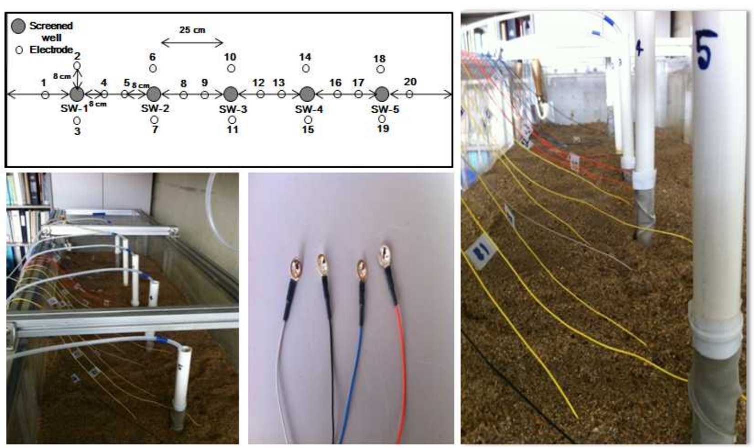


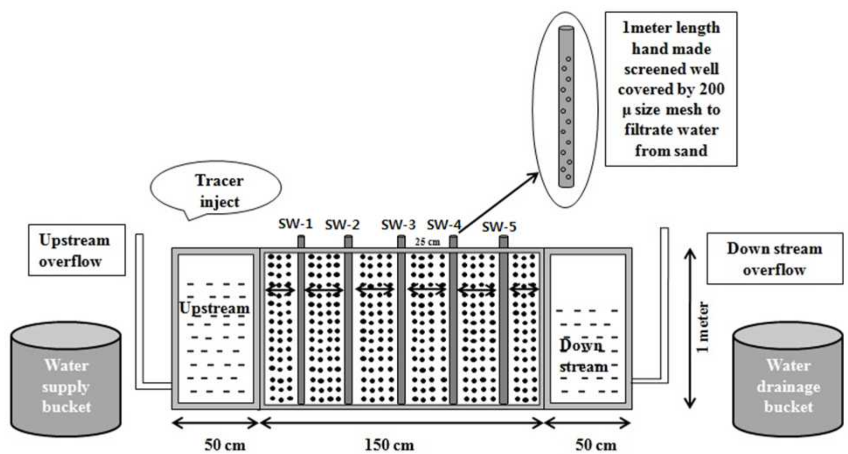
Kuhlman (2016, per. comm.)

Used
Fuel
Disposition

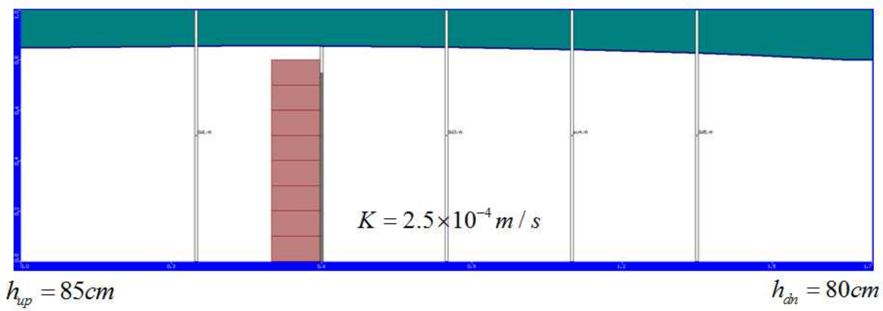
Streaming potential testing – experimental setup

