SAND2017-4132PE

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PRESENTATION FOR TASKS A, C AND F

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DECOVALEX-2019 3nd Workshop, Stockholm, Sweden

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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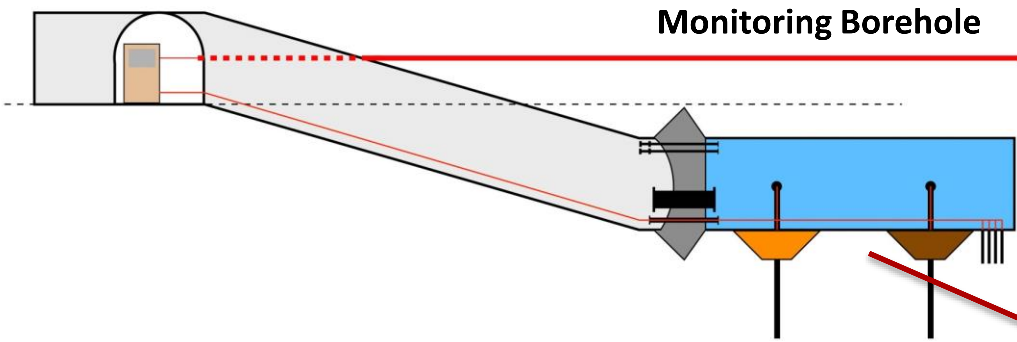
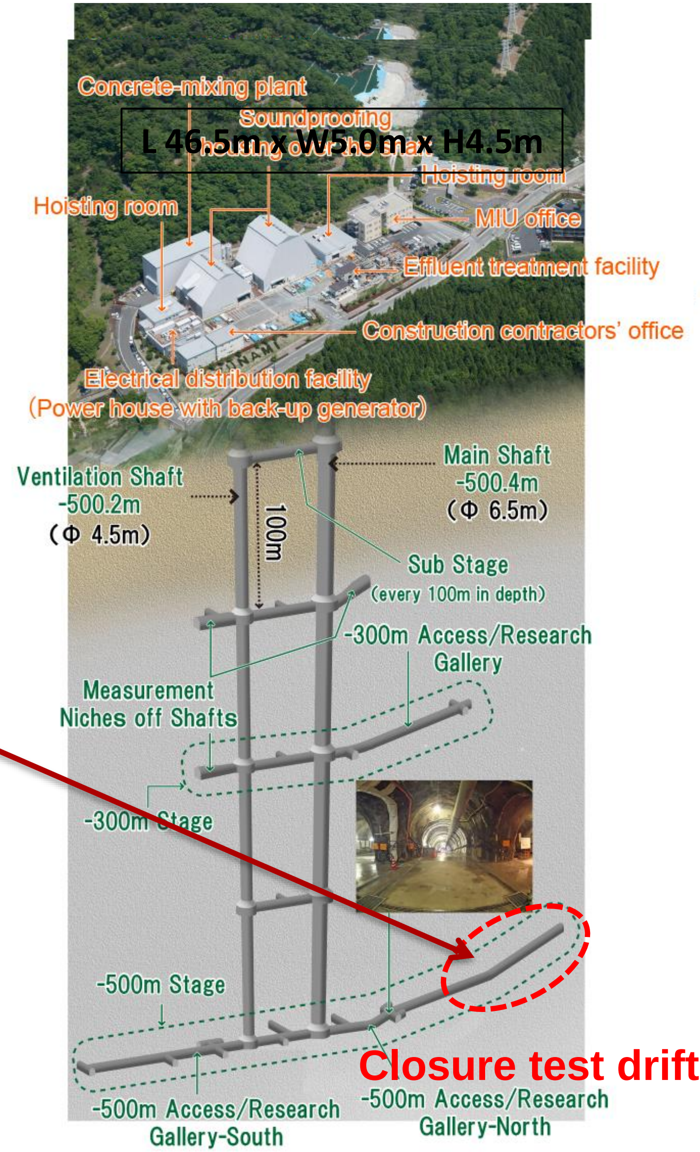
DECOVALEX Task C

<u>GREET(Groundwater REcovery Experiment in Tunnel)</u> : Preliminary test (drift closure and water-filling) to estimate the recovery process in granitic rock

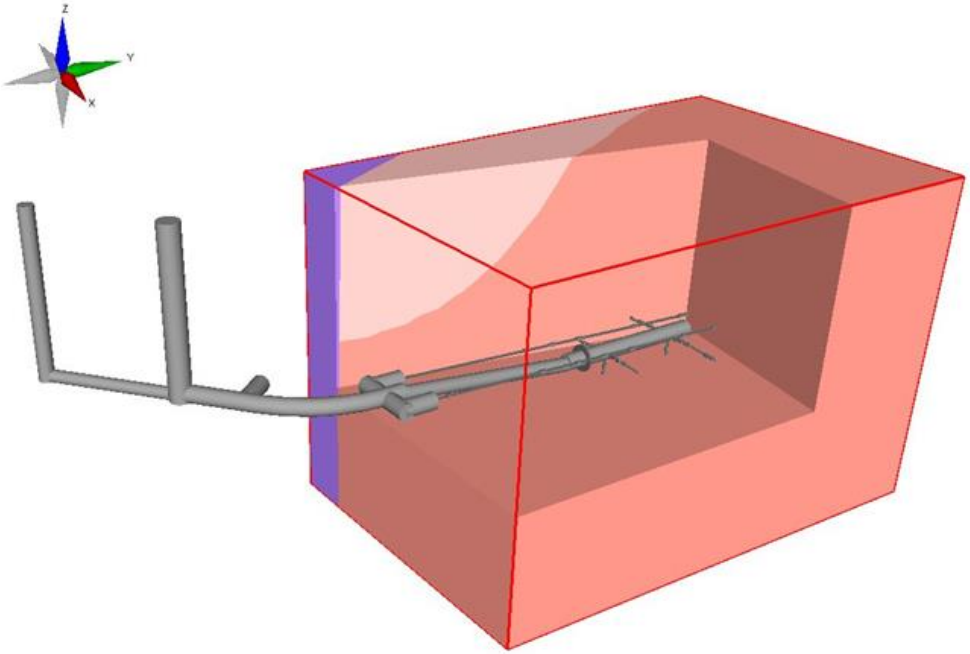


L 46.5m x W5.0m x H4.5m

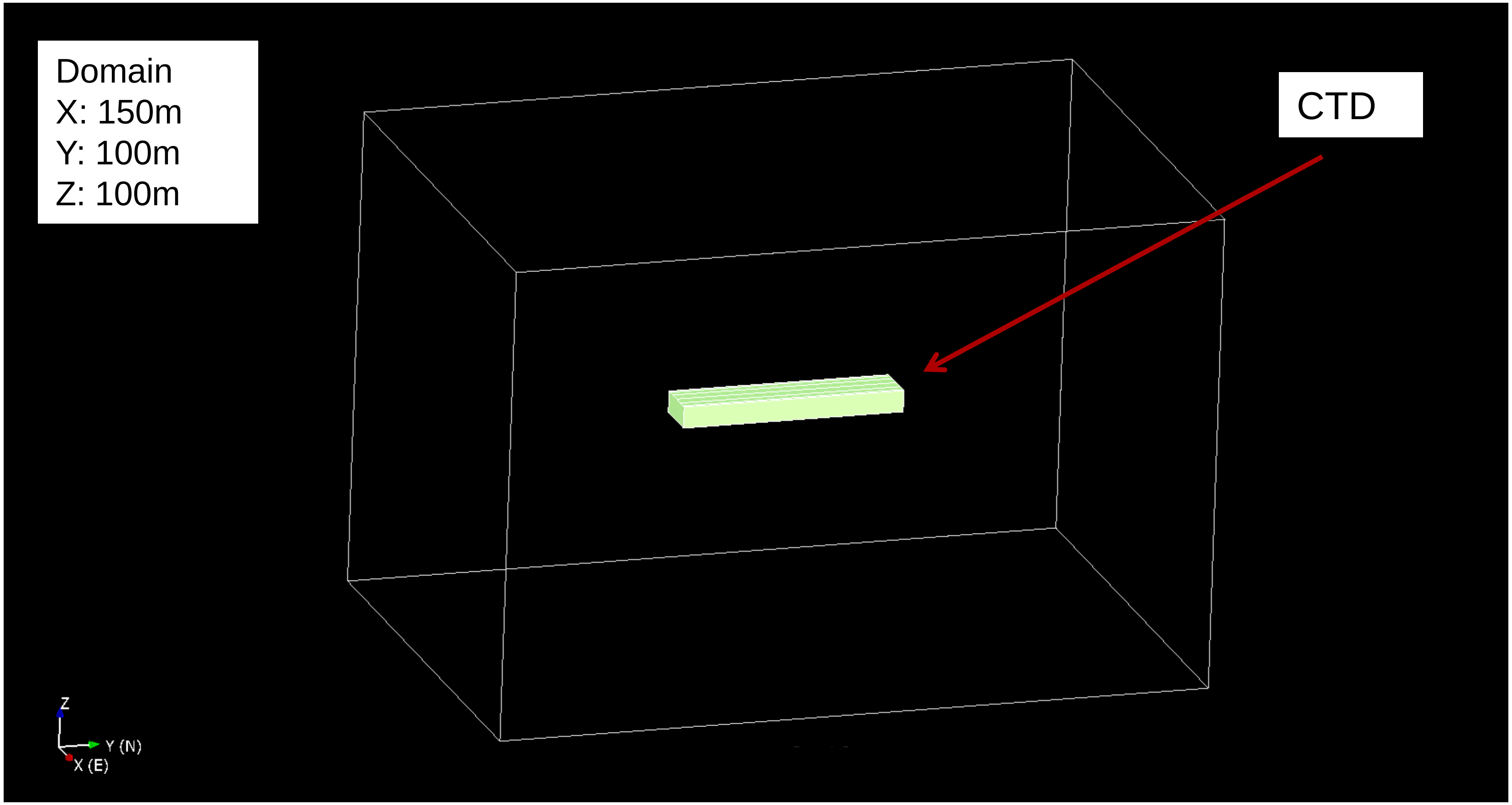


Sandia Tasks

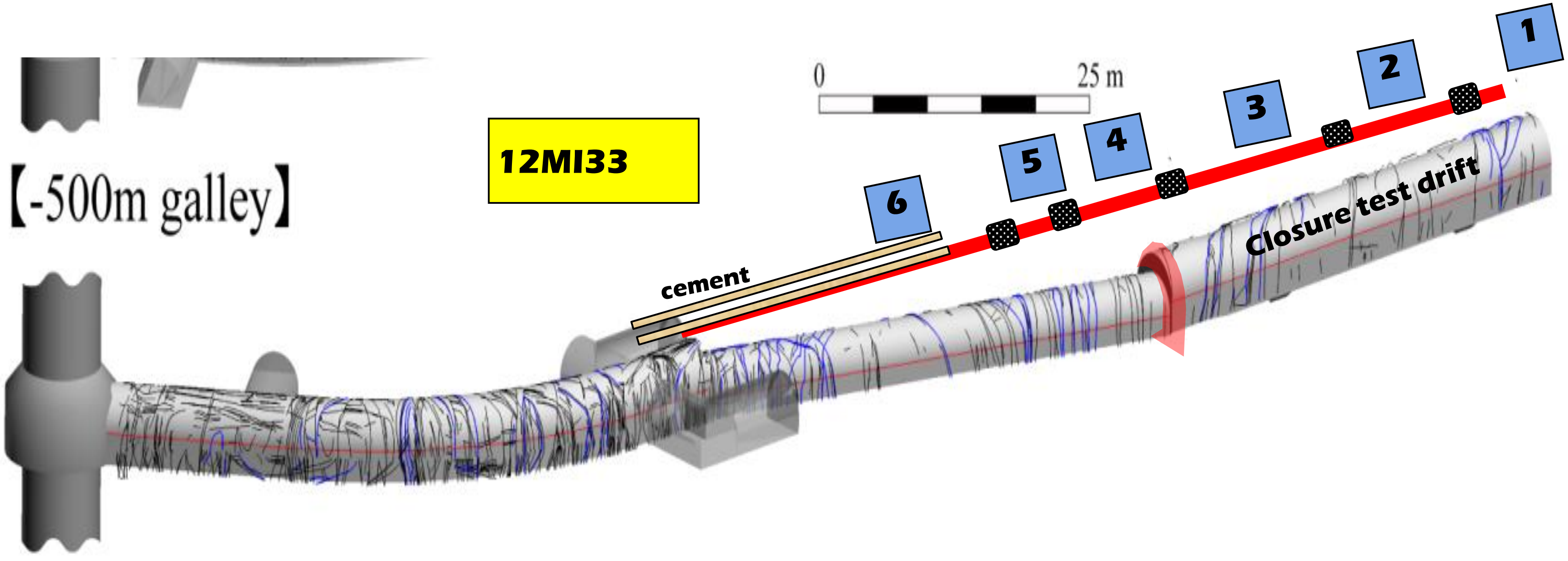
- ➢ Fracture models using field data.
- ➢ Inflow rate



