SAND2018-5475PE

Spent Fuel Waste Science & Technology

DR Crystalline Disposal R&D: An Overview

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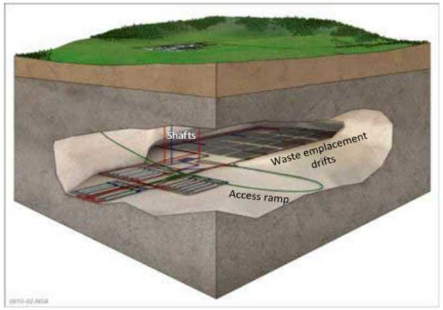
Crystalline Disposal R&D Work Packages

- **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 components of deep geologic repository in crystalline rocks: EBS & fractured NS**
  - Better characterization and understanding of fractured media and fluid flow and transport in such media
  - Designing effective engineered barrier systems for waste isolation
  - Assisting GDSA to develop a TSPA model for a reference case
- **Fully leverage international collaborations**
  - Korean Atomic Energy Research Institute
  - Äspö Hard Rock Laboratory (Sweden)
  - DECOVALEX (UK, France, Canada, Japan, etc.)
  - Colloid Formation & Migration Project (Switzerland)
  - Crystalline club
  - Others

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



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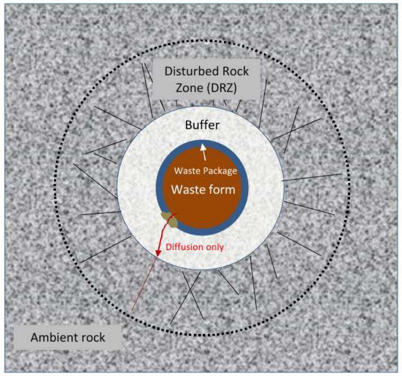
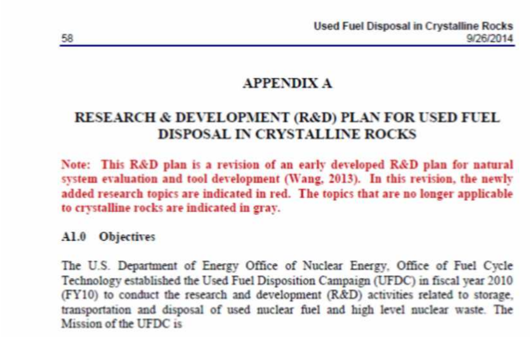