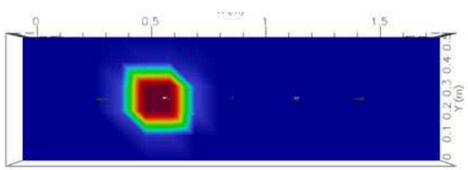




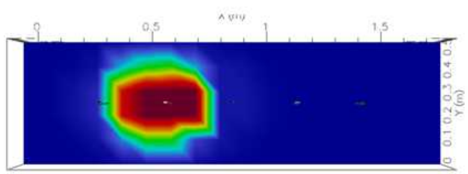


Numerical simulation of tracer test

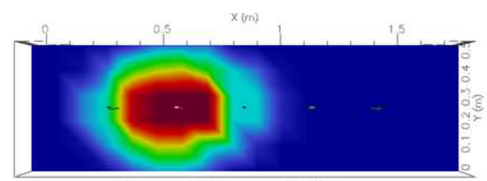




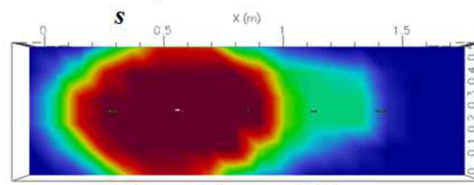
Elapsed time = 200 *s*



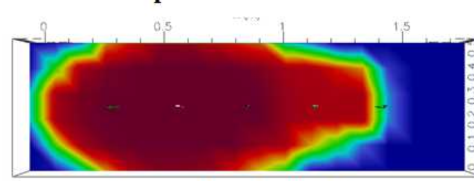
Elapsed time = 1200 *s*



Elapsed time = 2200 *s*



Elapsed time = 6800 *s*

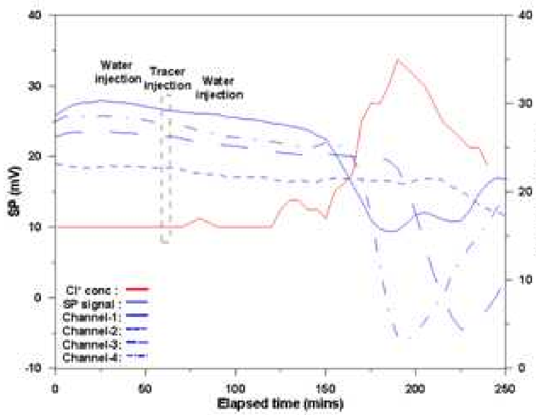


Elapsed time = 9400 *s*

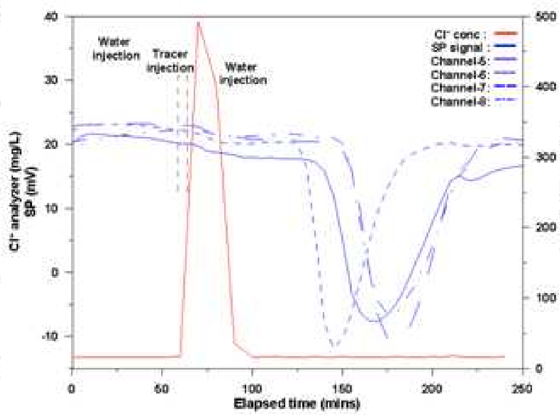
Used Fuel Disposition

Streaming potential testing

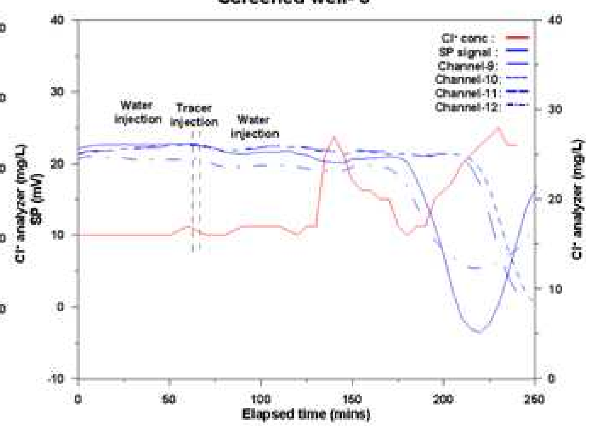
Screened well- 1



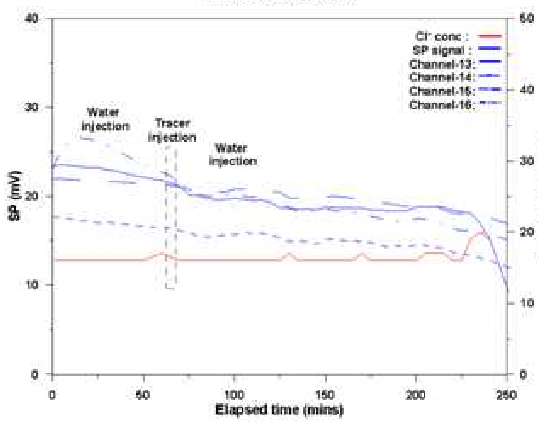
Screened well- 2



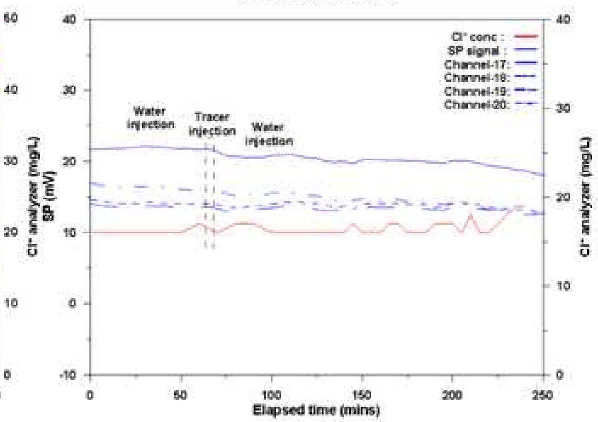
Screened well- 3



Screened well- 4



Screened well- 5



Hydrologic Borehole Tracer Testing

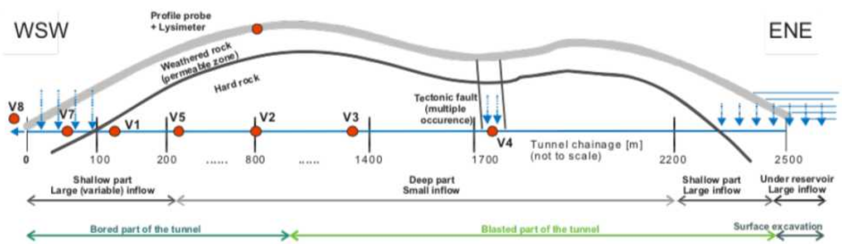
- The contractor shall conduct hydrologic testing in their existing granite boreholes to provide data and experience to increase the likelihood of success in the deeper and larger-diameter DOE-NE deep borehole project.
- Tracer testing will be conducted using a three-packer system in the KAERI deep granite borehole that allows testing between two adjacent packed-off borehole intervals.
- Injection will occur into one interval and recirculation pumping will occur into another interval. A push-pull (injection followed by withdrawal from the same packer) tracer test will be conducted before and will overlap with a vertical dipole tracer test (injection of tracer from one packer and withdrawal with recirculation from another packer).
- Different tracers will be used in the push-pull and vertical dipole tracer tests, to allow interpretation of both tests independently.
- The contractor shall be responsible for instrumentation, testing and data acquisition. SNL and the contractor will work jointly on experimental design and data interpretation.

General observations

- **Clear objectives are the key to the success**
  - KURT data for development reference cases
  - KURT data for discrete fracture network model demonstration
- **Need substantial commitment for actual technical work**
  - Funding for actual technical work
  - Face-to-face meeting
  - Need stable and predictable funding
- **Opportunities**
  - Newly extended tunnel
  - In-situ Engineered Barrier System (EBS) testing program
  - Fluid flow and transport in major fracture zones
  - Inclusive & responsive
  - Able to directly participate in experimental design

DECOVALEX – Task 2: Multiple environmental tracer test at Bedrichov Tunnel, Czech Republic

			Model 2 (V6)	Model 3 (V2)	Model 4 (V4)
	tunnel depth [m]		-39	-140	-91
	thickness of shallow zone [m]		-20	-15	-20
parameter group 2	K shallow [m/s]		1.00E-06	1.00E-06	1.00E-06
	K fract [m/s]		1.14E-07	1.29E-10	2.35E-08
POR2	K deep [m/s]		5.47E-10	3.17E-12	4.04E-10
	n shallow		0.02	0.02	0.02
	n fract		0.04354	0.00004	0.073
	n deep		0.0225	0.00004	0.073
	dispersion length (L/T) (m)		1-May	1-May	1-May
	tortuosity		1	1	1
	diffusion coef. (m^2/s)		6.00E-10	6.00E-10	6.00E-10



Tracers: $\delta^{18}O$, $\delta^{2}H$, ^{3}H, CFC

PFLOTRAN

- **3D integral finite volume**
- **Multi-physics:**
  - Multiphase, heat and fluid flow and reactive transport
- **Massively parallel**
- **Here we used Richards Mode with flow equation:**

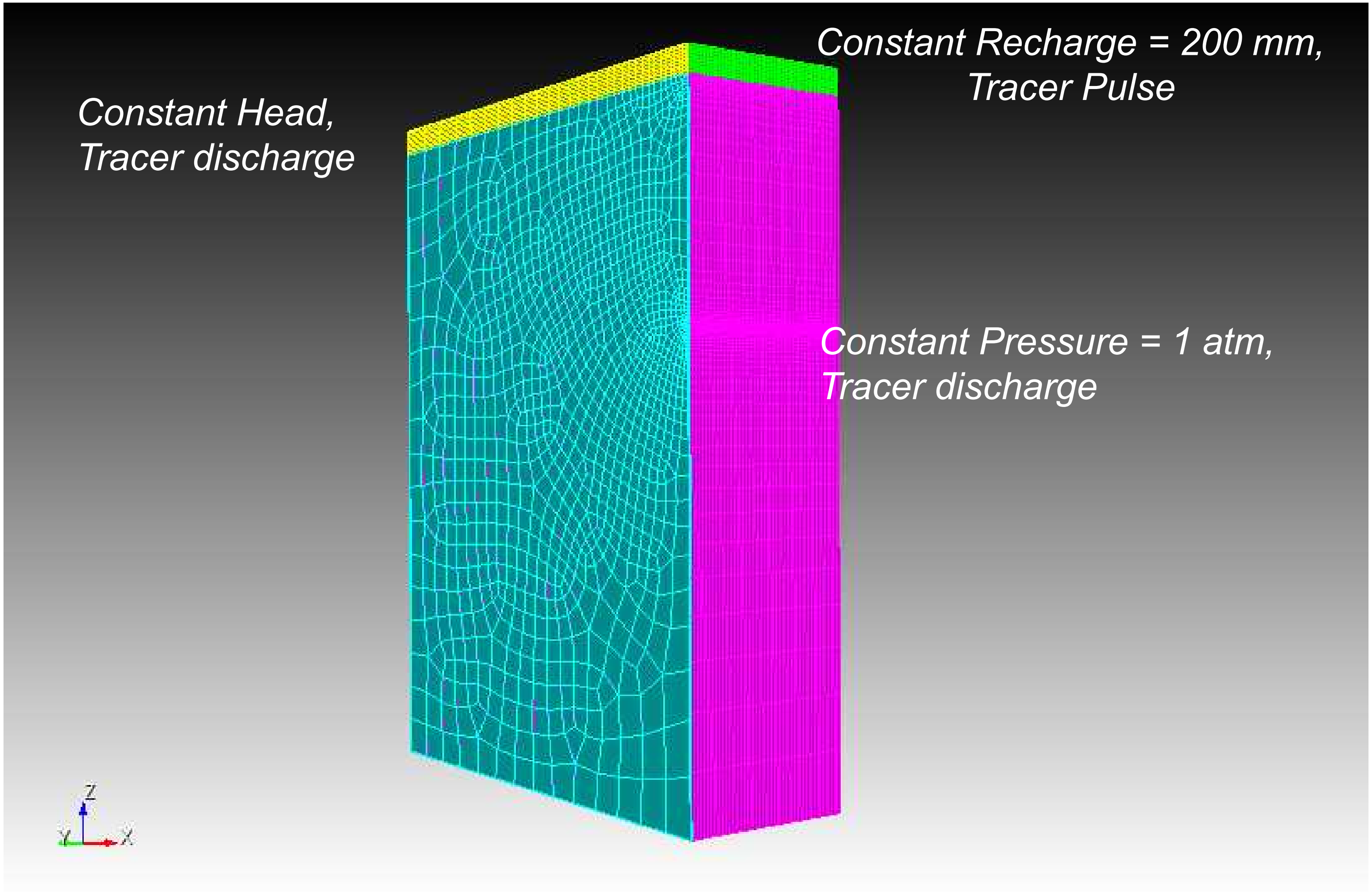
$$\frac{\partial}{\partial t}(\phi s q) - \nabla \cdot (\rho q) = Q_w$$