Modeling Domain

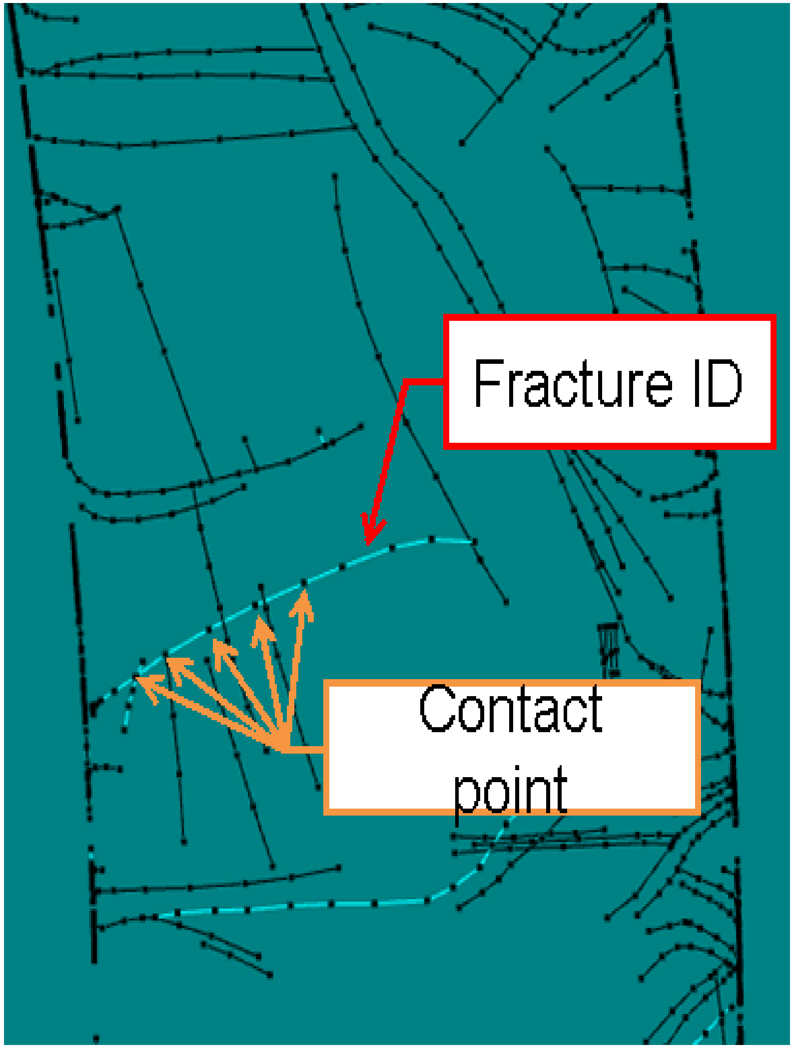


Available Fracture Data



- Trace data for Access Drift, Inclined Drift, and Closure Test Drift (CTD)
- 2,023 fractures
- Type of fata: trace length, dip, strike, alteration, and flow range
- Aperture: not measured

Trace Data Description



[Trace length column]
This column shows three-dimensional trace length. The value were calculated by sum of distance of all contact point.

[Inflow column]
N: no inflow
W: Wet (< approximately 0.1 l/min)
D: Drop (> approximately 0.1 l/min)
F: Flow (> approximately 1.0 l/min)
n.d.: No data. But no inflow was identified.

[Alteration column]
non-alt: The fracture without the alteration halo
alt: The fracture with alteration halo

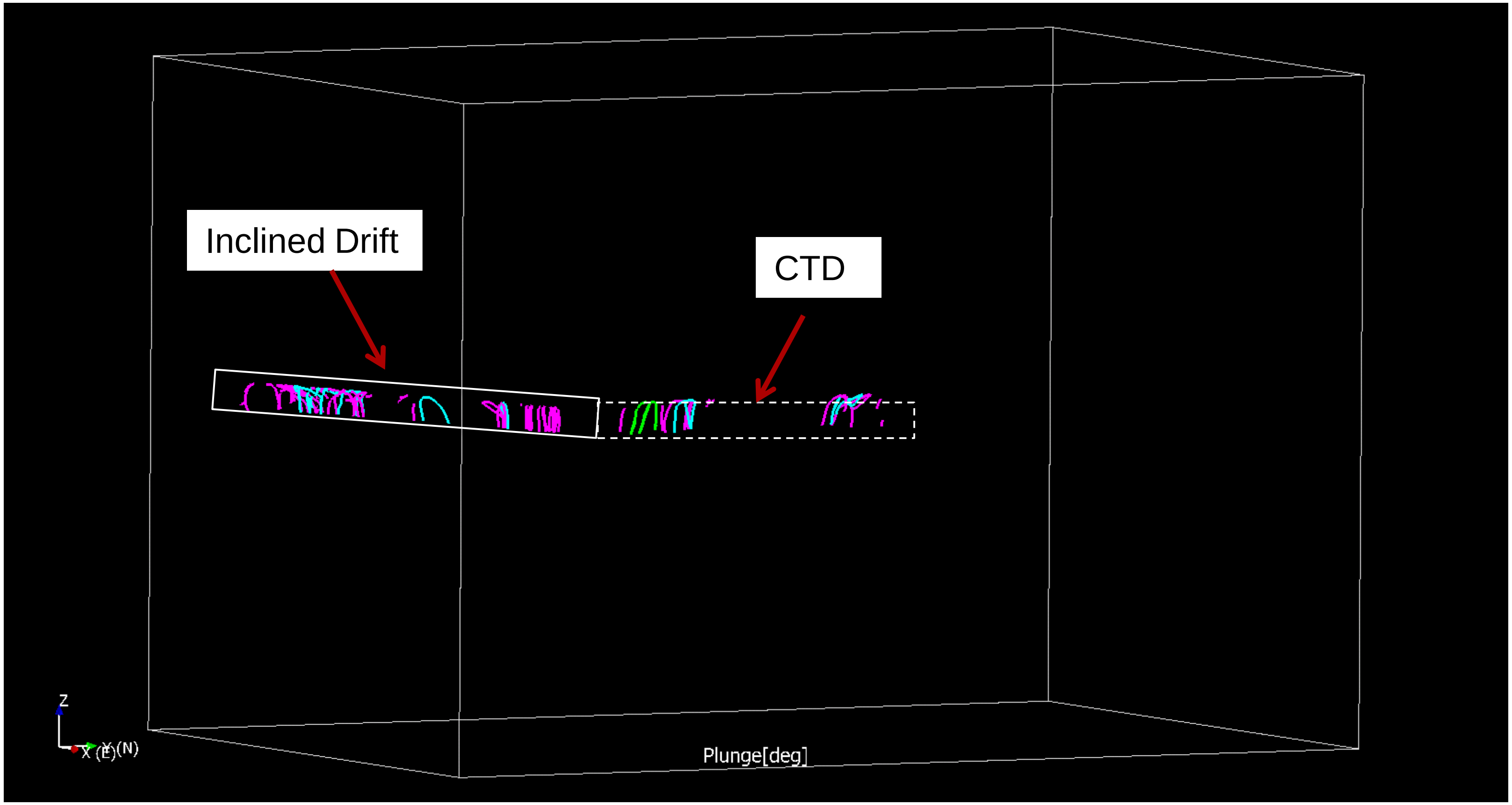
[Fracture fillings column]
carb: Carbonate such as calcite
chl: Chlorite and/or sericite
cly : Unconsolidated clayey fillings including smectite

Importing Trace Data into Model

- The model includes Inclined Drift and CTD.
- The Access Drift is outside of the modeling domain.
- Fractures included in the model are fractures with observed flow (F, D, and W).

- CTD (total number of fractures 233):
  - 4 Flow fractures (F), q>1.0 l/min
  - 15 Drop fractures (D), q>0.2 l/min
  - 3 Wet fractures (W), q<0.1 l/min
- Inclined Drift (total number of fractures 477)
  - 14 Flow fractures (F), q>1.0 l/min
  - 42 Drop fractures (D), q>0.2 l/min

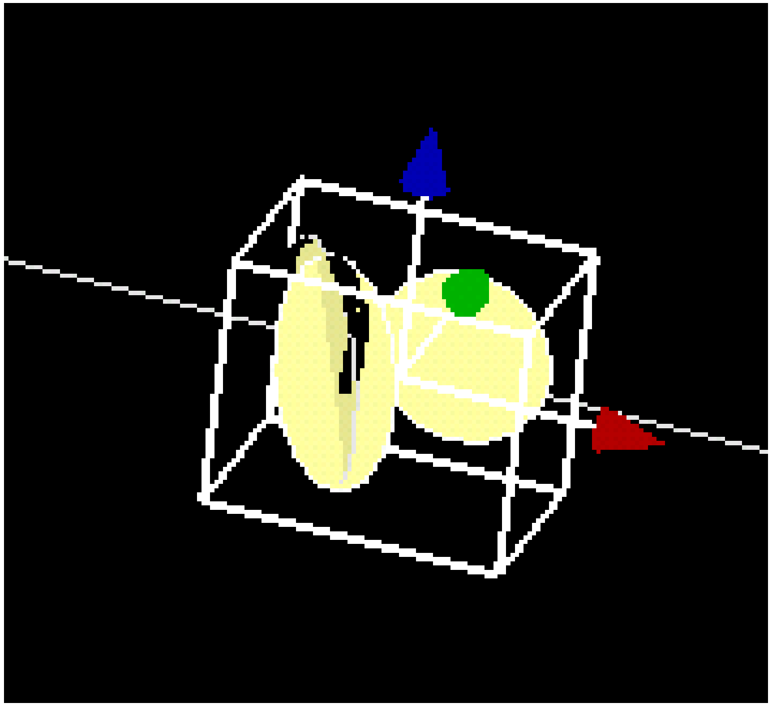
Trace Data Included in the Model



- Blue - Flow fractures
- Purple - Drop fractures
- Green - Wet fractures

Generating Fractures from the Trace Data

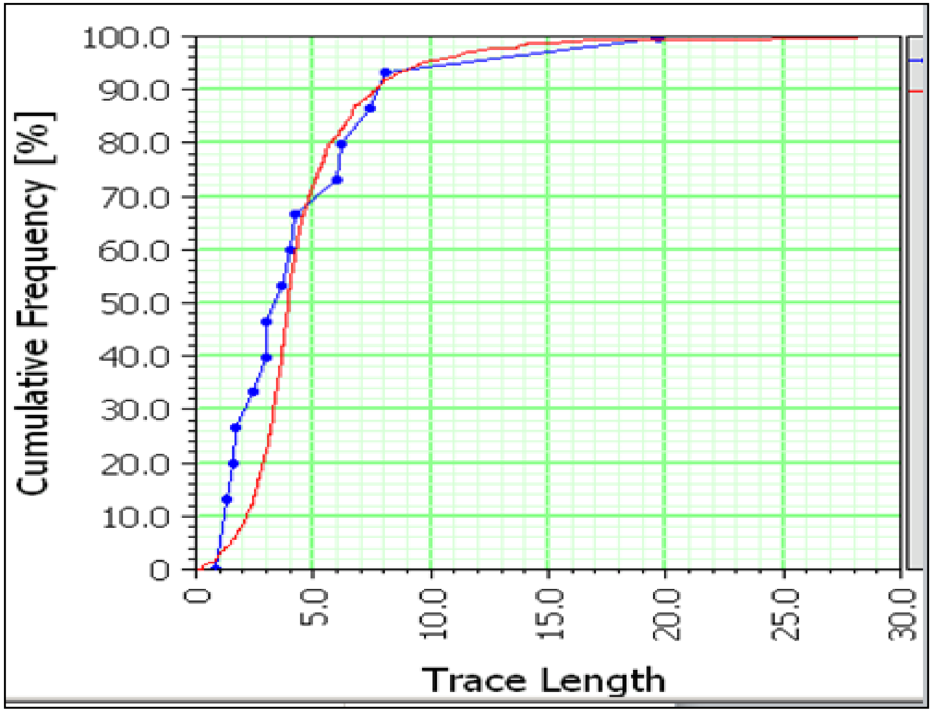
- The dip direction and dip angle of the fracture are derived from the plane containing the fracture traces.
- The trace length is approximated by the power law distribution.
- The parameters of the power law distribution (min radius and α) are used to define the fracture size.