58 Used Fuel Disposal in Crystalline Rocks
9/26/2014

APPENDIX A

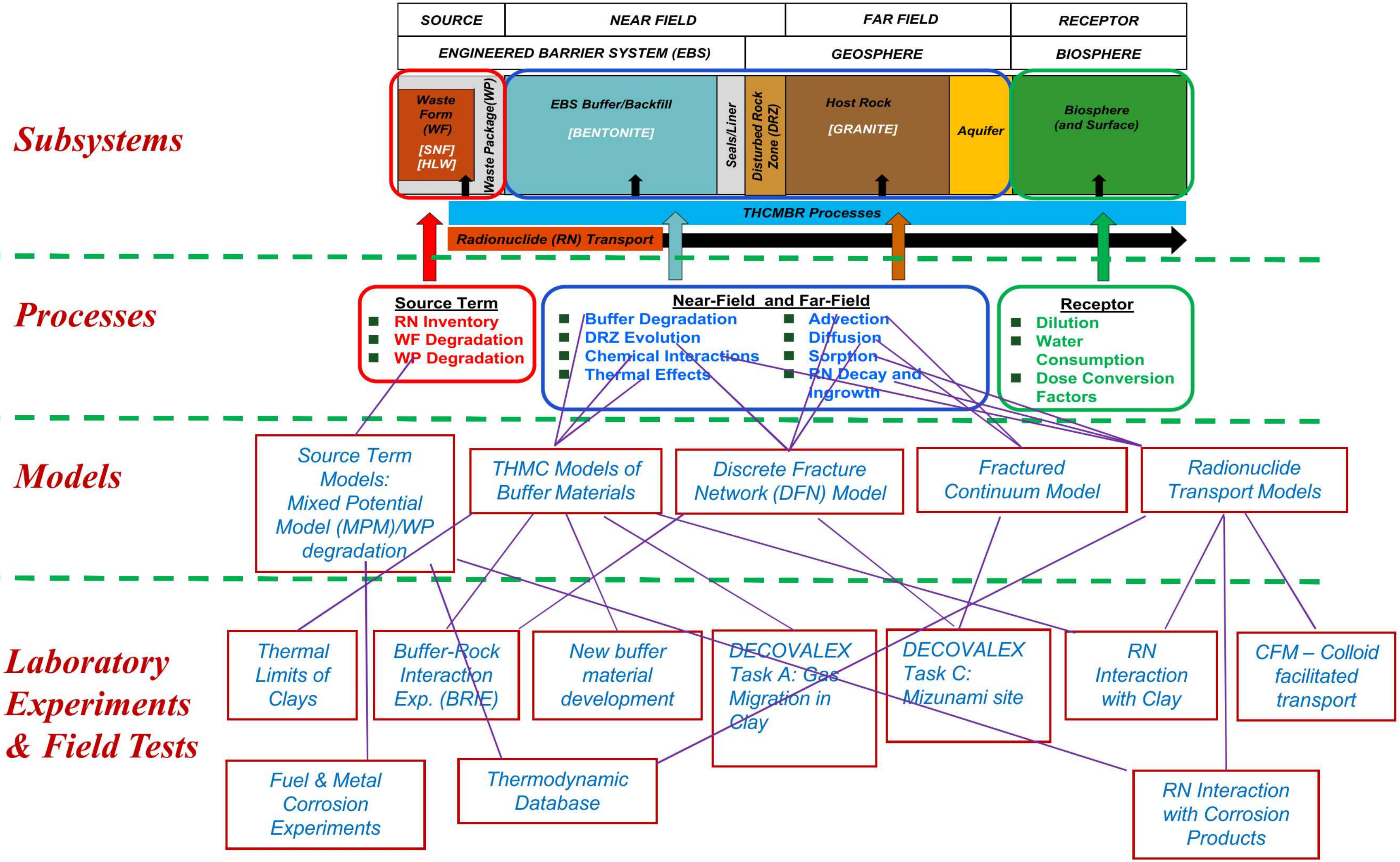
RESEARCH & DEVELOPMENT (R&D) PLAN FOR USED FUEL DISPOSAL IN CRYSTALLINE ROCKS

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 The topics that are no longer applicable to crystalline rocks are indicated in gray.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

Experimental & modeling activities for used fuel disposition in crystalline rocks



Subsystems

SOURCE	NEAR FIELD	FAR FIELD	RECEPTOR
ENGINEERED BARRIER SYSTEM (EBS)		GEOSPHERE	BIOSPHERE

- Waste Form (WF) [SNF] [HLW]
- Waste Package(WP)
- EBS Buffer/Backfill [BENTONITE]
- Seals/Liner
- Disturbed Rock Zone (DRZ)
- Host Rock [GRANITE]
- Aquifer
- Biosphere (and Surface)

THCMBR Processes

Radionuclide (RN) Transport

Processes

Source Term
- RN Inventory
- WF Degradation
- WP Degradation

Near-Field and Far-Field
- Buffer Degradation
- DRZ Evolution
- Chemical Interactions
- Thermal Effects
- Advection
- Diffusion
- Sorption
- RN Decay and Ingrowth

Receptor
- Dilution
- Water Consumption
- Dose Conversion Factors

Models

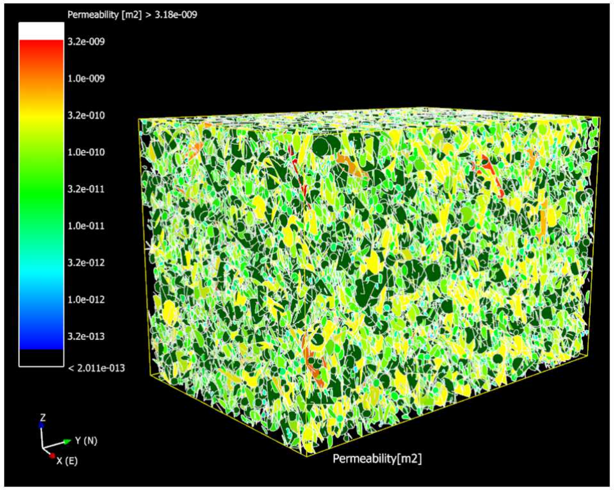
- Source Term Models: Mixed Potential Model (MPM)/WP degradation
- THMC Models of Buffer Materials
- Discrete Fracture Network (DFN) Model
- Fractured Continuum Model
- Radionuclide Transport Models