- **And the multi-component reactive transport equation:**

$$\frac{\partial}{\partial t}\left(\phi \sum_{\alpha} s_{\alpha} \Psi_j^{\alpha}\right) + \nabla \cdot \sum_{\alpha} (q_{\alpha} - \phi s_{\alpha} D_{\alpha} \nabla) \Psi_j^{\alpha} = Q_i - \sum_{m} v_{jm} I_m - \frac{\partial S_j}{\partial t}$$

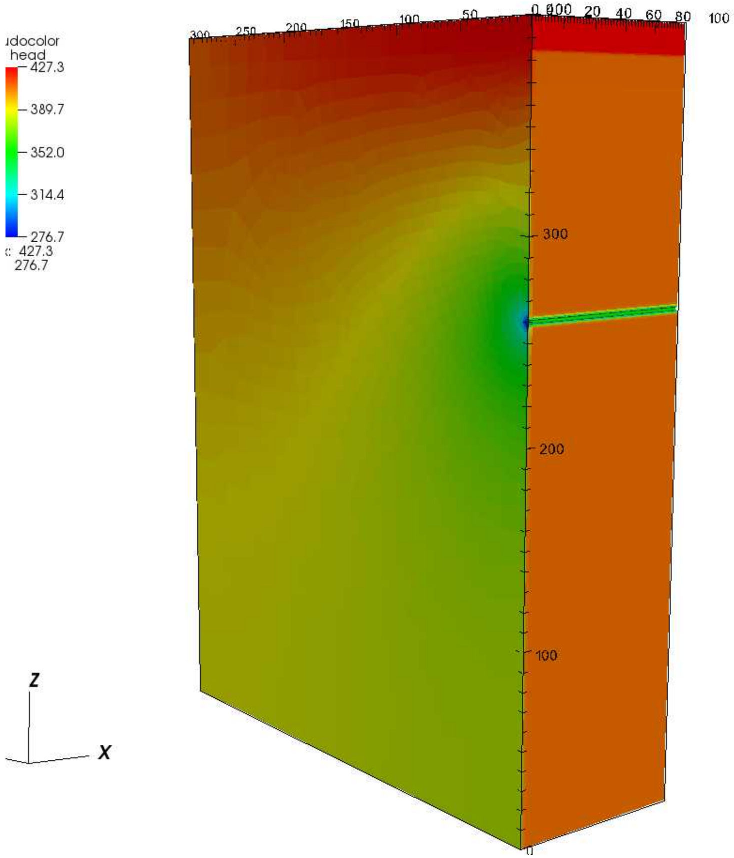
- **PFLOTRAN is 3D only, thus fractures must be treated as a 3D portion of the domain**

Model domain

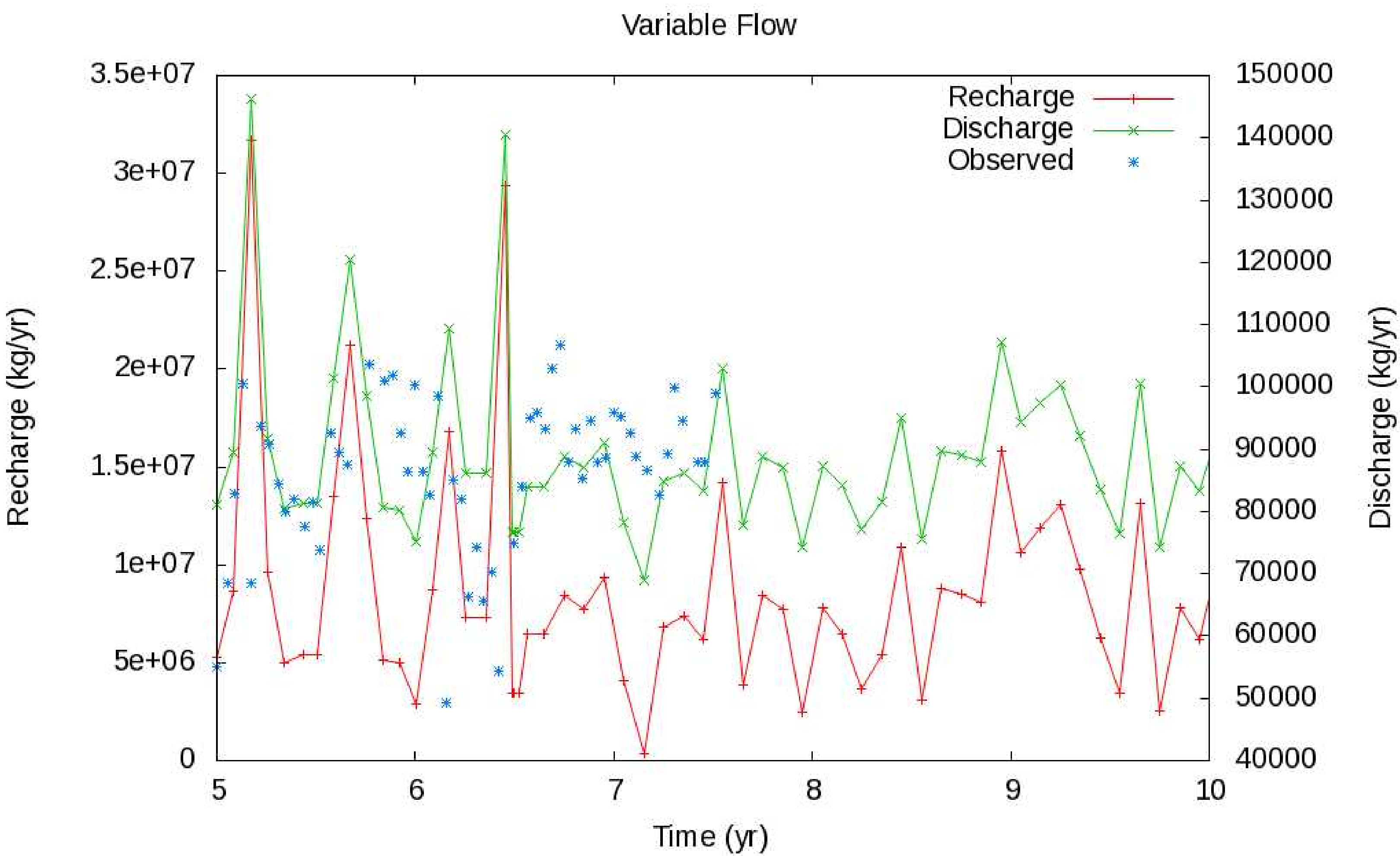


Initial Conditions – Transient Flux

- **Model "spin up"**
  - First assumed fully saturated column at hydrostatic pressure
    - *Set tunnel to atmospheric pressure*
    - *Set recharge to 200 mm across the top*
    - *Run model until steady state achieved for initial flow field*
  - Assign average tracer concentration throughout
  - These initial condition are used in transient simulation where transient tracer concentration and recharge are applied across the top
    - *Recharge 20% of monthly average*
    - *Isotope composition inverse distance weighted precipitation composition*