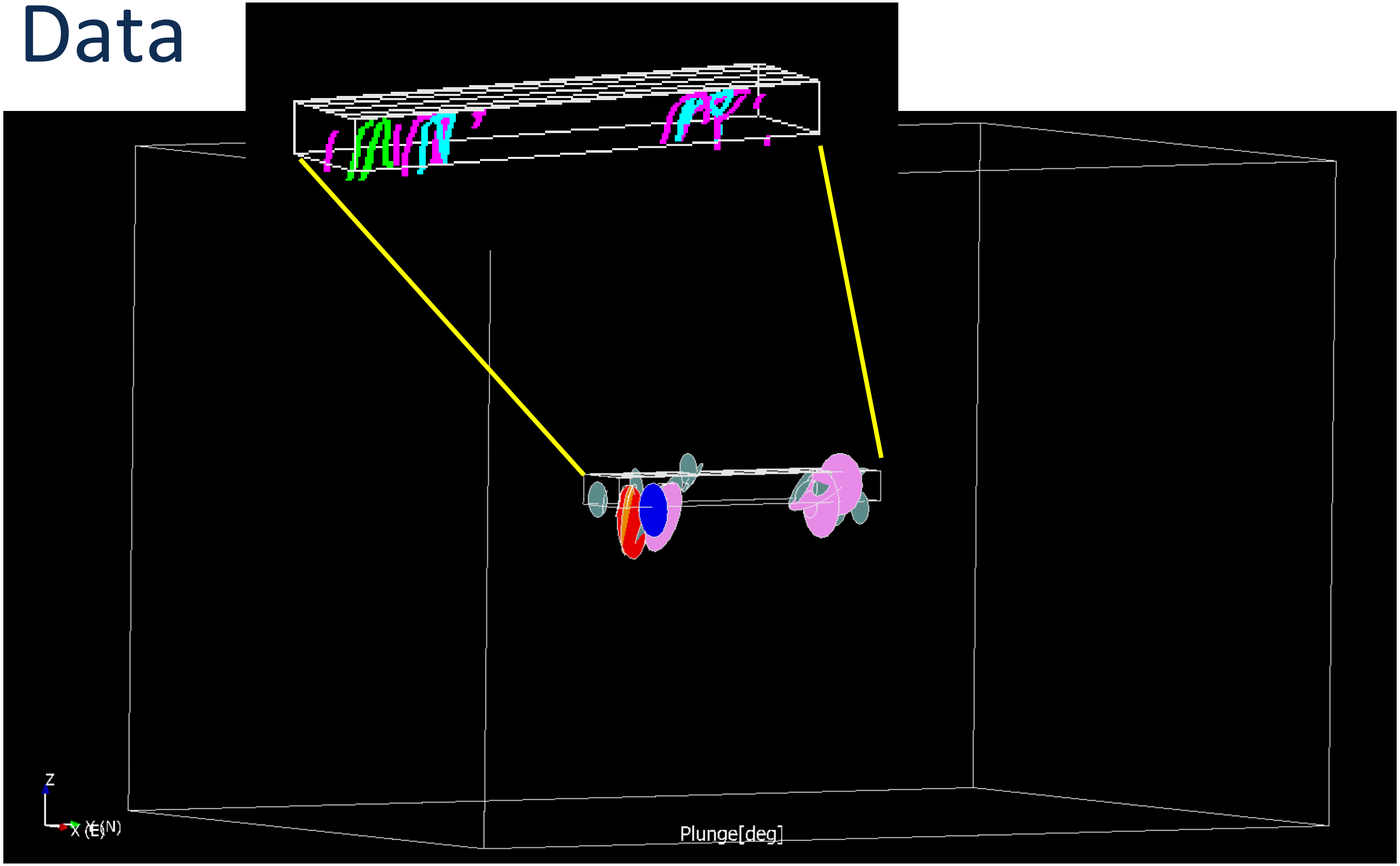
Power Law Distribution Parameters

Parameters	CTD D	CTD F	CTD W	Inclined F	Inclined D
Minimum Radius (m)	1.92	4.22	4.0	2.94	1.97
α	3.48	3.76	3.43	3.98	3.45
Significance	0.998	0.997	0.976	0.997	0.392