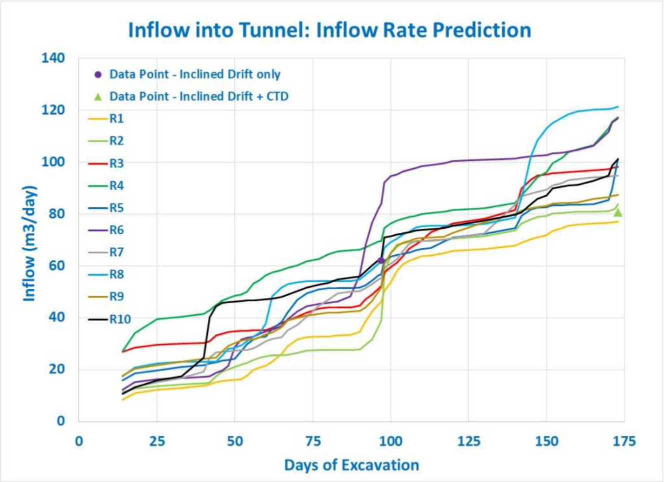
Laboratory Experiments & Field Tests

- Thermal Limits of Clays
- Buffer-Rock Interaction Exp. (BRIE)
- New buffer material development
- DECOVALEX Task A: Gas Migration in Clay
- DECOVALEX Task C: Mizunami site
- RN Interaction with Clay
- CFM – Colloid facilitated transport
- Fuel & Metal Corrosion Experiments
- Thermodynamic Database
- RN Interaction with Corrosion Products

Highlights of accomplishments

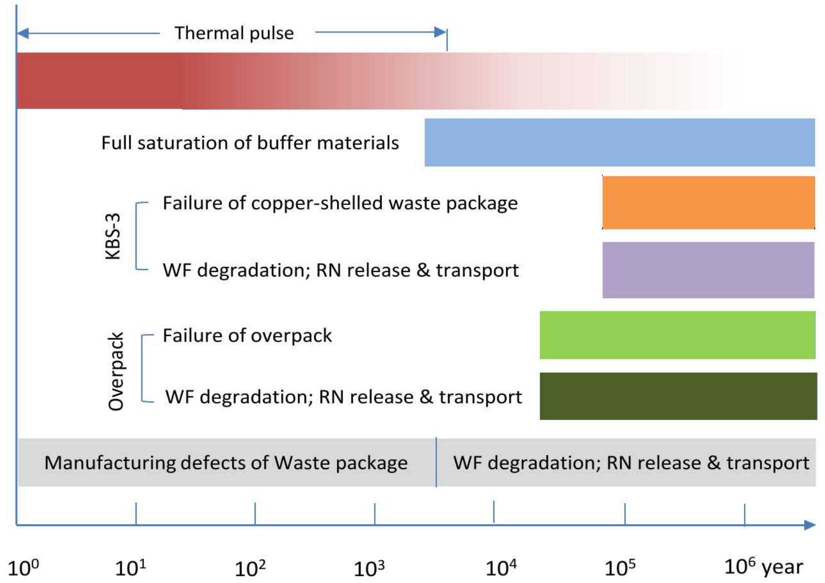
- Developed a reference case for the disposal concept.
- Won R&D 100 award for discrete fracture network (DFN) simulation package.
- Established a general framework for synthesizing field data into a fracture network model.
- Advanced THMC modeling capability for buffer materials.
- Advanced mechanistic understanding of RN interactions with both engineered and natural materials.
- Developed new models for waste form degradation
- Leverage materials science for engineered material development.
- Established strong international collaborations.



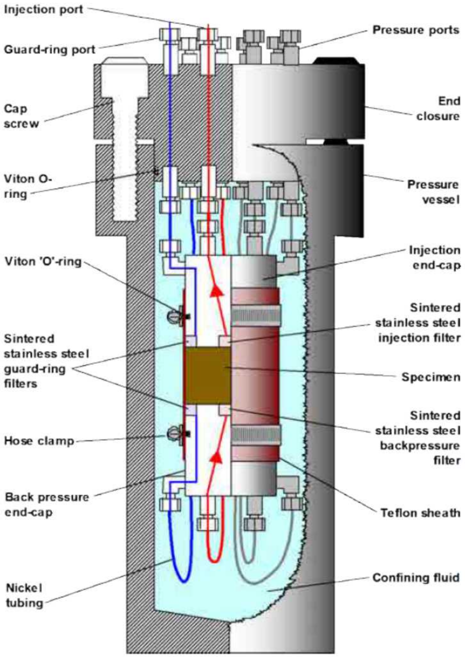


Future work

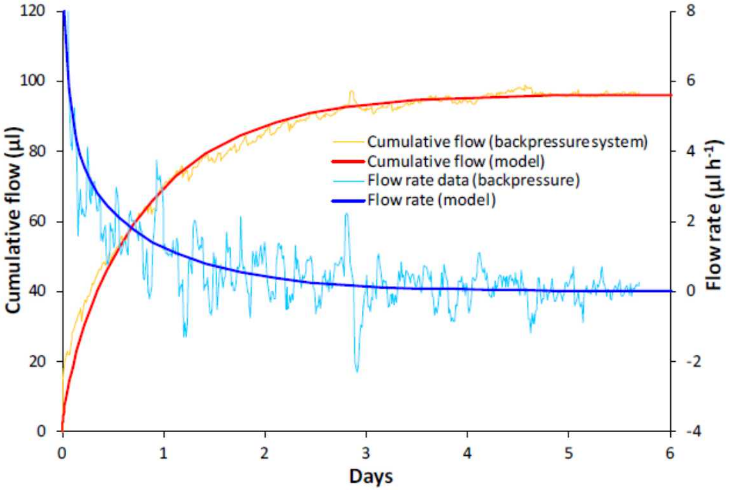
- Develop a sensible GDSA model for sensitivity analyses.
- Move model development more towards model validation with real data.
- Develop reduced order models for incorporation into the GDSA model.
- Continue with buffer material development.
- Develop and refine EBS models, especially WP degradation models.