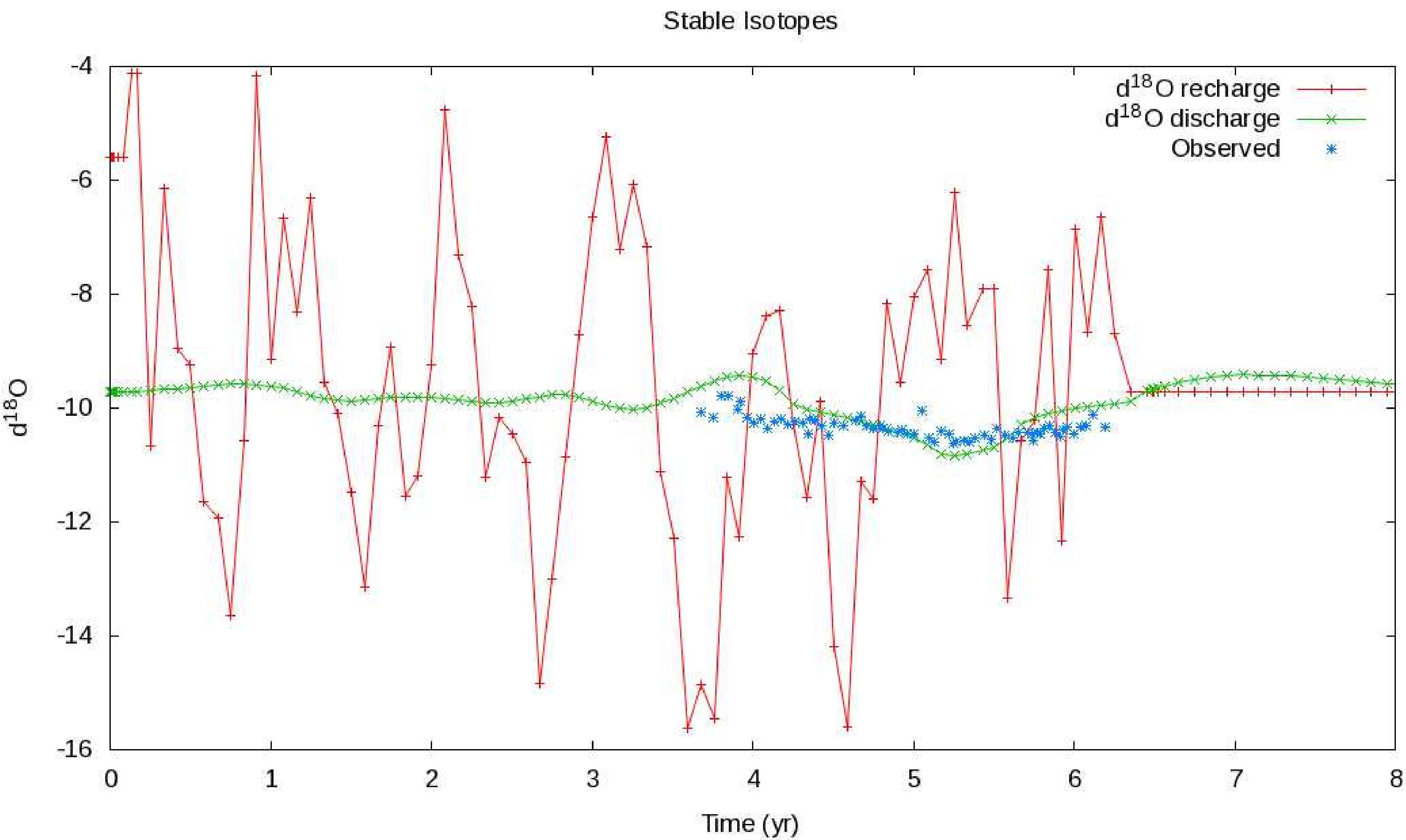


Modeled and Observed Discharge – M2,V6



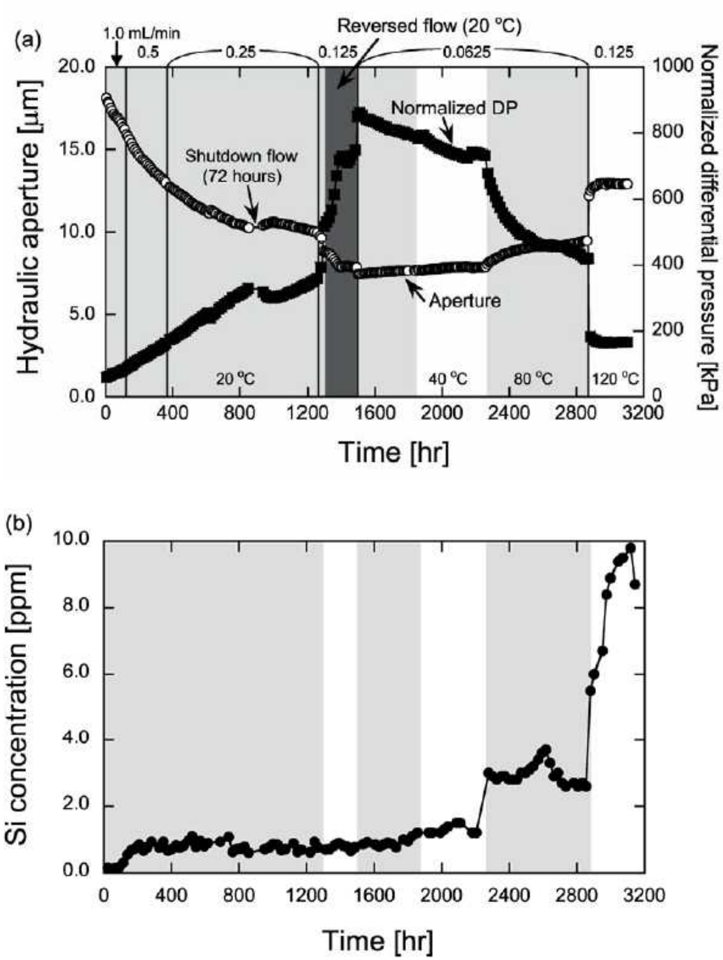
Used Fuel Disposition

Modeled and Observed $\delta^{18}O$ – M2,V6

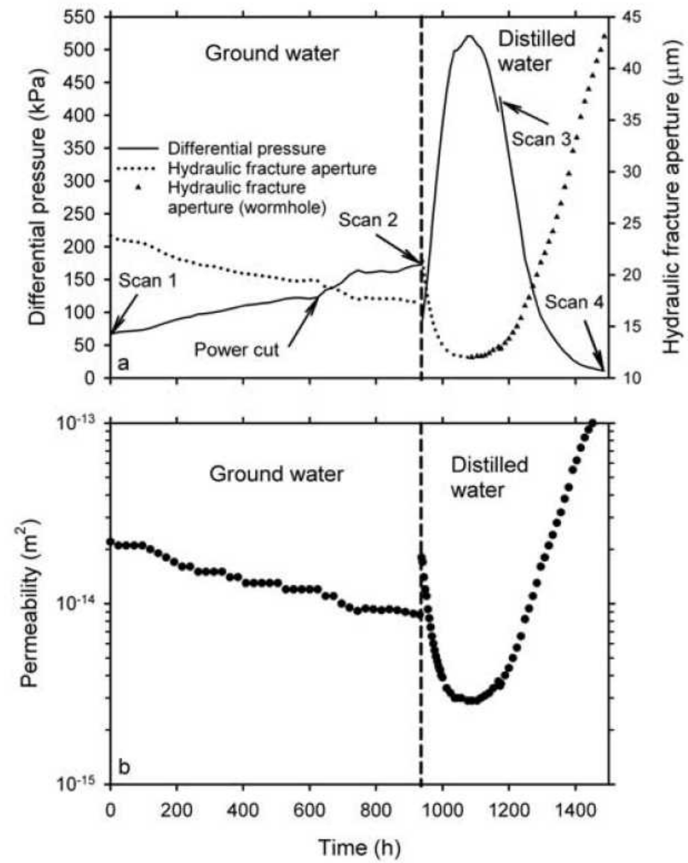


Used
Fuel
Disposition

DECOVALEX Task C1: On fracture opening and closure



Yasuhara et al. (2006)