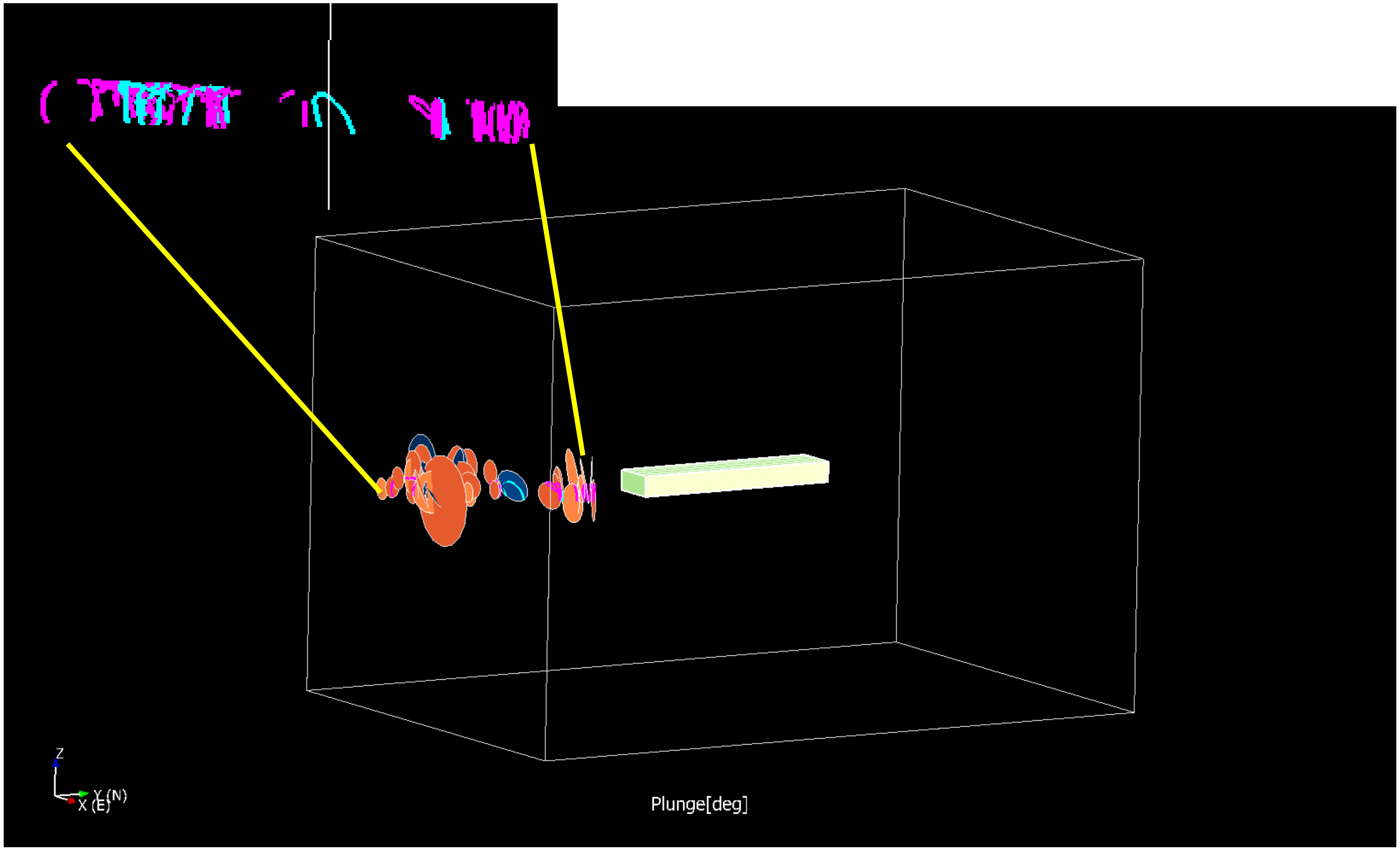
CTD Fracture Set D



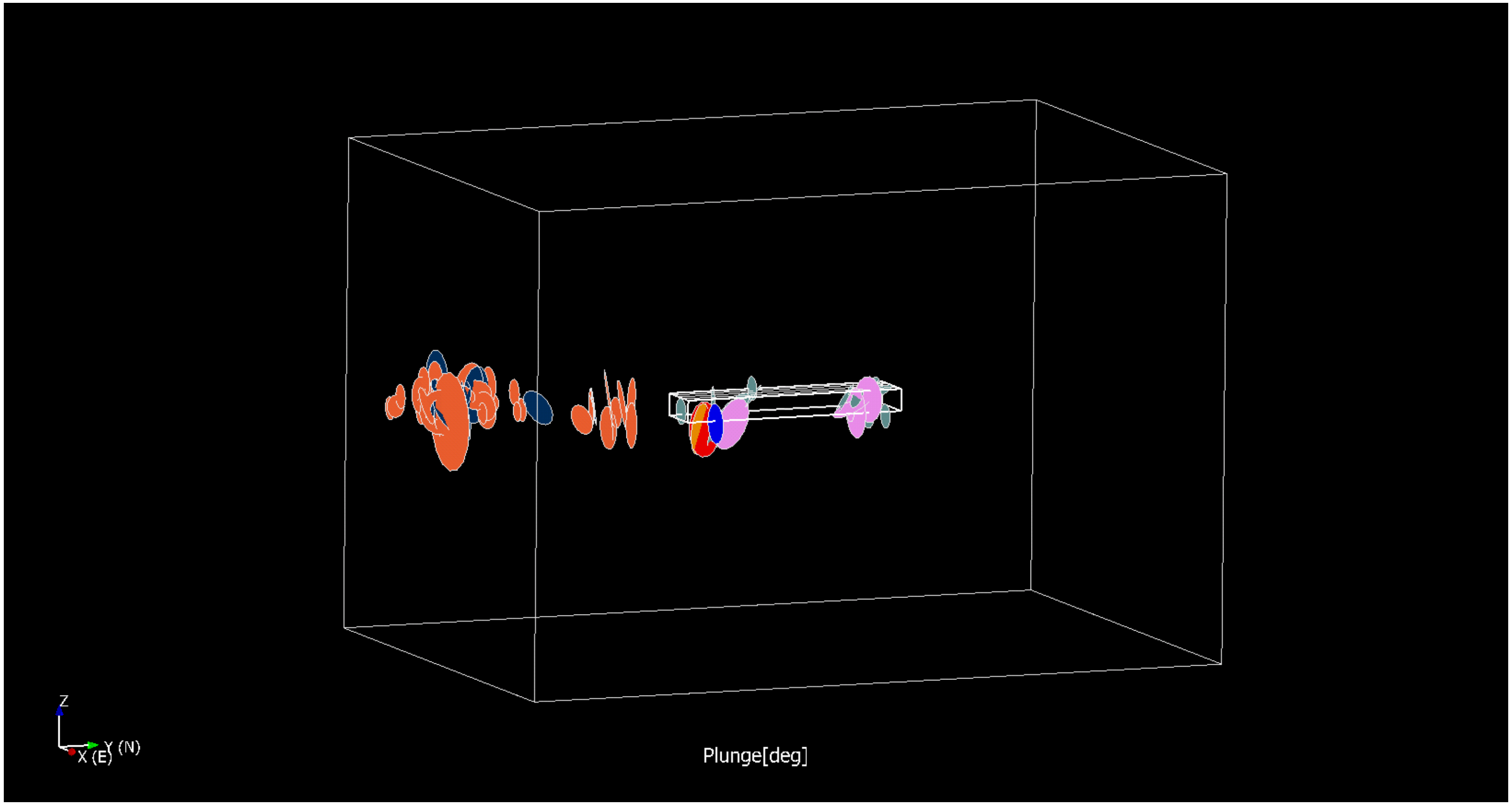
CTD Fractures Generated from Trace Data



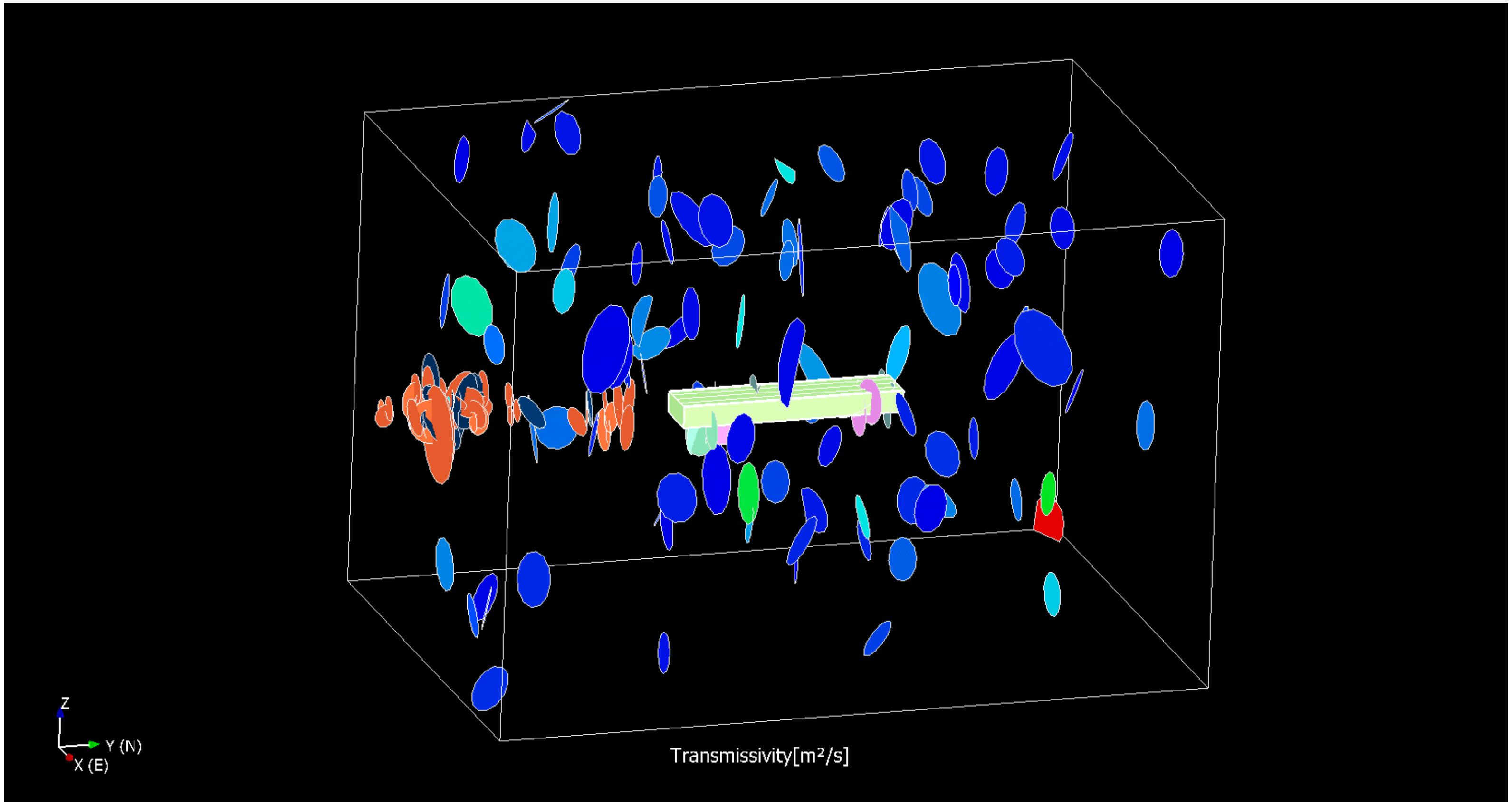
Inclined Drift Fractures Generated from Trace Data



Inclined Drift and CTD Fractures

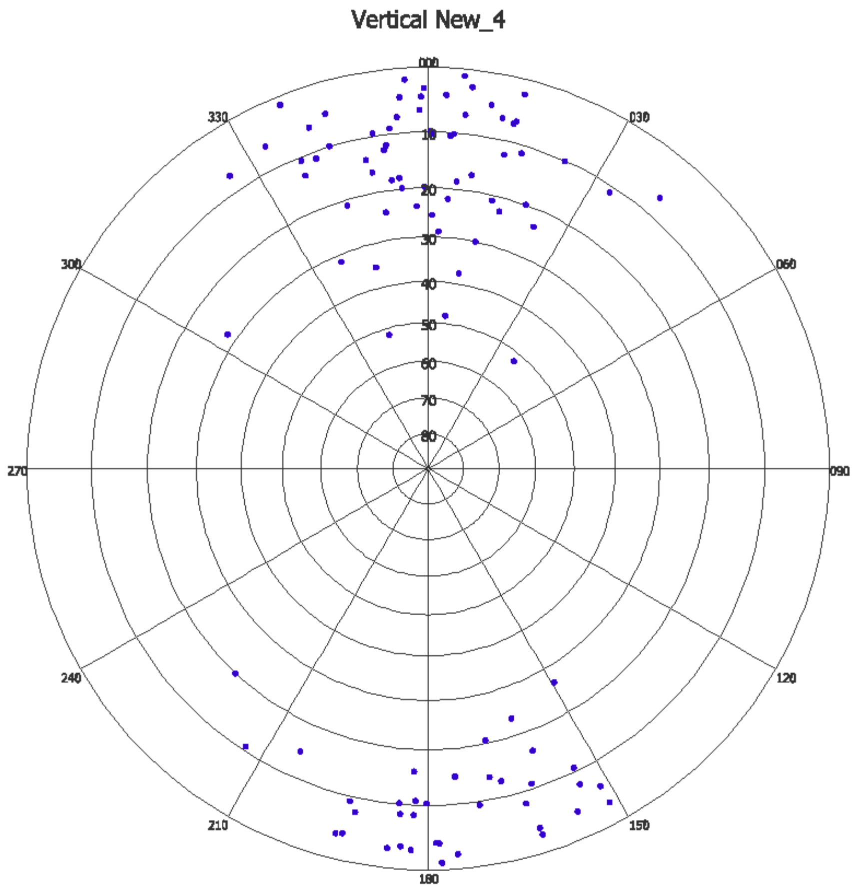


Stochastic Vertical Fractures



- Generated using power law distribution with min radius=4.0 m and α=3.5.

Stochastic Vertical Fracture Stereogram



Converting DFN to Continuum Model with Oda Method

- Oda calculates permeability tensors in three dimensions for each cell.
- Oda tensor is a simplification of Darcy's Law for flow through an isotropic porous medium.
- The fracture permeability (k) is projected onto the plane of the fracture and scaled by the ratio between the fracture volume (porosity) and the volume of the grid cell.

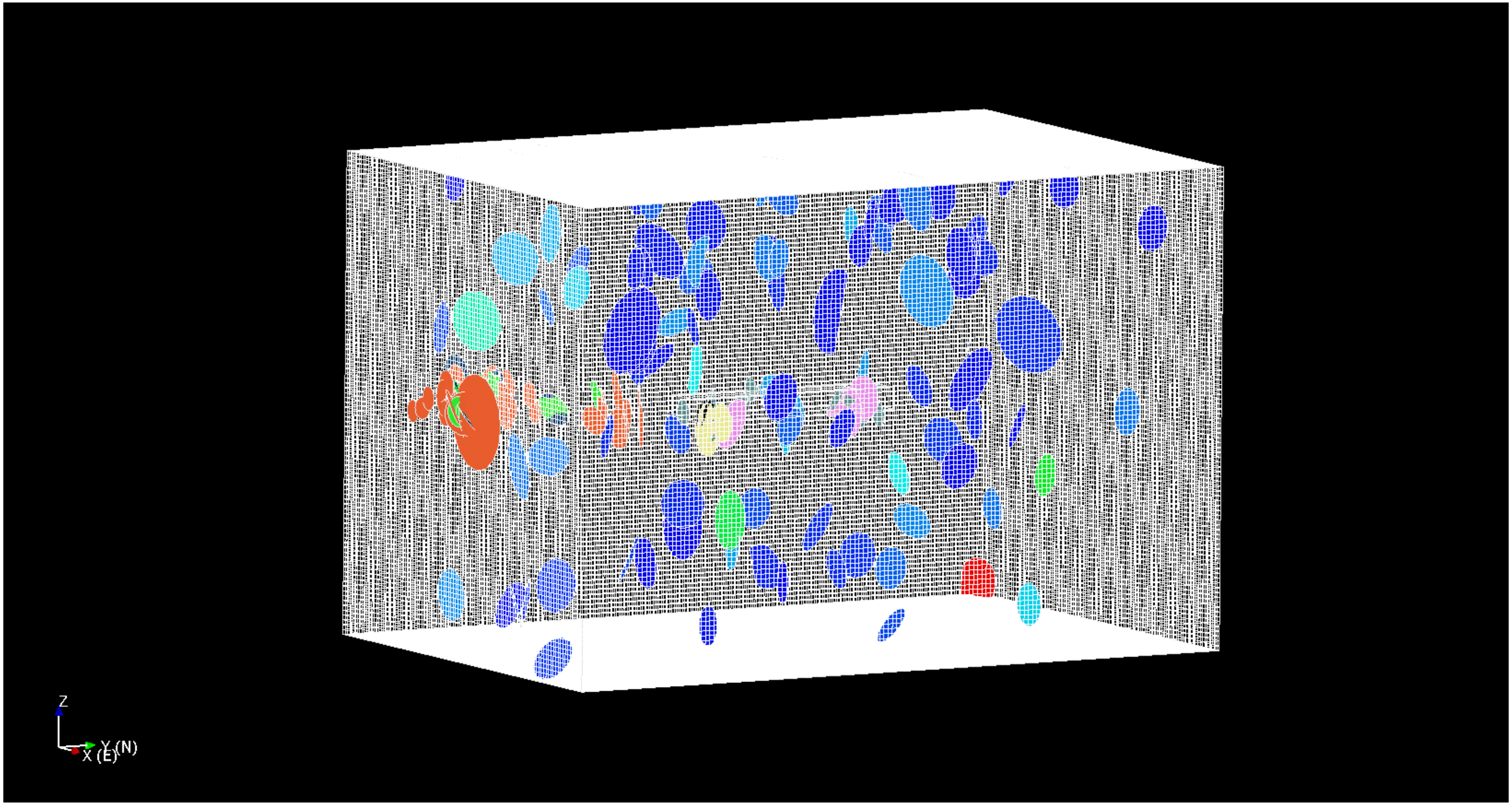
$$F_{ij} = \frac{1}{V} \sum_{k=1}^{N} A_k T_k n_{ik} n_{jk}$$

Fij = fracture tensor
V = grid cell volume
N = total number of fractures in grid cell
Ak = area of fracture k
Tk = transmissivity of fracture k
nik, njk = the components of a unit normal to the fracture k

$$k_{ij} = \frac{1}{12}\left(F_{kk}\delta_{ij} - F_{ij}\right)$$

kij = permeability tensor
Fij = fracture tensor
δij = Kroenecker's delta

Orthogonal Grid, 1mx1mx1m cell size



Future Work for Fracture Characterization

- Define fracture permeability pdf for each group of fractures (F, D, and W) generated from trace data for CTD and Inclined Drift.
- Analyze other data available for this area to understand how many fracture sets are present and what are their properties.
- Generate stochastic fractures based on the properties of the trace data and other available data.
- Define fracture permeability pdf for each set of stochastic fractures.
- Generate representative number of realizations (50 or more) of the stochastic fractures in the modeling domain.
- Convert DFN realizations into continuum model for flow and transport simulations.
- Analyze the connectivity of the stochastic and trace data based fracture networks.
- Sensitivity analysis related to fracture size and properties of both, trace based and stochastic fractures.

CTD-Scale Flow and Transport Simulations - Model Setup

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- Domain: 150 m x 100 m x 100 m
  - with cell size of: 1 m x 1 m x 1 m
- Number of Elements: 1,500,000
- Porosity: Anisotropic
- Permeability: Anisotropic
- Initial Conditions: Hydrostatic pressure
- Boundary Conditions:
  - Pressure at Specified Location

Fluid Flow Simulation

- PFLOTRAN numerical simulator
- Estimate inflow rate and other requested output
- Steady state flow to be utilized for the following:
  - to estimate effective permeability for each realization
  - To generate flow field for transport simulation
- Darcy's law and east face flux to be used to calculate effective permeability:

$$q = \frac{-k_{eff}\Delta P}{\mu L}$$

q = flux,
k_{eff} = effective permeability,
ΔP = pressure difference,
μ = dynamic viscosity
L = distance between west and east faces

Transport Simulations: Tracer Breakthrough Curves Evaluation:

- PFLOTRAN numerical simulator to be used (advection-diffusion)
- Porosity and steady state flow fields for each realization utilized as input to transport simulations
- Simulate transport through domain
- Output used to calculate normalized breakthrough curve for each realization
- Include chemistry to hydrology
- Provide requested transport output

Data Needs for Flow and Transport Modeling

- There is a need for input data and definition of required output in the modeling of flow and transport
- For the CTD-Scale model:
  - Initial and boundary conditions, and other input parameters
  - Experimental data for comparison of pressure and tracer data
- For Large-Scale Model
  - Initial and boundary conditions and other input parameters
  - Experimental data for comparison of pressure and tracer data
- Type of output for comparison with other models
  - Inflow rate
  - Transport
  - Chemistry

Evaluation of Geochemical Trends in Groundwater Chemistries in Crystalline Rock

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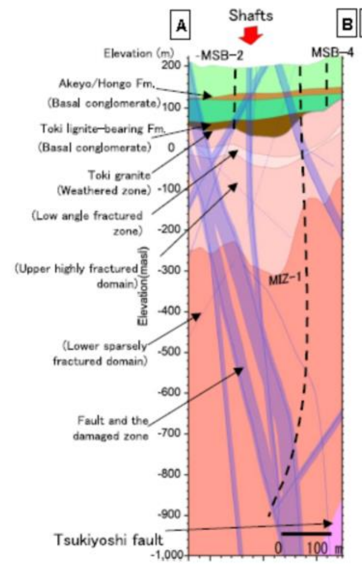
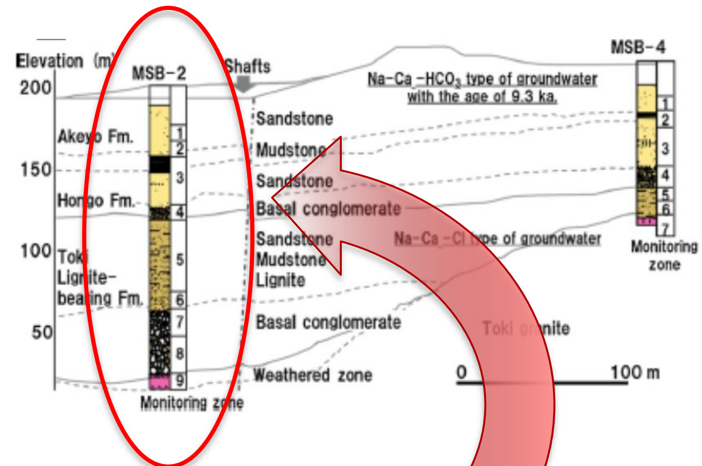
- GREET (Groundwater REcovery Experiment in Tunnel)
- Geochemical evaluation of groundwater site data (JAEA GREET website; Iwatsuki et al., 2005 & 2015)

