



# Modeling Reactive Transport And Fracture Stimulation in Geothermal Systems and Hydrocarbon Reservoirs

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# Motivation and Outline

## Overall Motivation:

Evaluate and predict coupled Thermal-Hydrological-Mechanical-Chemical (THMC) processes in Enhanced Geothermal Systems with applications to Unconventional Hydrocarbon Reservoirs

- Develop a reasonable geological, hydrological, and geochemical model
- Evaluate stimulation effectiveness
- Use geochemical and isotopic data to constrain fracture properties, porosity and permeability changes, heat transfer area
- Evaluate effects on permeability over periods of days to decades

## Outline:

- THMC Models/Code Development
- Newberry Volcano EGS 3-D THMC Model
- Results and Insights from the 2012/2014 EGS Stimulation and Modeling
- Preliminary Flowback Geochemical/Isotopic Data
- THMC Modeling of a Stimulated Reservoir
- Applications to Hydraulic Fracturing

# Use of Reactive Transport For Evaluation of THM Processes

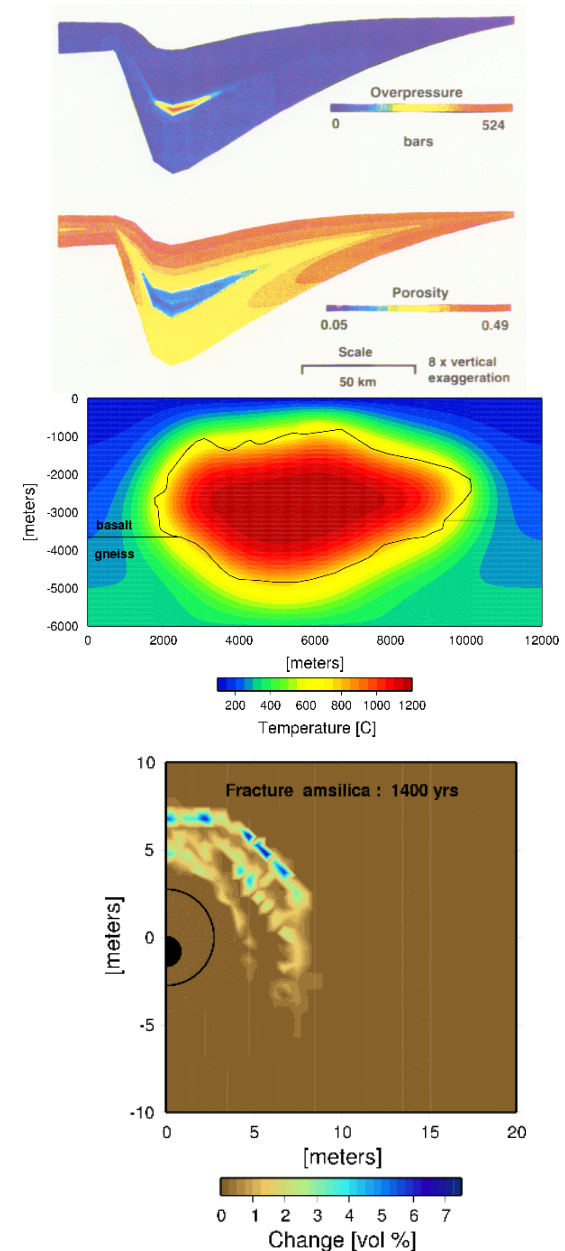
Water chemistry of injection/production fluids can be used as natural tracers for evaluating fracture surface area

Geochemical & isotopic systems are modified by water-rock interaction, mixing, degassing, allowing for better understanding of fluid sources/pathways

Introduced (Engineered )Tracers: conservative, reactive/sorbing and thermally-degrading for determining heat transfer area and connectivity

# Questions and Codes

- Can pressure solution and compaction lead to sealing and development of overpressured compartments in evolving sedimentary basins?
  - RCTSED: sedimentation, subsidence, fluid flow, diffusion-limited pressure solution, dissolution/ precipitation kinetics, compaction, subcritical crack growth (*Sonnenthal & Ortoleva, 1994*)
- Which processes control the differentiation of mafic magmas and is some layering the result of reactive infiltration of melt/fluids?
  - RCTMAG: multicomponent crystallization, heat transport, porous melt flow and convection, chemical & Soret diffusion (*Sonnenthal & McBirney, 1998, 2007*)
- What thermal, hydrological, and chemical effects will result from emplacing nuclear waste in the subsurface?
  - TOUGHREACT: multicomponent, multiphase reactive transport (*Xu, Sonnenthal, Spycher, & Pruess, 2001; 2006; 2011*)