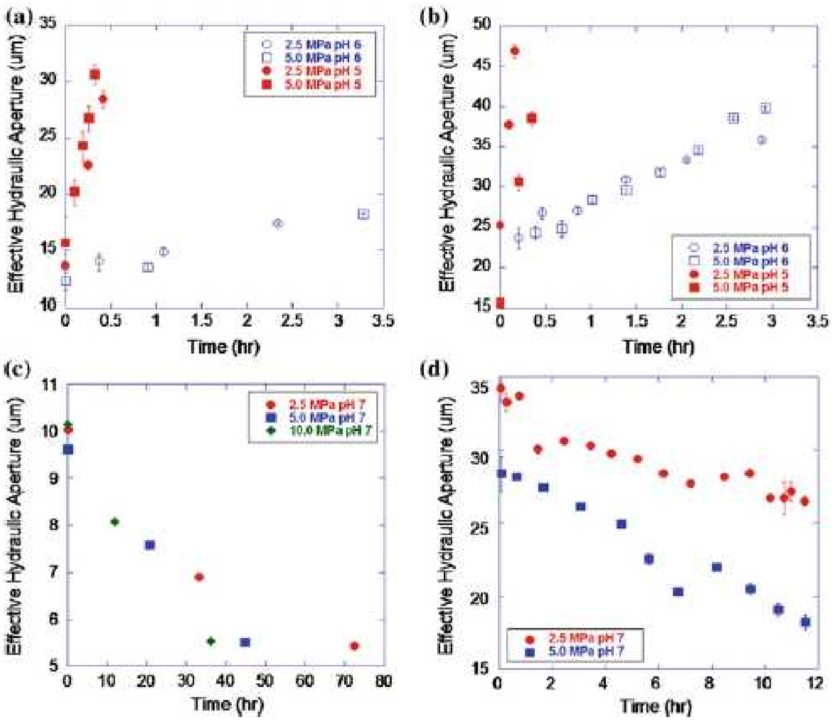


Polak et al. (2004)

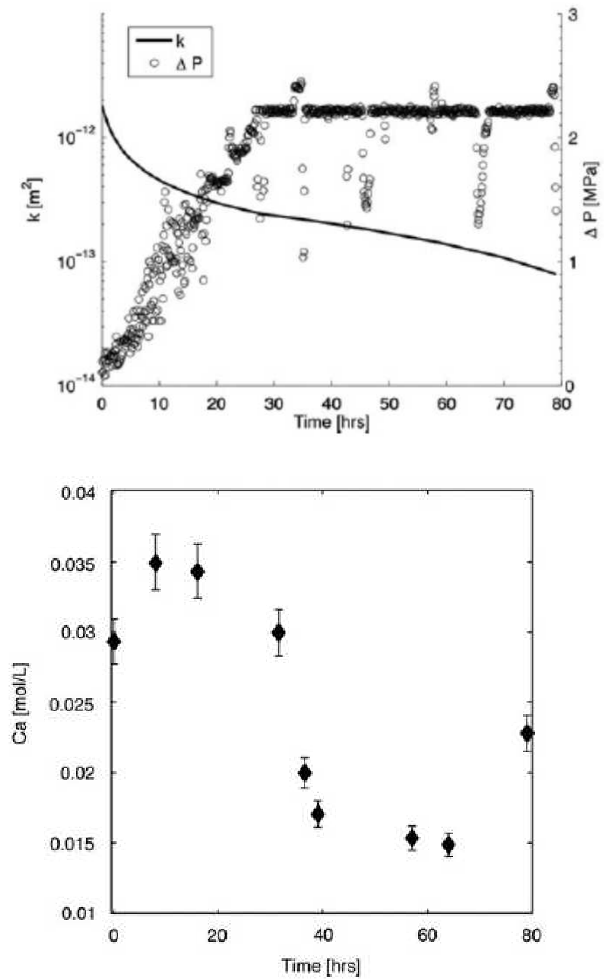
Sandia National Laboratories

Used
Fuel
Disposition

Fracture opening and closure



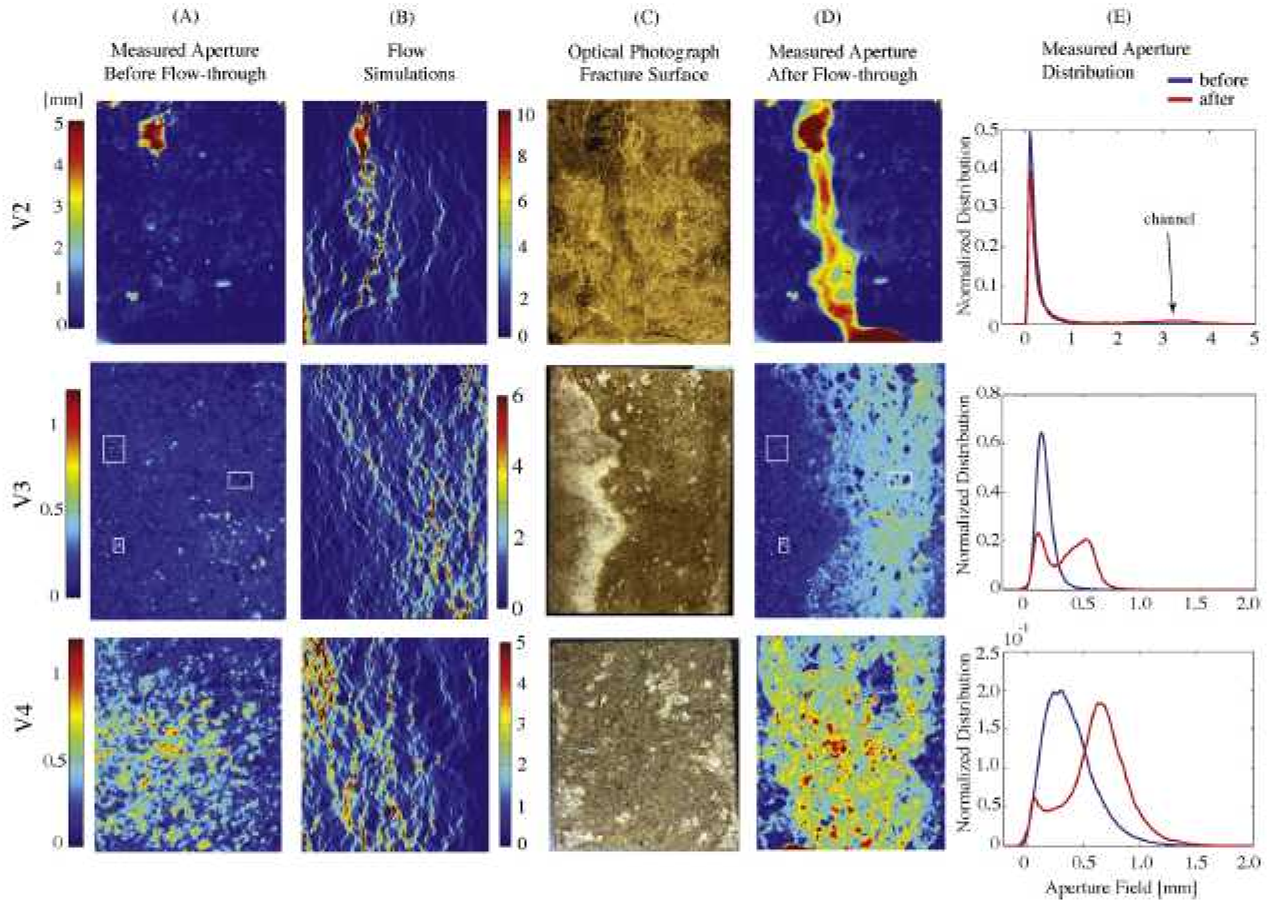
McGuire et al. (2013)



Ellis et al. (2013)