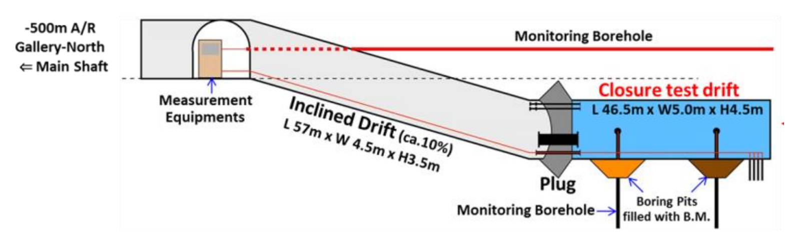




- DECOVALEX-19 Task C:
  - **Current focus: geochemical evaluation of groundwater chemistry trends**
  - Evaluation of monitoring hydrological and geochemical site data (e.g., Closure Test Drift - CTD)
  - Interactions with host-rock and barrier materials

Monitoring Borehole MSB-2 Evaluation

Closure Test Drift - CTD



GREET: Groundwater Chemistry Site Data

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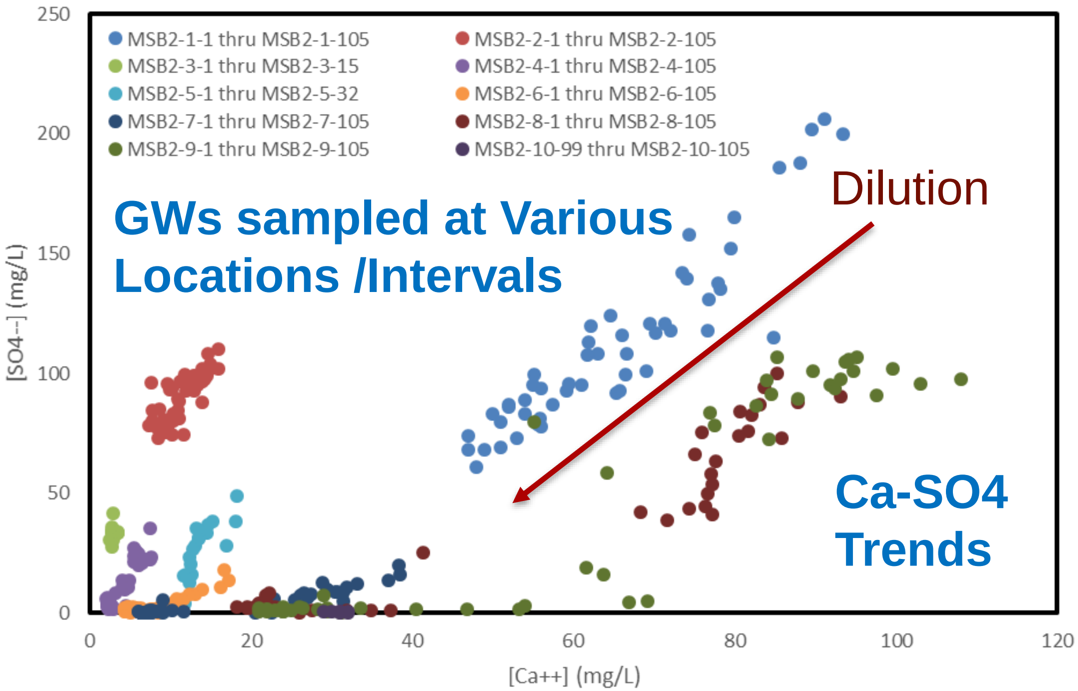
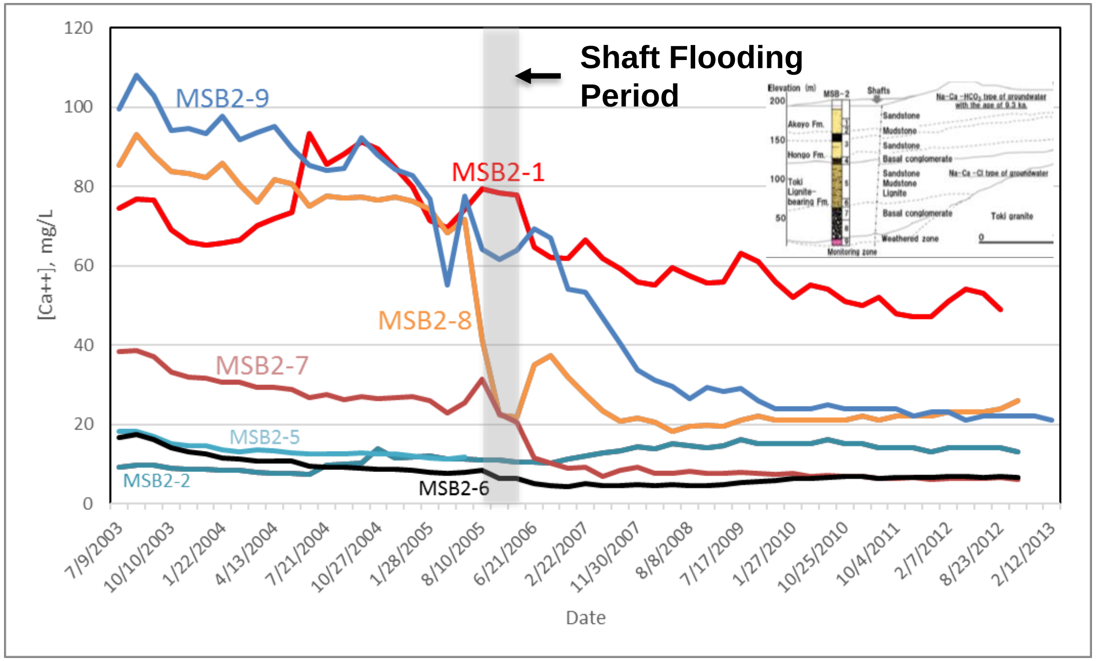
MSB2 Monitoring Borehole Total Data (Ca & SO_4)



- Dilution → Overall, applies to major constituents:
  - Ca, SO_4, K, Na
- Trend variations in different zones
  - e.g., Na, Cl concentrates in certain zones

- Evaluate geochemical trends:
  - Time -> Separate flood event
  - Location -> Spatial correlation for chemical trends
- Geochemical modeling
  - EQ3/6 code simulations
    - Reaction path modeling (dilution, mixing)
    - Aqueous speciation
      - Charge imbalances
      - GW chemical evolution
    - GW saturation state
    - Mineralogic interactions

GREET: Groundwater Chemistry Site Data: MSB2 monitoring borehole



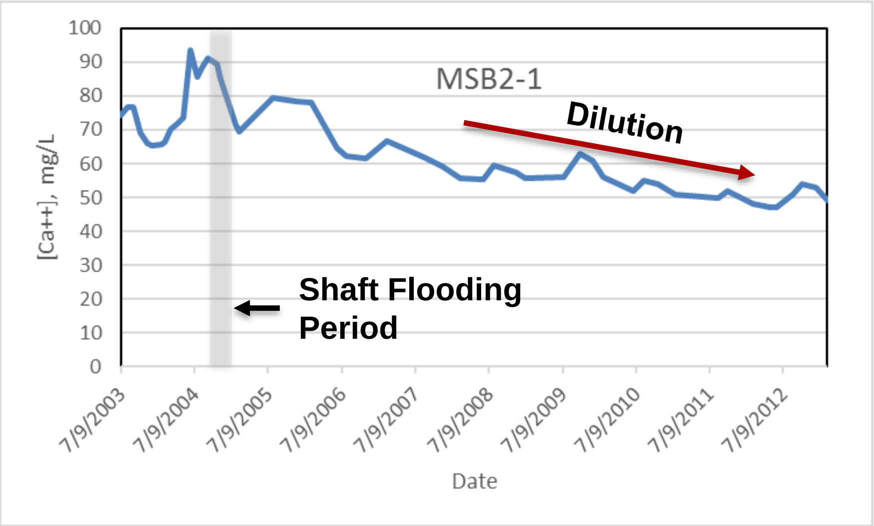
- Evaluate geochemical trends:
  - Time -> Separate trends from flood event
  - Zones -> Spatial fluid mixing between zones
- Geochemical modeling
  - EQ3/6 code simulations
    - Reaction path modeling
      - Pure water dilution of MSB2-1 analysis
      - Mixing of waters from different zones (mixing MSB2-7 with MSB2-1 groundwater)
      - No mineral saturation considered
    - Geochemical speciation
      - Assess bicarbonate concentrations
      - Charge balancing

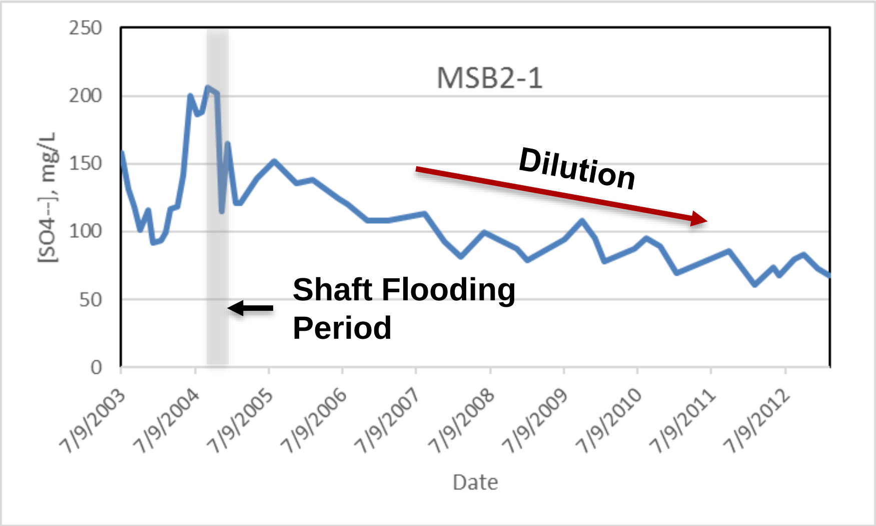
Goals:

- Explore evaluation of groundwater mixing in boreholes using geochemical modeling
- Assess application of geochemical tools to predict groundwater chemistry

GREET: Groundwater Chemistry Site Data: MSB2 monitoring borehole

MSB2 Monitoring Borehole Zone 1: Dilution with time





GW mixing Modeling:

- $[Ca^{++}]$ and $[SO_4^{--}]$ selected as dilution indicators
- Only post shaft flooding GW composition considered
  - Large variations in pre shaft-flooding data
  - Only data showing progressive dilution trends
- Other aqueous species will be considered in subsequent evaluations

GREET: EQ3/6 GW mixing Simulation: MSB-2 monitoring borehole (Zones 1 & 7)

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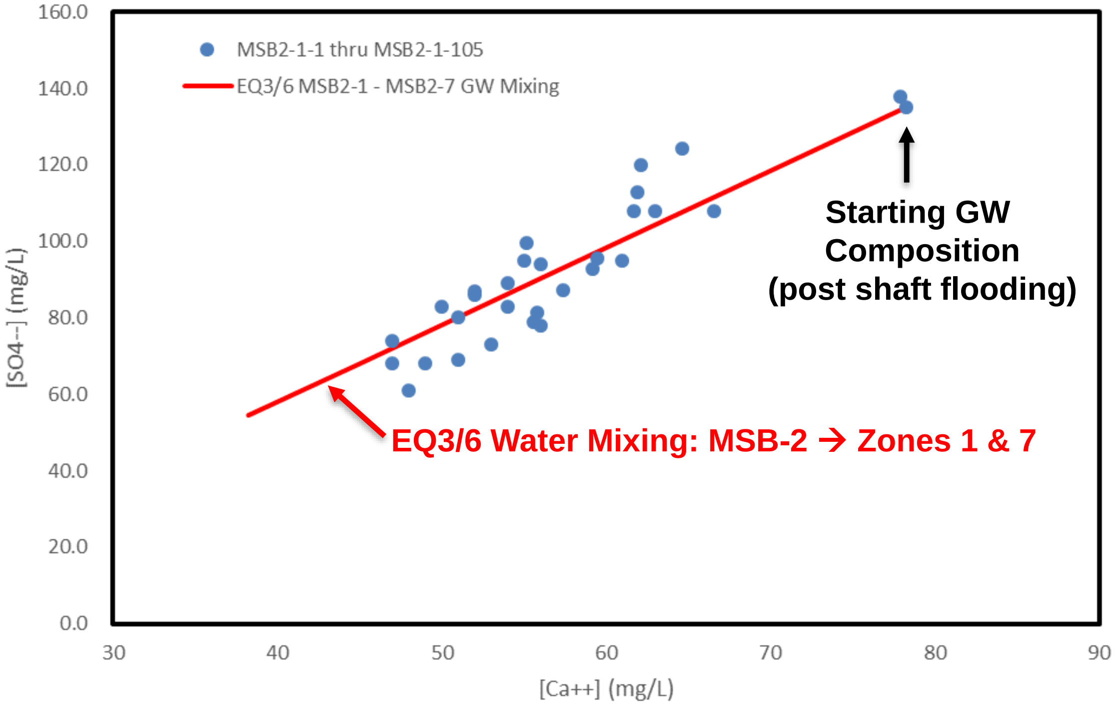

TODO Next:

- Consider different starting GW compositions: MSB2-1 & MSB2-4
- Consider other GW chemistries: MSB4, WR's, Galleries
- Simulate mineral saturation effects: e.g., calcite

- Evaluate dilution trends:
  - EQ3/6 simulation of MSB-2 GW mixing of Zones 1 & 7
  - Test flood water provenance: likely from MSB-2, Zones 7 & 8 (Iwatsuki et al. 2015)
- Simulation Results
  - Ca vs SO_4 dilution trend is represented by the GW mixing for MSB-2, Zones 1 & 7
  - Simulation predicts increases in [Na] & [Cl] as observed but at higher concentrations
  - Assess discrepancies in predicted trends
    - Fresh water input?
    - Mixing with a more dilute water?