# TOUGHREACT-ROCMECH Coupled Flow / Heat / Mechanics / Reactive Transport Code

Fluid/Heat Flow

Pass calculated pressure, temperature

Mechanics - Solve for Stress, strain, failure strain

Aqueous and Gaseous Species Transport

Reactive Chemistry (Water-Gas-Minerals)

Porosity/permeability changes

# TOUGHREACT V3.0-OMP Capabilities

## Processes:

- Multiphase fluid and heat flow: extended TOUGH2 V2 (Pruess, et al., 1999)
- Transport: advection and diffusion in both liquid and gas phases
- Chemical reactions:
  - Aqueous complexation
  - Surface complexation:
    - Double diffuse layer, constant capacitance, and non-electrostatic
    - Molality, mole-fraction, or equivalent-based formulation
    - Dynamically linked to mineral amounts/surface area
  - Redox equilibrium/disequilibrium
  - Mineral dissolution/precipitation
  - Gas dissolution/exsolution
  - Cation exchange (multi-site)
  - Linear Kd adsorption
  - Decay

## Special Features:

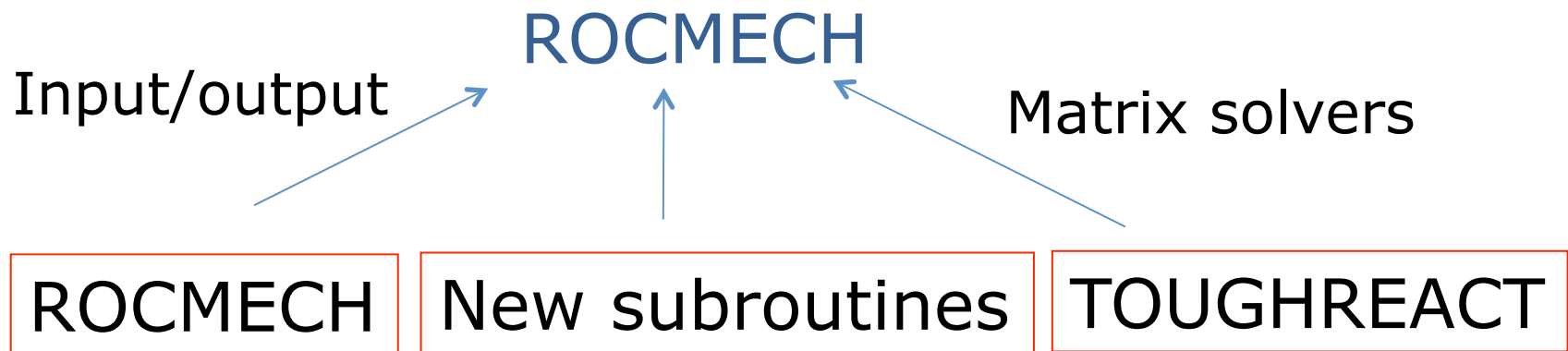
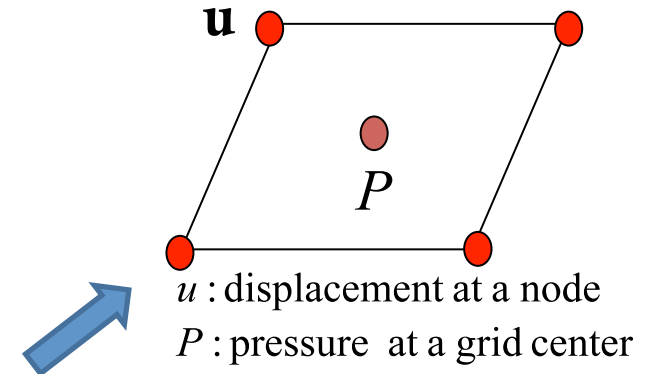
- Shared memory parallelization of chemical reactions
- Changes in porosity due to mineral dissolution and precipitation
- Porosity-permeability-capillary pressure coupling
- Aqueous and gaseous species active in flow, transport, and reaction
  - Equilibrium and kinetic reactions (solid & aqueous, biodegradation)
- Porous and fractured media
- Any number of chemical species
- Stand-alone thermodynamic database
- Physical and chemical heterogeneities
- Single-phase wellbore model
- Temperature- and mineralogy-dependent heat capacity and thermal conductivity
- Sedimentation (simple 1D advection)