DECOVALEX Task A: Modeling advective gas flow through low permeability materials



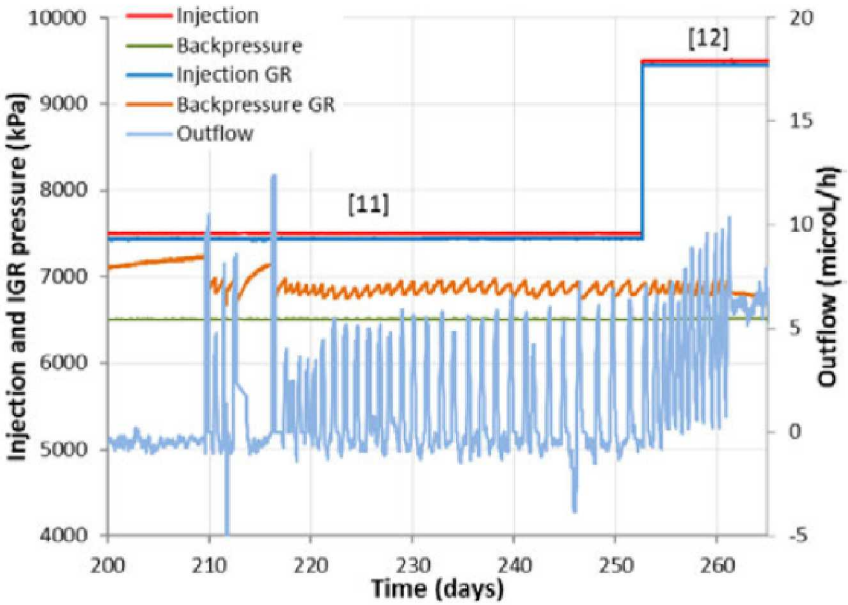
FORGE Report D4.17 (Harrington, 2013)



$$\nabla.\left(\frac{k_i}{\mu_w}\left(\nabla p_w + \rho_w g \nabla z\right)\right) = \phi\beta\frac{\partial p_w}{\partial t} + \frac{\partial}{\partial t}(\nabla.\mathbf{u})$$

$$\frac{E}{2(1+\nu)}\nabla^2\mathbf{u} + \frac{E}{2(1+\nu)(1-2\nu)}\nabla(\nabla\cdot\mathbf{u}) - \nabla p_w = 0$$

Dynamic behaviors of the system



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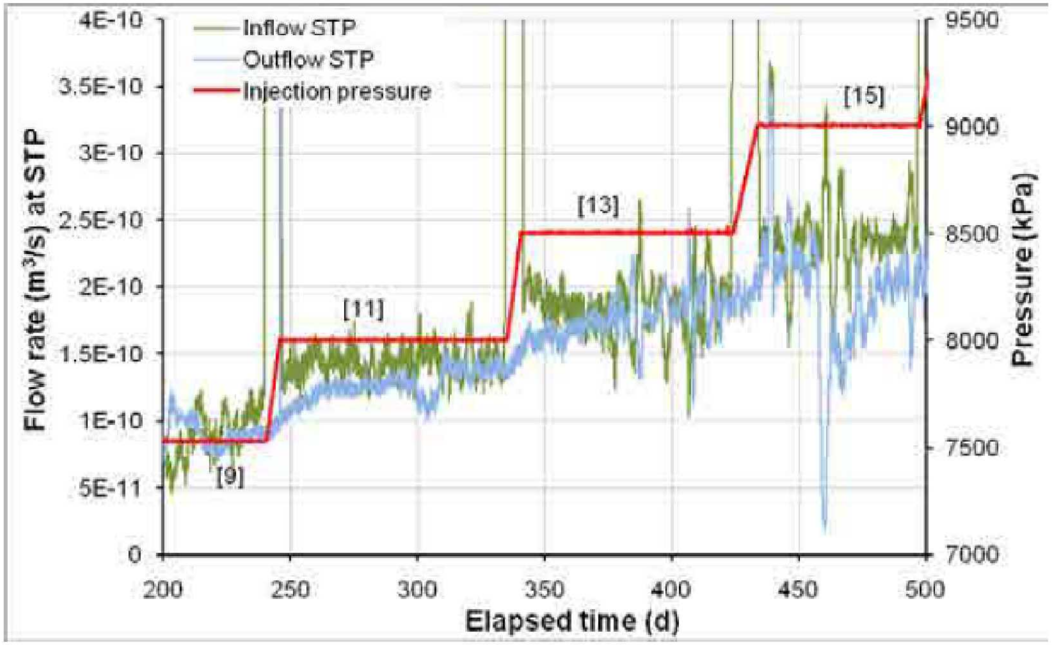
Dynamic behaviors of the system (cont.)