Closure Test Drift (CTD): H-C Model

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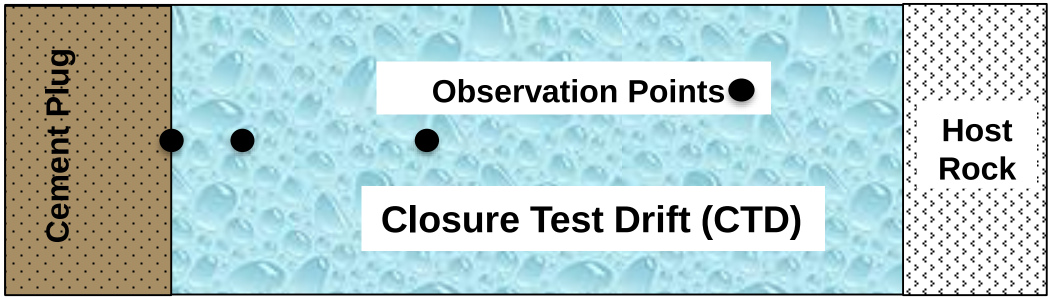
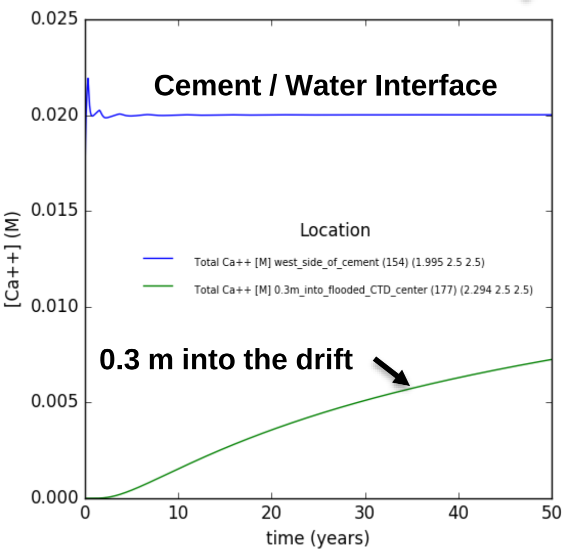
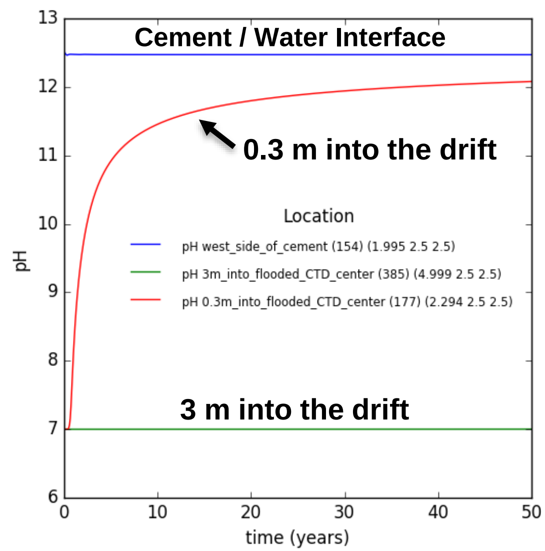
PFLOTRAN 1D Reactive Transport Modeling

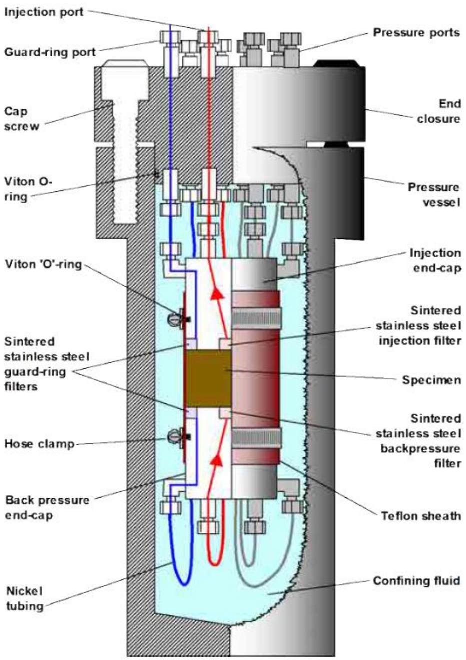




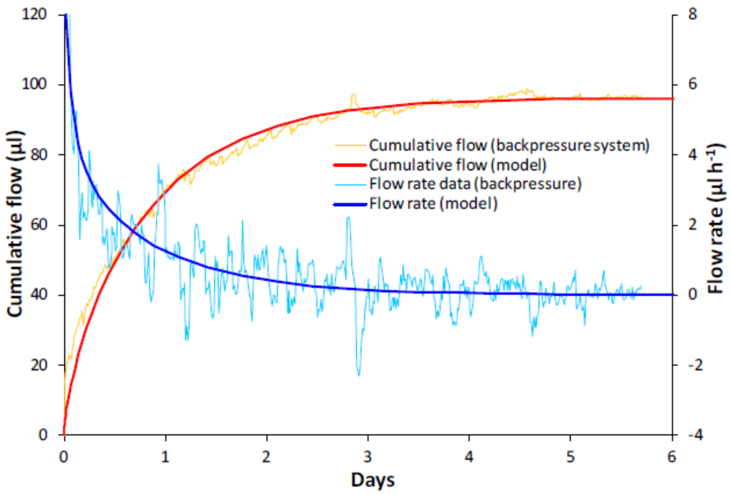


- H-C (Reactive-transport - RT) modeling
  - **PFLOTRAN** RT simulation tool
  - 1D reactive-transport model
    - Cement plug / CTD region
    - Flooded CTD region modeled as a high porosity / high permeability domain
    - Diffusion only
    - OPC cement composition
    - Diluted “fresh” water composition in flooded domain
    - THERMODDEM thermodynamic database including cement phases
  - Effects of cement interactions on bulk water chemistry
    - As expected, large changes in pore & bulk fluid composition at the vicinity of the cement / water interface (see Figs.)
    - Increases in Ca & pH can be significant even at 30 cm from the interface
    - Next: Sensitivity analyses on transport parameters, kinetic rates, aqueous species profiles

What does the noise mean?



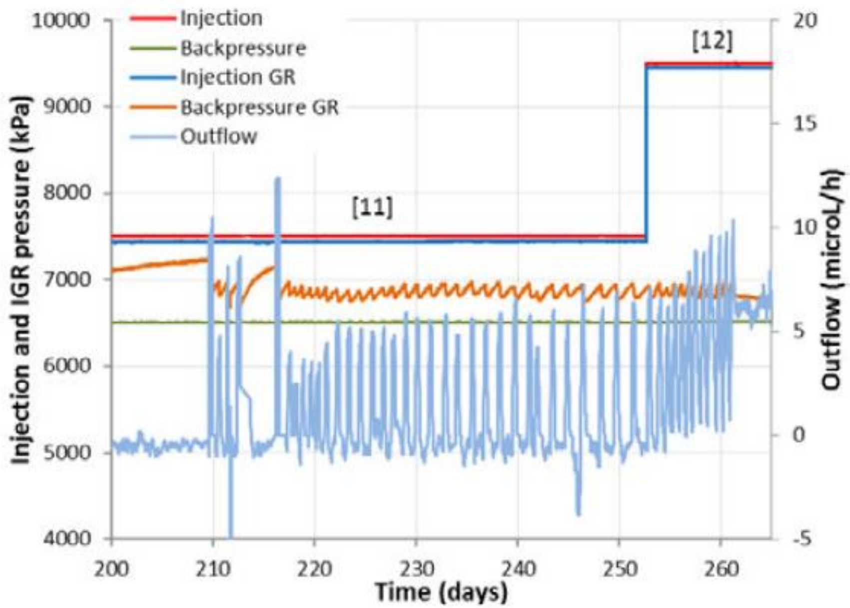
FORGE Report D4.17 (Harrington, 2013)



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

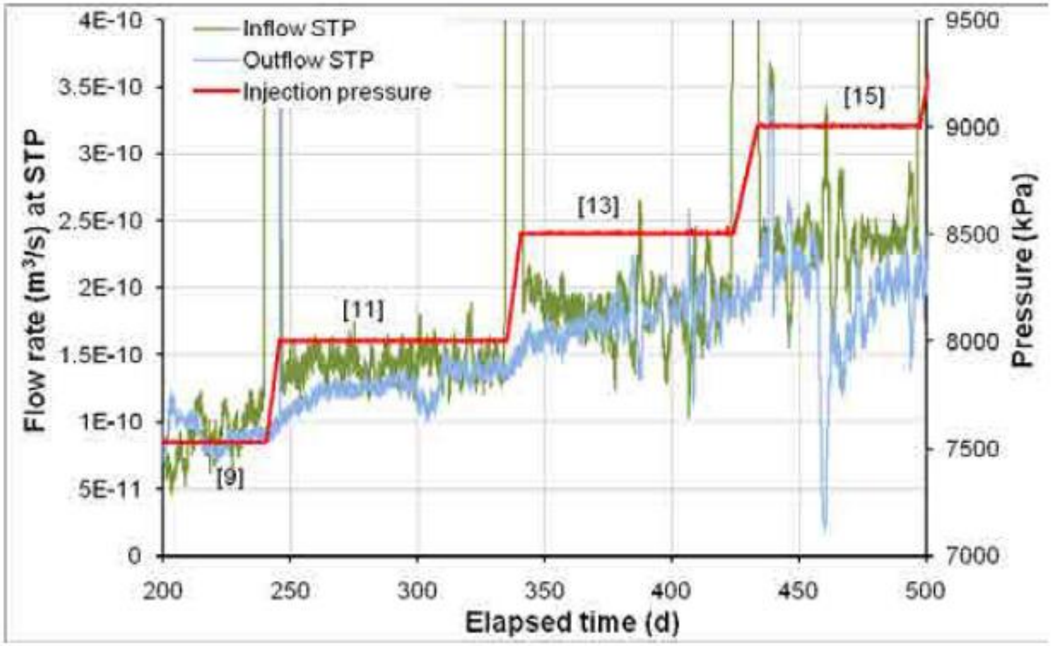
$$\frac{E}{2(1+\nu)} \nabla^2 \mathbf{u} + \frac{E}{2(1+\nu)(1-2\nu)} \nabla (\nabla \cdot \mathbf{u}) - \nabla p_w = 0$$

Dynamic behaviors of the system



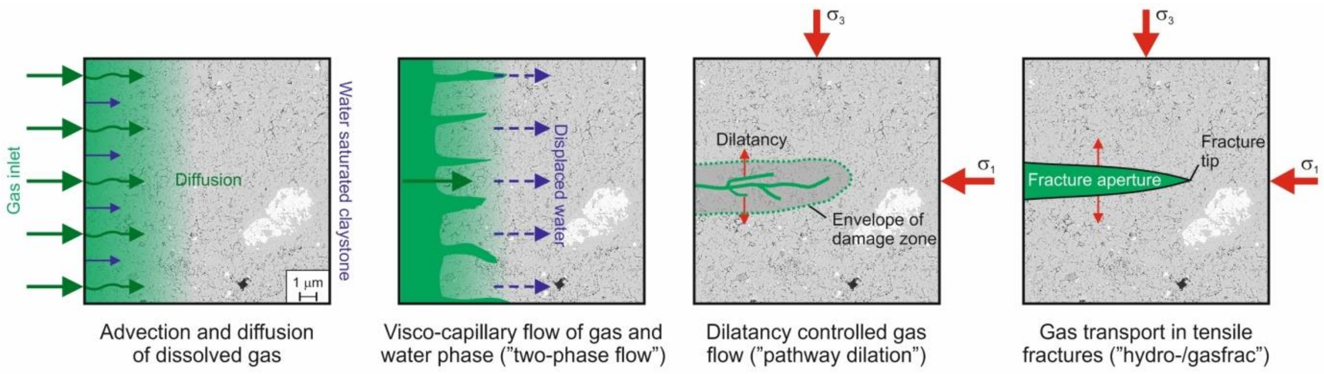
FORGE Report D4.17 (Harrington, 2013)

Dynamic behaviors of the system (cont.)