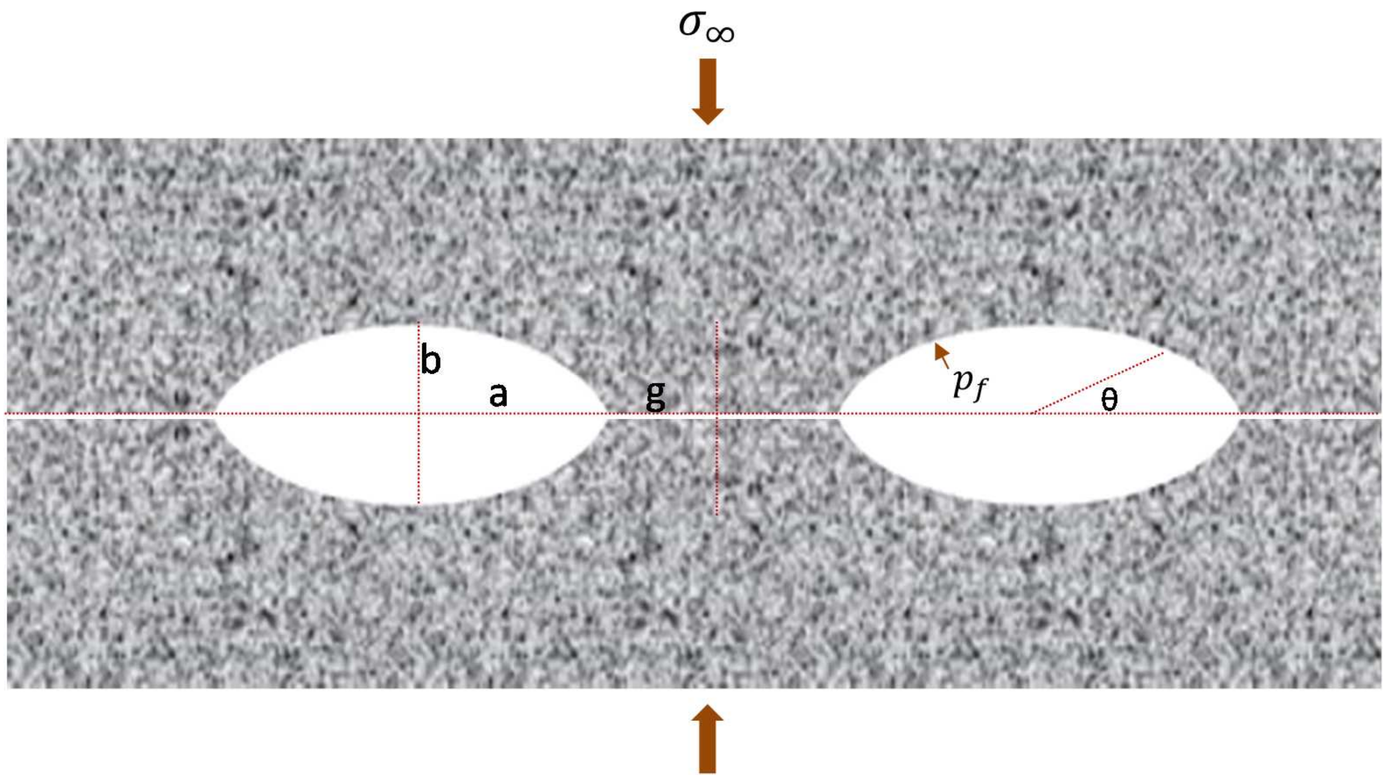
Used
Fuel
Disposition

Fluid flow channeling



Elkhoury et al. (2013)

Geometrical Representation of Fracture



Used
Fuel
Disposition

Local Stress

At a fracture contact:

$$\sigma_\infty = p_f(1 - f_c) + \sigma_c^n f_c$$

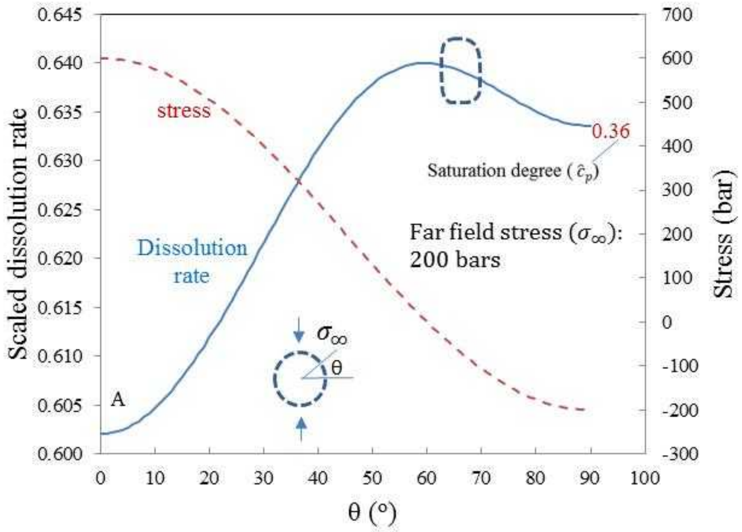
$$\sigma_c^t = p_f$$

On an aperture channel surface:

$$\sigma_p^n = p_f$$

$$\sigma_p^t(\theta) = p_f - \frac{(1-m^2)(-\sigma_\infty+2p_f)+2\sigma_\infty(m-cos2\theta)}{1+m^2-2mcos2\theta}$$

where $m = (a-b)/(a+b)$



Chemical potential

Chemical potential at a fracture channel surface:

$$\mu_s(\theta) = \mu_s^0 + \frac{1}{2}[\sigma_p^n(\theta) + \sigma_p^t(\theta)]v_s + \Delta G_s(\theta)$$

Chemical potential of a dissolved species:

$$\mu_a = \mu_a^0 + RTlnc_p + p_f v_a$$

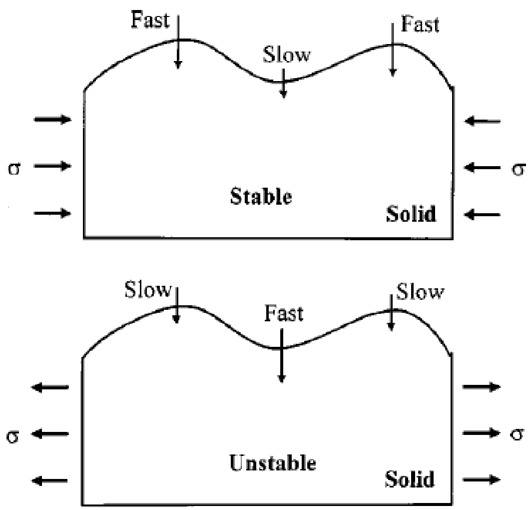
Strain energy at an aperture surface:

$$\Delta G_s(\theta) = \beta v_s[\sigma_p^n(\theta)^2 + \sigma_p^t(\theta)^2]$$

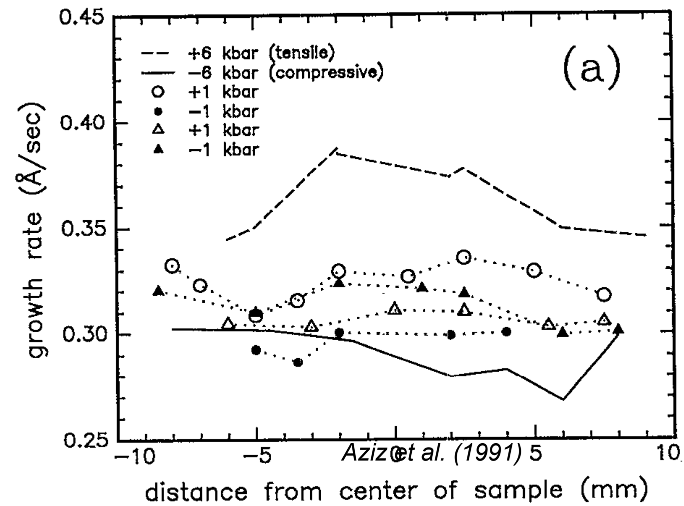
Chemical affinity (A_p) for mineral dissolution at an aperture surface:

$$A_p = \mu_s(\theta) - \mu_a = \mu_s^0 + \left\{\frac{1}{2}\left[\sigma_p^n(\theta) + \sigma_p^t(\theta)\right] + \beta\left[\sigma_p^n(\theta)^2 + \sigma_p^t(\theta)^2\right]\right\} v_s$$
$$+\Delta G_s(\theta) - \mu_a^0 - p_f v_a - RTlnc_p$$