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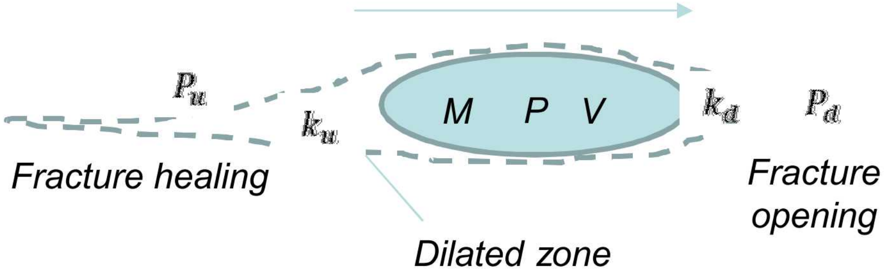
Bubble migration under a pressure gradient



P_u k_u M P V k_d P_d

Fracture healing

Dilated zone

Fracture opening

$$\frac{dM}{dt} = k_u(P_u - P) - k_d(P - P_d)$$

$$k_u = k_u^0 P \qquad k_d = k_d^0 P \qquad M = \frac{PV}{RT}$$

Continuous logistic equation

$$\frac{dP}{dt} = \lambda_1 P\left(1 - \frac{P}{K}\right)$$

$$\lambda_1 = \frac{\left(k_u^0 P_u + k_d^0 P_d\right)RT}{V} \qquad \lambda_2 = \frac{\left(k_u^0 + k_d^0\right)RT}{V} \qquad K = \frac{\lambda_1}{\lambda_2}$$

Delay logistic equation

$$\frac{dP}{dt} = \lambda_1\left(1 - \frac{P}{K}\right)\int_{-\infty}^{t} G(t-s)p(s)ds$$

$$\frac{dP}{dt} = \lambda_1\left(1 - \frac{P}{K}\right)\int_{-\infty}^{t} \alpha e^{-\alpha(t-s)}p(s)ds$$

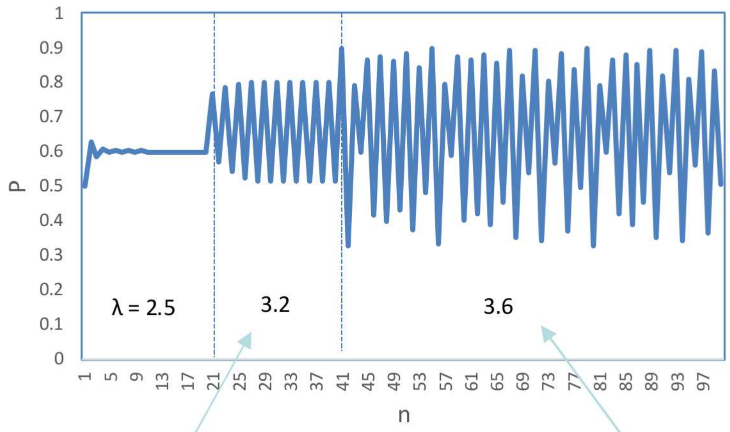
Logistic map: An illustration

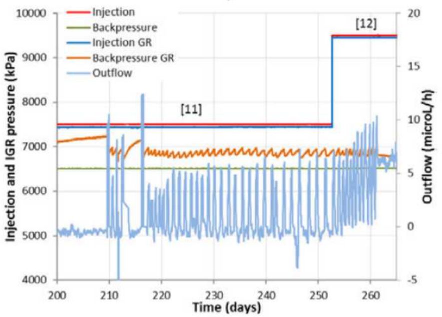
$$\frac{dP}{dt} = \lambda_1 p\left(1 - \frac{P}{K}\right)$$