FORGE Report D4.17 (Harrington, 2013)

Dynamic instability

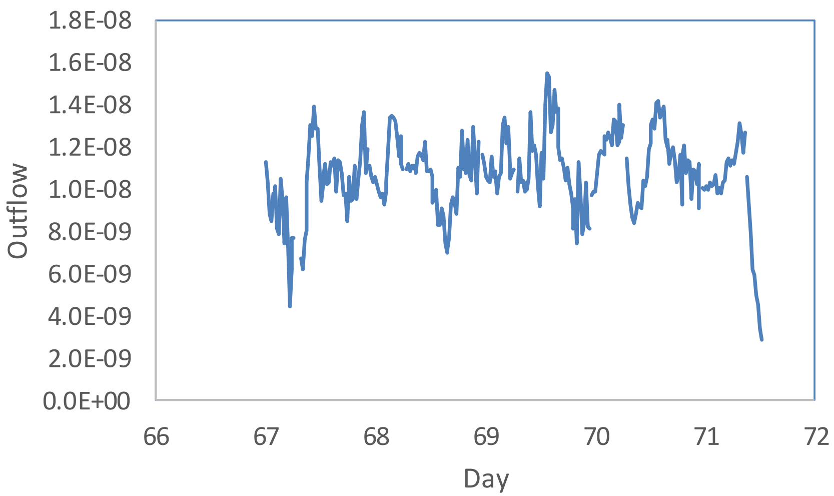


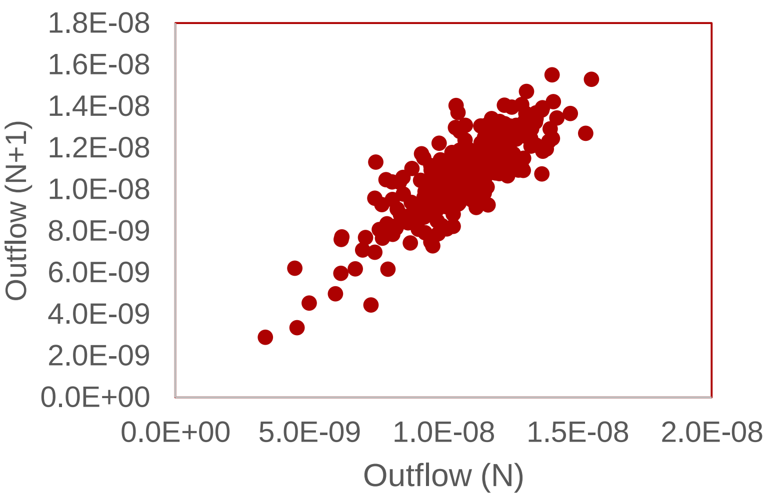
In clay-rich system considerable evidence exists suggesting gas flow is accompanied by the creation of preferential pathways and dilation of the clay

- Channeling of gas percolation front
- Instability of the movement of individual gas bubbles

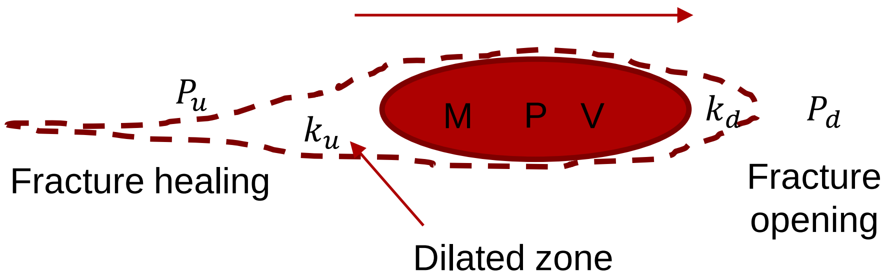
Harrington & Tamayo (2016)

Not completely random: Behavior in an embedded space





Bubble migration under a pressure gradient



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

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

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

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

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

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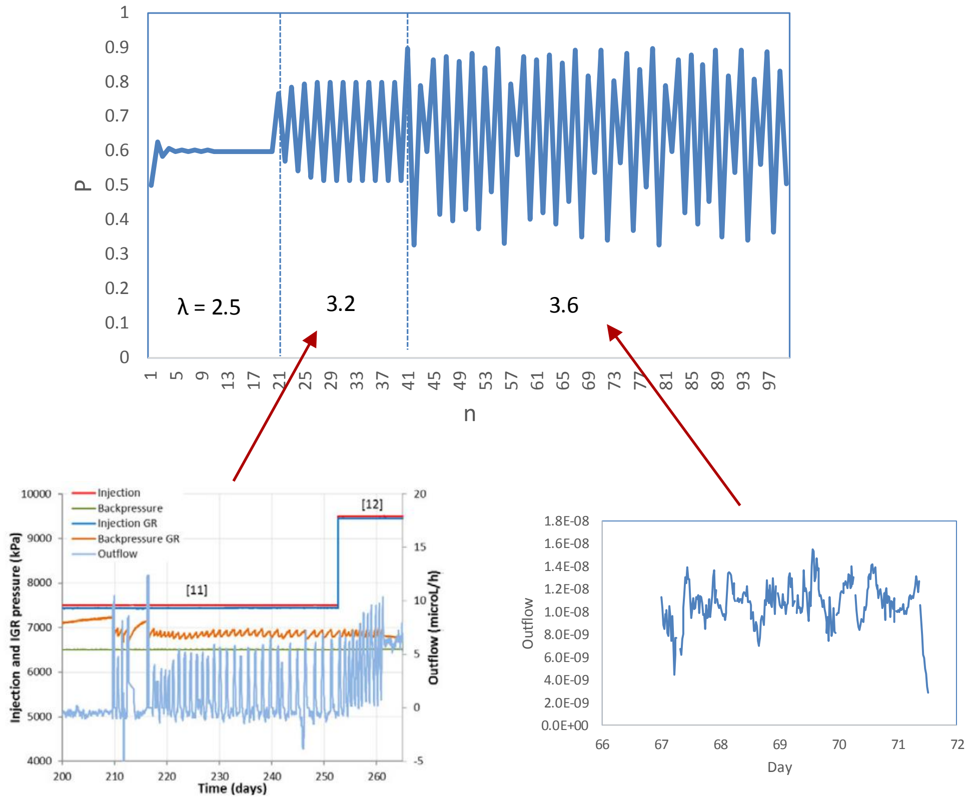
Logistic map: An illustration

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

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

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

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



FORGE Report D4.17 (Harrington, 2013)

Schedule

Activity	Spring 2016	Autumn2016	Spring 2017	Autumn 2017	Spring 2018	Autumn 2018	Spring 2019	Autumn 2019
Stage1: 1D flow (laboratory)	Wksp 1	Wksp 2						
Stage 2: Spherical flow (laboratory)			Wksp 3	Wksp 4				
Interim reporting								
Stage 3: Field scale flow					Wksp 5	Wksp 6		
Stage 4: Gas flow in natural clay							Wksp 7	Wksp 8
Final Reporting								

Next steps

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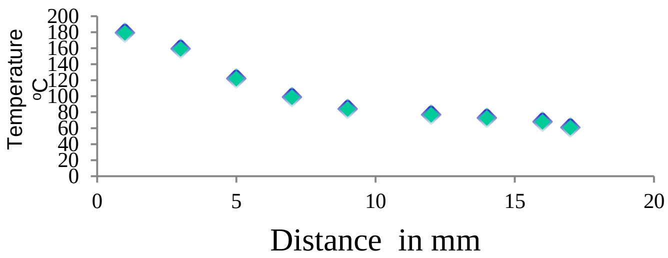
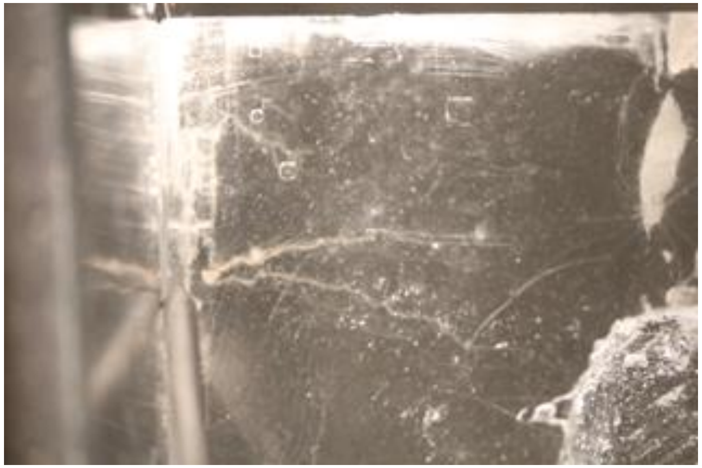
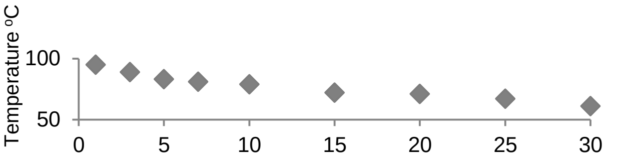
- Complete the mathematical formulation and analysis for single bubble movement.
- Complete the formulation for the channeling of a gas percolation front.
- Consider how to incorporate the instability analysis into a 2D or 3D continuum model.

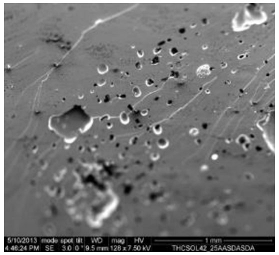
Observations: Temperature effect

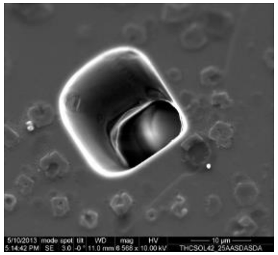




Caporuscio et al. (per. Comm.)