Stress-activated mineral dissolution



Yu and Suo (2000)



Aziz et al. (1991)

Dissolution rate at an aperture surface:

$$R(\theta) = k e^{-\frac{\Delta G^{\#} + \sigma_p^t(\theta) v^{\#}}{RT}} \left(1 - e^{-\frac{A_p}{RT}}\right)$$

$$= k e^{-\frac{\Delta G^{\#} + \sigma_p^t(\theta) v^{\#}}{RT}} \left[1 - \frac{C_p}{K(\theta)}\right]$$

Reaction-diffusion at a fracture contact

Concentration of dissolved species at a fracture contact:

$$c_c = e^{\frac{\mu_s^0 - \mu_a^0 + \frac{1}{2}(\sigma_c^n + \sigma_c^t)v_s - p_f v_a + \Delta G_s(contact)}{RT}}$$

Mineral dissolution rate at a fracture contact :

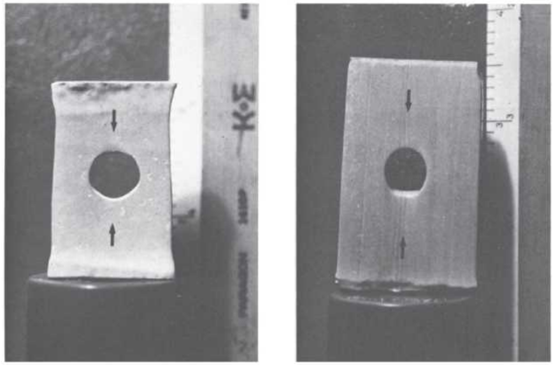
$$R(contact) = \frac{De^{-\frac{\Delta G_D^{\ddagger}}{RT}} w(c_c - c_p)}{2g^2}$$

Water film thickness:

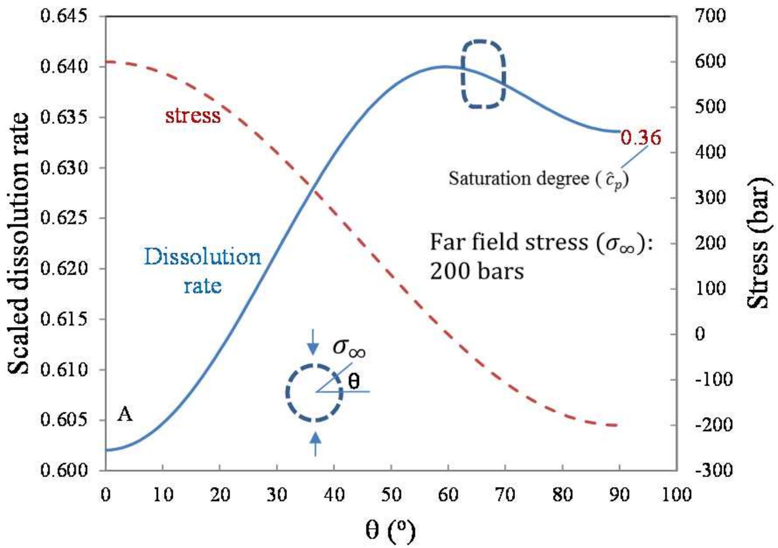
$$w = \lambda(\sigma_c^n - p_f)^{-\gamma}$$

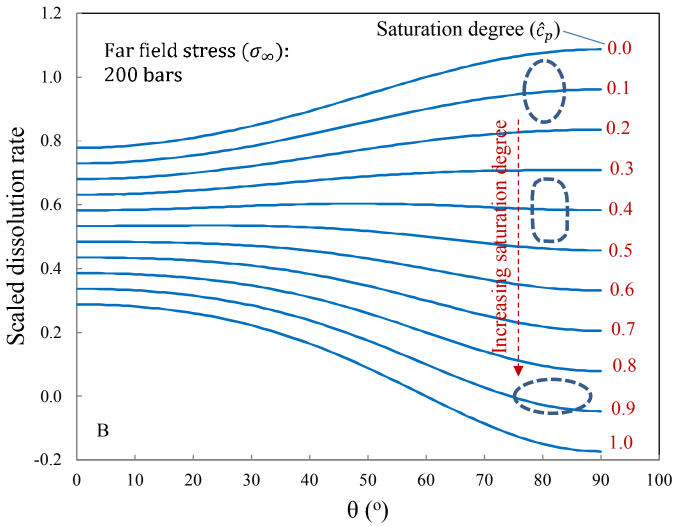
Shape evolution of a circular channel

$$r(\theta) = e^{-\frac{\sigma_p^t(\theta) v^{\#}}{RT}} \left\{ 1 - \frac{\hat{c}_p}{e^{\frac{\left[0.5\sigma_p^t(\theta) + \beta \sigma_p^t(\theta)^2\right] v_S}{RT}}} \right\}$$



Sprunt and Nur (1977)

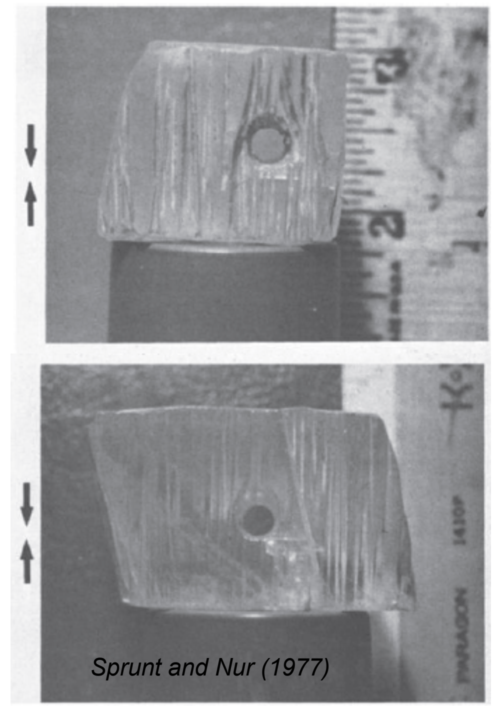




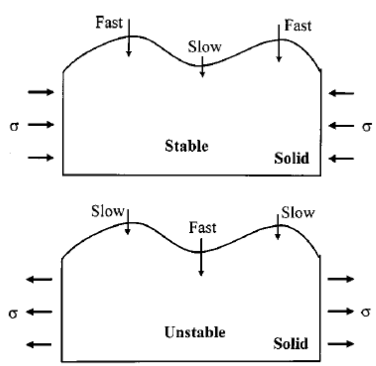
Shape evolution of a circular channel

Material & solution	Axial load (bars)	Hole shape
	In salt solution	
Salt undersaturated 1	30	Flattened circle
Salt undersaturated 2	12	Flattened circle
Salt undersaturated 3	13	Flattened circle
Salt saturated 1	15	Ellipse perpendicular
Salt saturated 2	14	Ellipse perpendicular
	In dilute hydrochloric acid	
Solenhofen limestone 3	129	Ellipse parallel
Solenhofen limestone 4	66	Ellipse parallel
Solenhofen limestone 6	45	Ellipse perpendicular
Oak Hall limestone 1	297	Ellipse perpendicular
Oak Hall limestone 3	324	Ellipse perpendicular
Oak Hall limestone 4	170	Ellipse perpendicular
Oak Hall limestone 5	262	Ellipse perpendicular
Kasota limestone	59	Ellipse perpendicular
Marble 1	220	Flattened circle
Marble 2	187	Flattened circle
Marble 3	91	Flattened circle
Water lime 1	48	Irregular
Water lime 1	42	Irregular
Water lime 1	29	Irregular
Chalk 1, Kansas	39	Irregular
Chalk 2, Kansas	24	Irregular