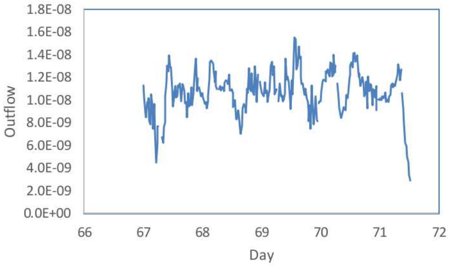
$$P_{n+1} = P_n + \lambda_1 P_n\left(1 - \frac{P}{K}\right)\Delta t$$

$$\lambda = 1 + \lambda_1 \Delta t$$

$$\boxed{p_{n+1} = \lambda p_n(1 - p_n)}$$

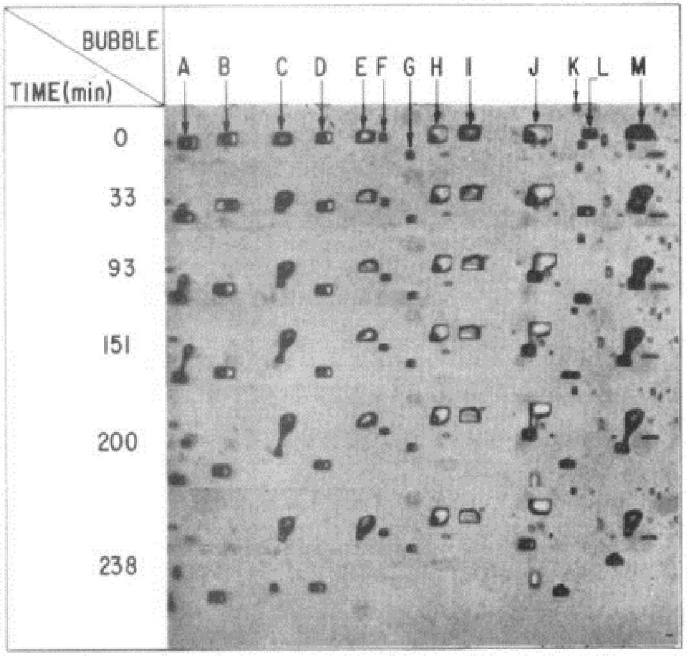


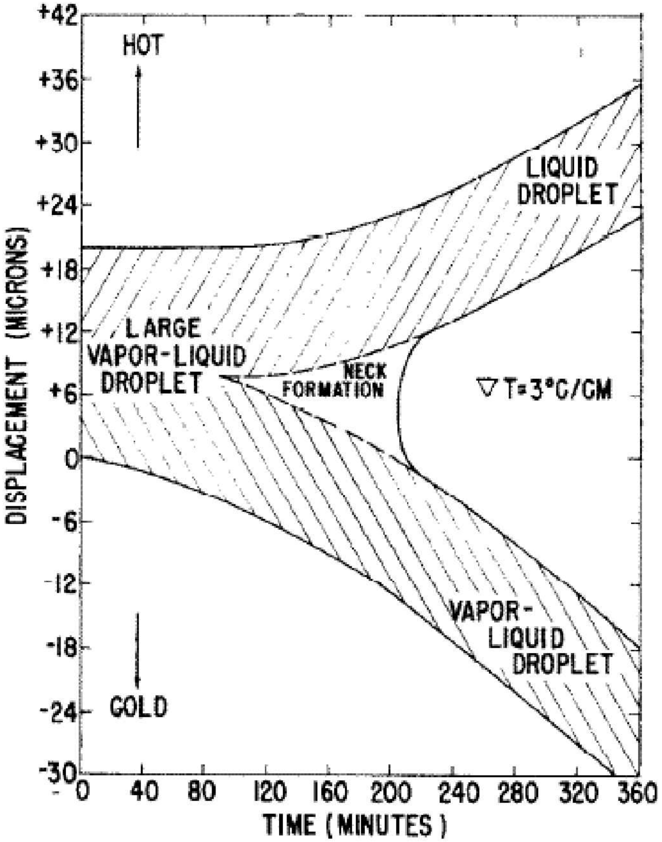




FORGE Report D4.17 (Harrington, 2013)