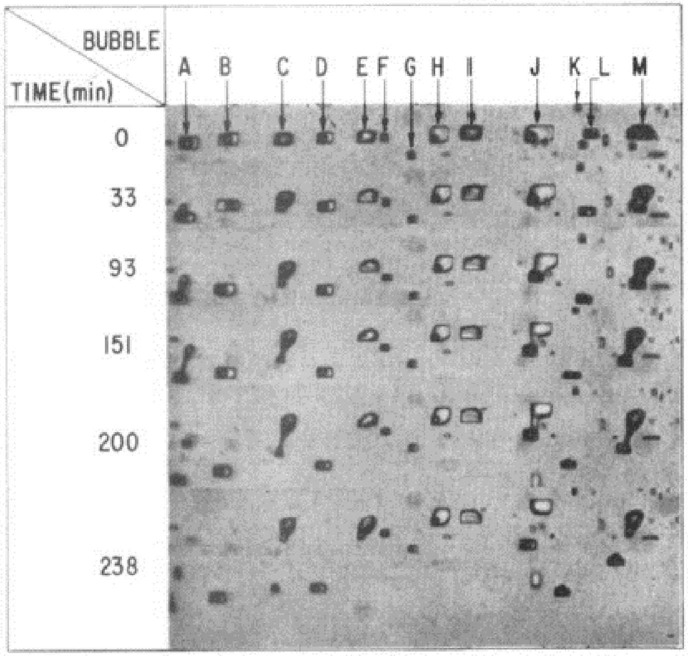


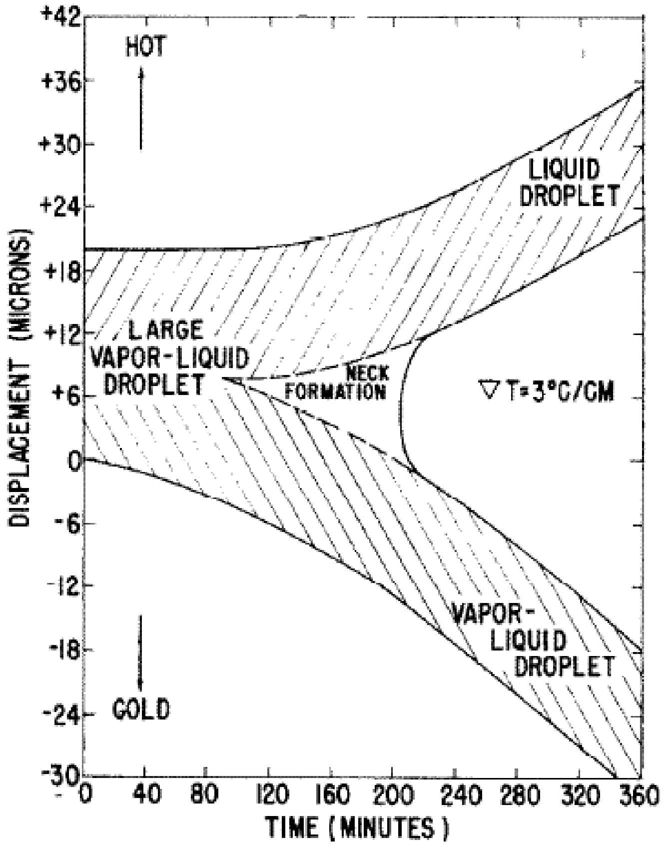




Interface instability and channeling

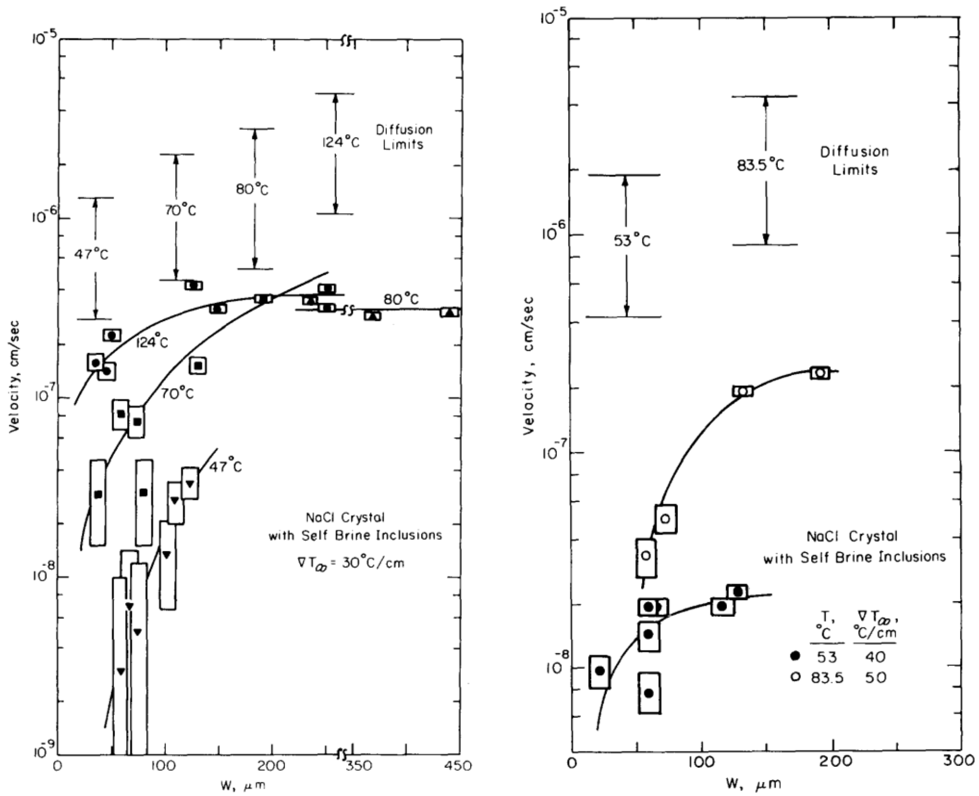
Observations: Biphase inclusions





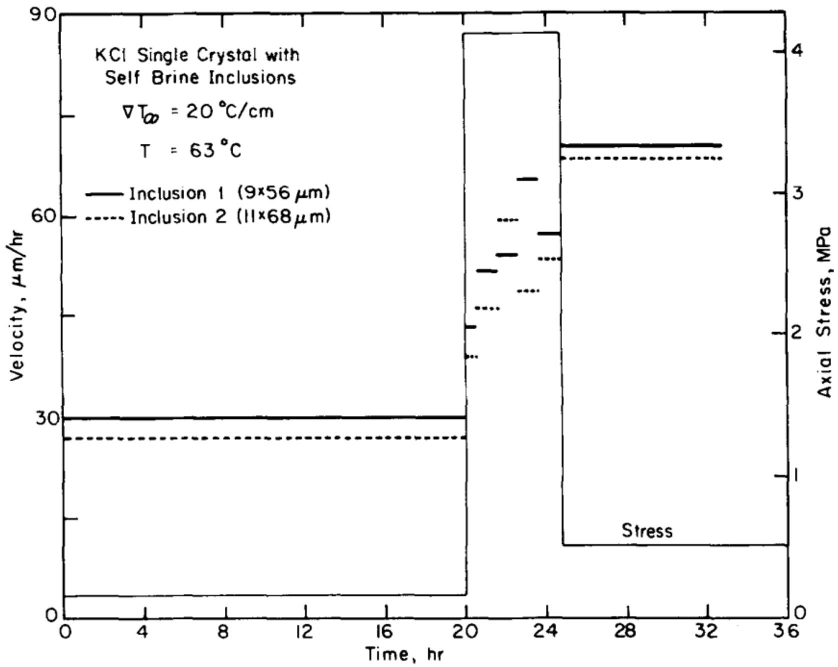
Anthony & Cline (1972)

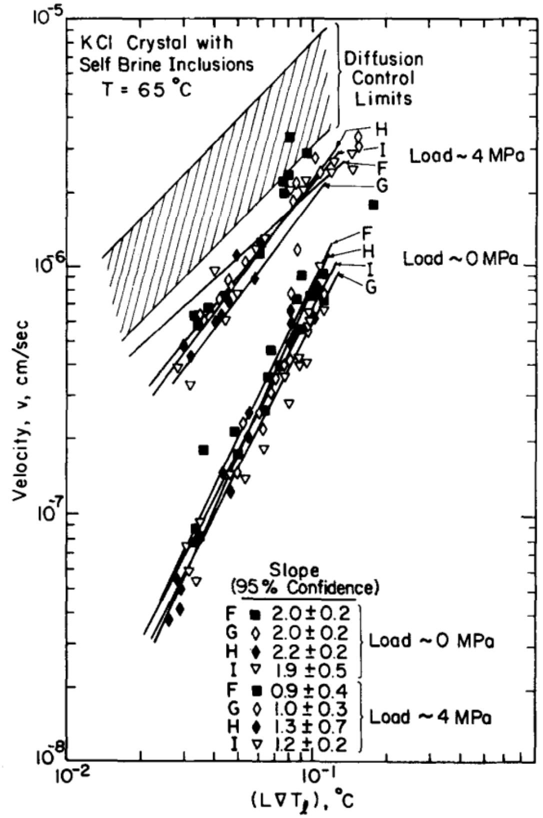
Observations: Size dependence



Olander et al. (1982)

Observations: Effect of stress





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:

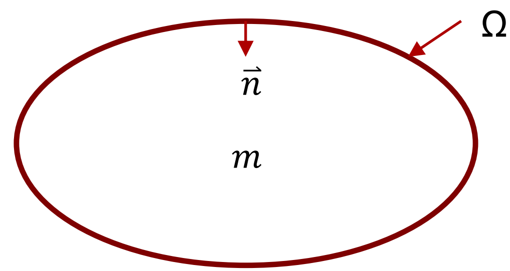
Ω(x, y, z, t) = 0

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

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

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

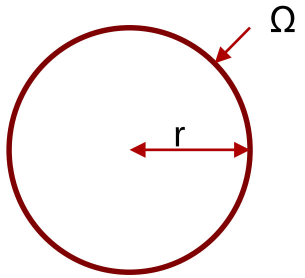
$$\kappa = -\vec{\nabla} \cdot \vec{n}$$



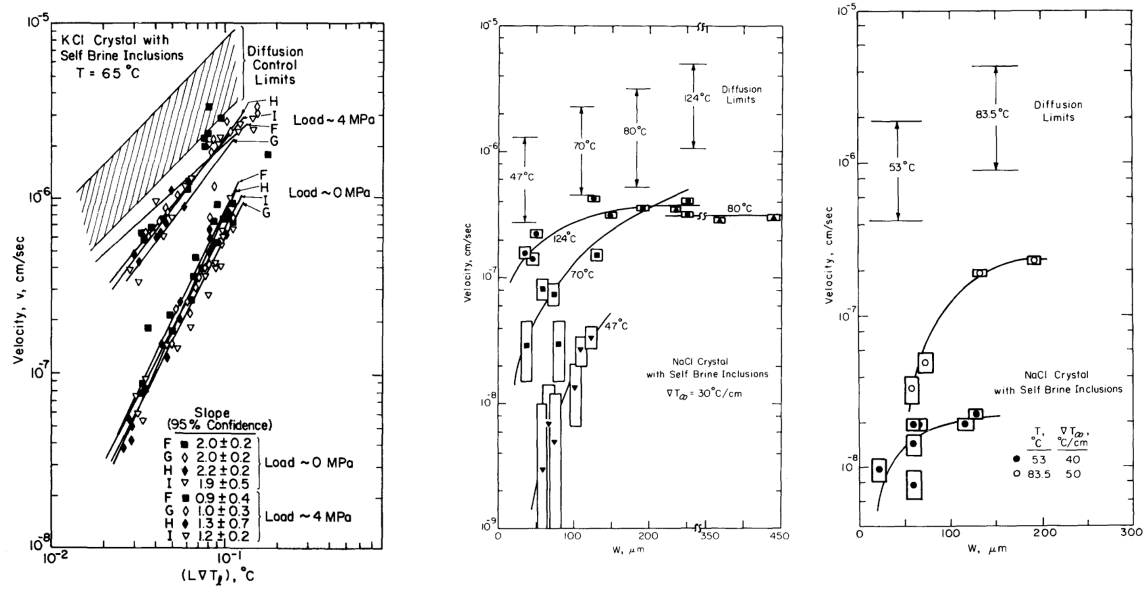
Questions:

- 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

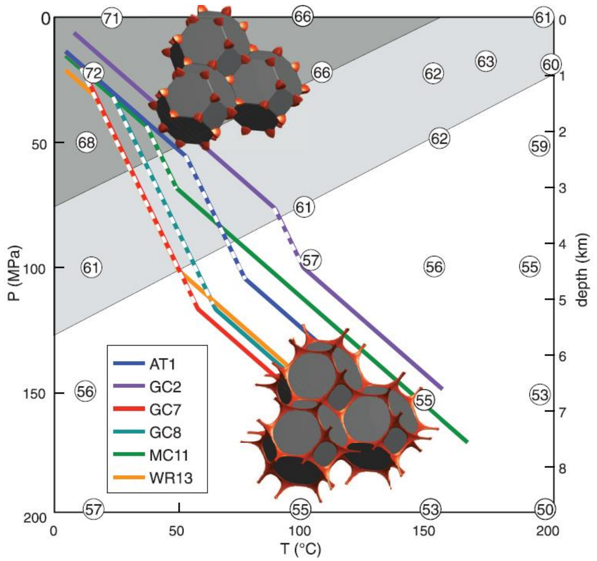


$$V_0 \approx \frac{V_m D K_d^0 \Delta H_r \alpha}{R T_0^2} e^{-\frac{2\gamma V_m}{R T_0 r}}$$



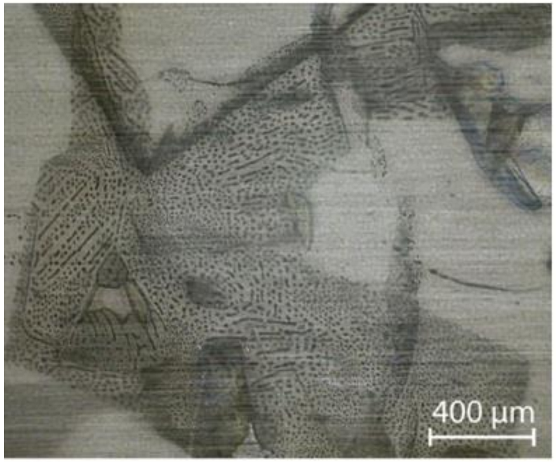
Olander et al. (1982)

Work in progress



Ghanbarzadeh et al. (2015)

$$\theta = 2\cos^{-1}[\gamma_{ss}/(2\gamma_{sl})]$$



Thiemeyer et al. (2015)

- Effect of stress on dihedral angle and percolation threshold
- Mechanism for the presence of fluid inclusions along grain boundaries

Schedule

	1. year		2. year		3. year	
	1. workshop	2. workshop	3. workshop	4. workshop	5. workshop	6. workshop
WP - 1						
Literature recherche						
Process definition/description						
Conceptuel modeling						
WP - 2						
Upscalling study (microscale - macroscale)						
Mathematical formulation						
Programm developement						
WP - 3						
Modelling against observation						