Sprunt and Nur (1977)



Sprunt and Nur (1977)



Yu and Suo (2000)

Conclusions:

- *Existing model assumption: Mineral dissolution on the free surface of a cavity embedded in a stress rock depends only on the normal stress exerted by a hydrostatic pore fluid pressure.*
- *The tangential stress and the stress-activation mechanism must be taken into account.*

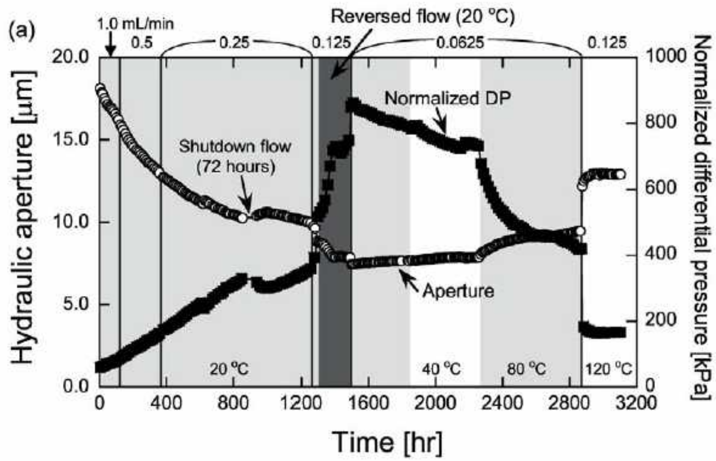
Criteria for channel opening and closure

$$\omega = R\left(\frac{\pi}{2}\right)/R(contact)\begin{cases} >1 & \text{channel opening} \\ <1 & \text{channel closure} \end{cases}$$

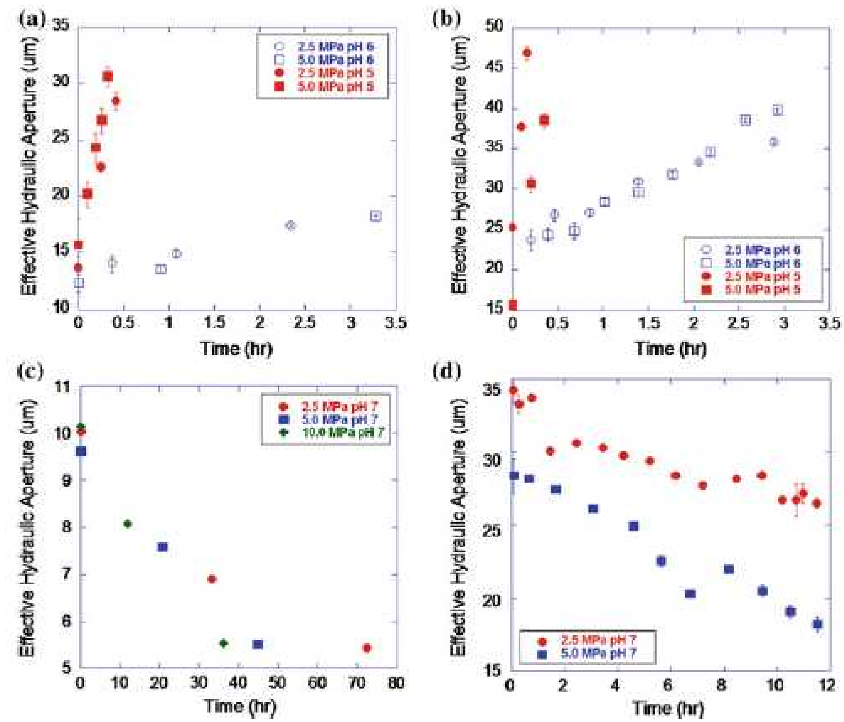
$$\omega \approx \frac{2g^2 k\sigma_\infty^\gamma}{\lambda K_{eq} D f_c^\gamma} \cdot \frac{\left(1-\hat{c}_p e^{\frac{\sigma_\infty v_s}{2RT}}\right)}{\left(1-\hat{c}_p e^{-\frac{\sigma_\infty v_s}{2 f_c RT}}\right)} \cdot e^{-\frac{\Delta G^{\#}-\Delta G_D^{\#}+\sigma_\infty(0.5 v_s/f_c - v^{\#})-\Delta H_r}{RT}}$$

Necessary condition for fracture opening:

$$\frac{2g^2 k\sigma_\infty^\gamma}{\lambda K_{eq} D f_c^\gamma} > 1$$

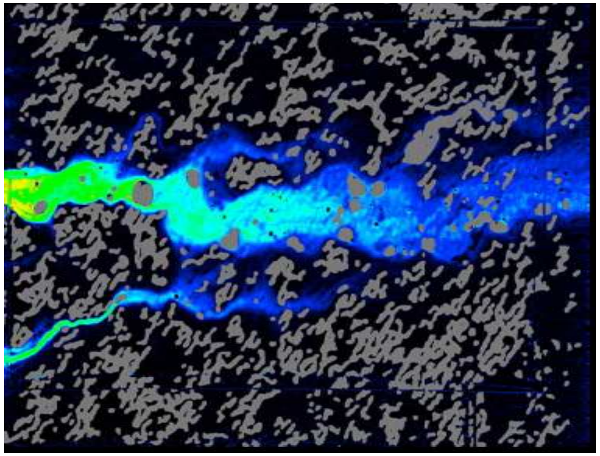


Yasuhara et al. (2006)

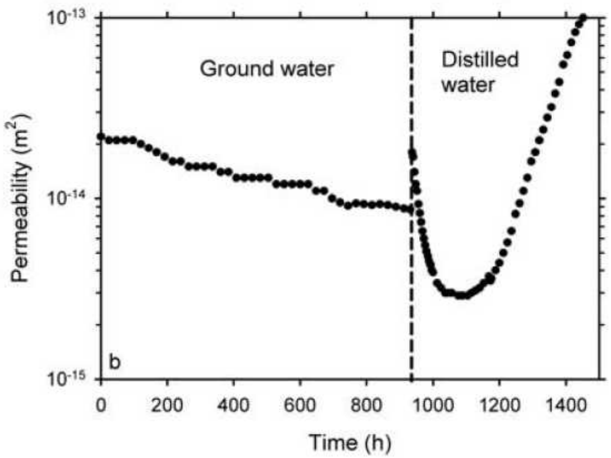


McGuire et al. (2013)

Infiltration instability and preferential channeling



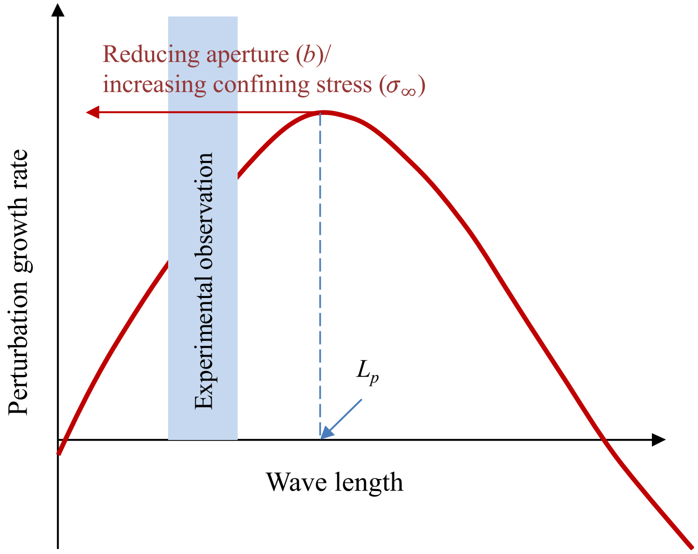
Dewiler (2010)



Polak et al. (2004)

Spacing of channels:

$$L_p \propto \frac{b^3}{k} e^{\frac{\Delta G^{\#} - \sigma_\infty v^{\#}}{RT}}$$



- *Spontaneous switching*
- *Appropriate scale for studying preferential channeling*