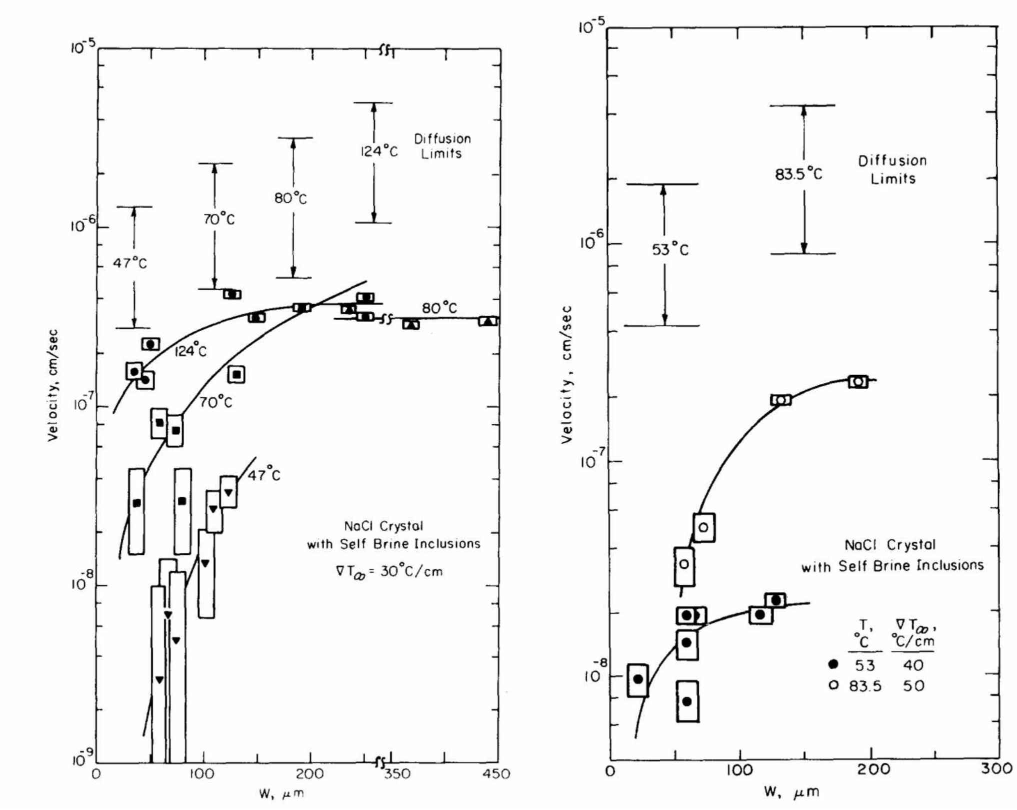
DECOVALEX Task F: Fluid inclusion and movement in tight rock





Anthony & Cline (1972)

Observations: Size dependence



Olander et al. (1982)

Fluid inclusion migration under a thermal gradient

Within Ω:

$$\frac{\partial m}{\partial t} = D\nabla^2 m$$

$$\frac{\partial T}{\partial t} = \alpha$$

On Ω:

NaCl(s) = NaCl(aq)

$$R_d = k(K_d - m)$$

$$K_d(T,\kappa) = K_d^0 e^{\frac{\Delta H_r}{RT}\left(\frac{T}{T_0}-1\right)+\frac{2\gamma V_m \kappa}{RT}}$$

Curvature effect

$$-D\vec{\nabla} m \cdot \vec{n} = R_d$$

Kinematics of Ω:

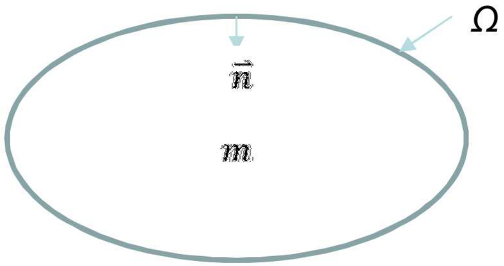
Ω(x, y, z, t) = 0

$$\vec{\nabla}\Omega \cdot \vec{V} + \frac{\partial \Omega}{\partial t} = 0$$

$$\vec{V} + V_0\vec{i} = -V_m R_d \vec{n}$$

$$\vec{n} = -\frac{\vec{\nabla}\Omega}{\|\vec{\nabla}\Omega\|}$$

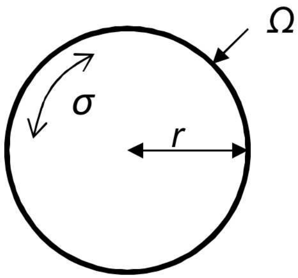
$$\kappa = -\vec{\nabla} \cdot \vec{n}$$



Questions:

- *Steady state shape of a fluid inclusion*
- *Morphological instability*
- *Dependence of inclusion movement on thermal gradient, size, solubility, etc.*
- *Effect on overall fluid movement*

Model analysis

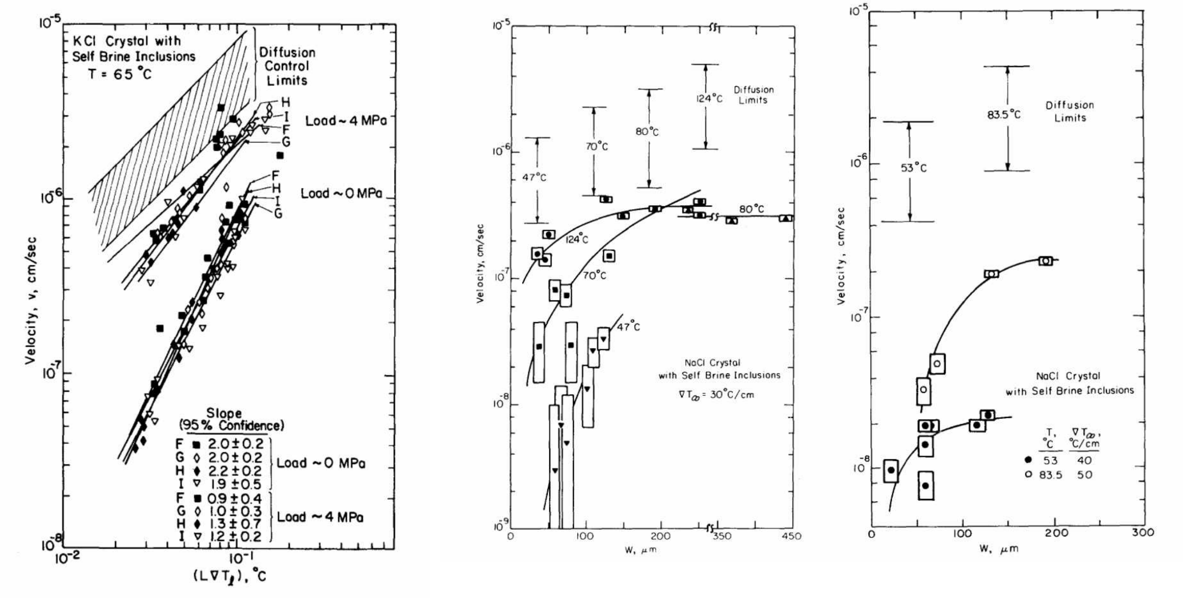


$$V_0 \approx \frac{V_m D K_d^0 \Delta H_r \alpha}{R T_0^2} e^{-\frac{2\gamma V_m}{R T_0 r}}$$

$$K_d^0 \propto e^{\frac{\Delta H_r}{R T_0} + \frac{\beta V_m \sigma^2}{R T_0}}$$

$$D \propto e^{\frac{\Delta \mathrm{E}}{R T_0}}$$

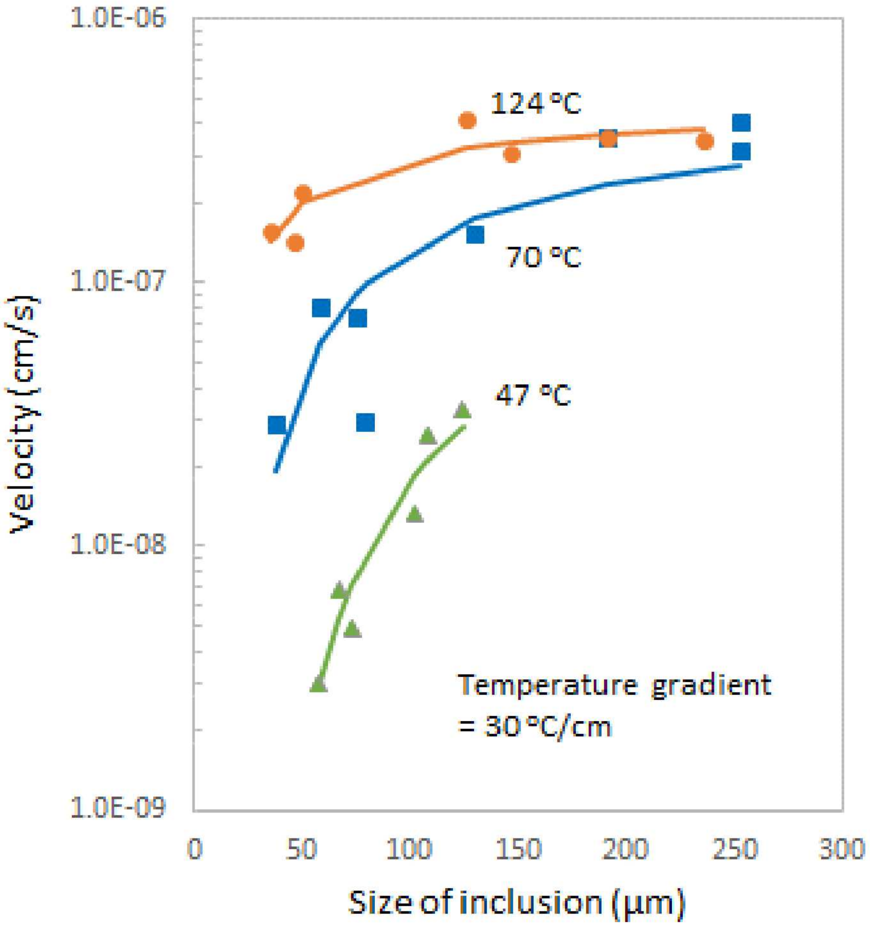
Wang (2017)



Data from Olander et al. (1982)

Model fitting

$$V_0 \approx \frac{V_m D K_d^0 \Delta H_r \alpha}{R T_0^2} e^{-\frac{2\gamma V_m}{R T_0 r}}$$



Data from Olander et al. (1982)

Model fitting (cont.)