<http://esd.lbl.gov/research/projects/tough/software/toughreact.html>

Sonnenthal et al., 2014; Xu et al., *Comp. & Geosci.*, 2006 and 2011

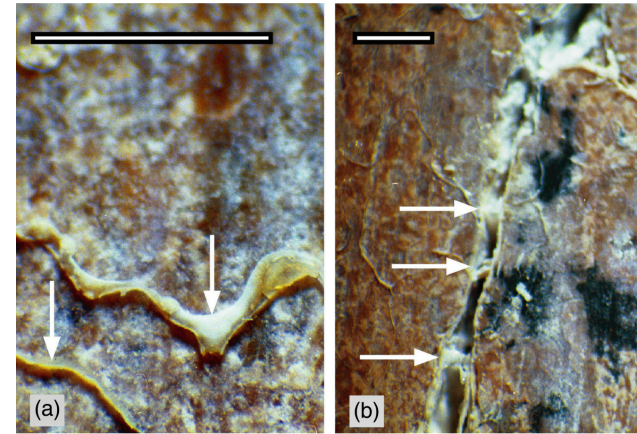
# THMC Modeling

- Written in Fortran 90/95
- Employ finite element method
- Enjoy highly stable space discretization
  - Mixed finite-volume (flow)/finite-element method (mechanics)
- Apply the most recent method for coupled flow-mechanics
- Extension to multiple porosity system (MINC)



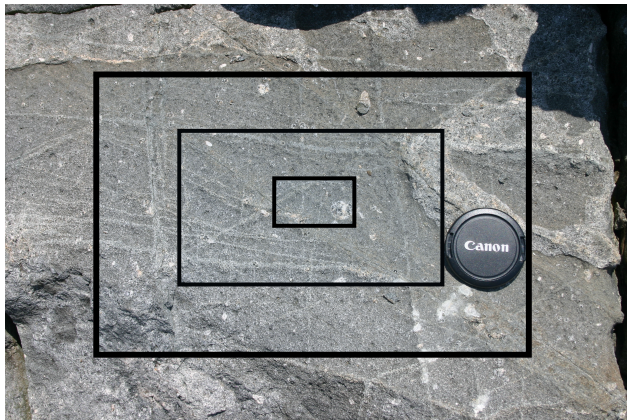
# Geochemically-Induced Permeability Changes in Multiphase Fractured Rocks

- **Single phase Systems:** Flow and alteration are typically enhanced in high permeability features
- **Multiphase Systems:** Capillary forces keep wetting liquids in lower permeability features (e.g. pore throats, fracture asperities)
  - Lower permeability features may experience more alteration
  - Extent of water-rock interaction depends on the wetted surface area
  - Gas transport important (e.g., H<sub>2</sub>O vapor, air, CO<sub>2</sub>, O<sub>2</sub>)



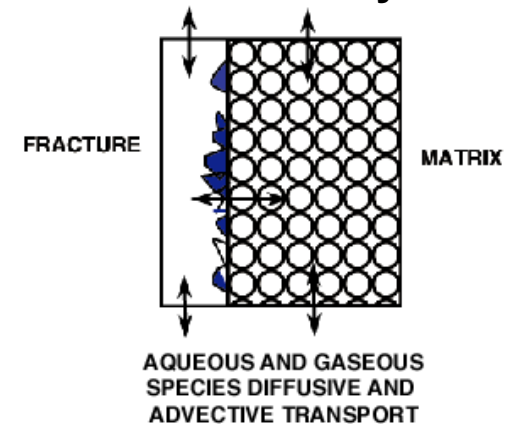
Experimental Results: Amorphous Silica in a Boiling Fracture (*Kneafsey et al., 2001, HLRWMC; Dobson et al., 2003, J. Cont. Hyd.*)

## Fracture Distributions/Networks



Isle au Haut, Maine

## Dual-Permeability Model





# Yucca Mountain Drift Scale Heater Test

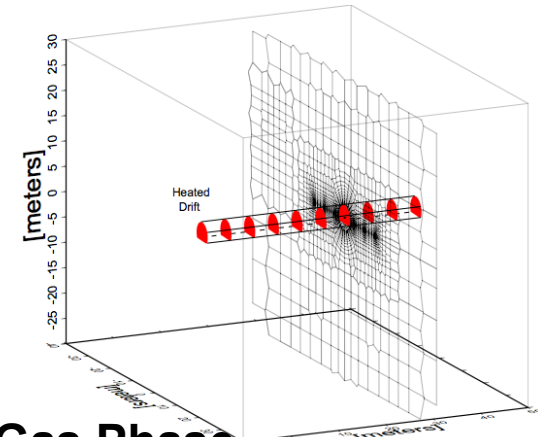
## Geochemical System

**Aqueous Species:**  $H^+$ ,  $Na^+$ ,  $Ca^{+2}$ ,  $Mg^{+2}$ ,  $K^+$ ,  $Al^{+3}$ ,  $SiO_2$ ,  $Fe^{+3}$ ,  $Cl^-$ ,  $F^-$ ,  $HCO_3^-$ ,  $SO_4^{2-}$ ,  $NO_3^-$ ,  $H_2^{18}O$ ,  $H_2^{16}O$ ,  $^{87}Sr/^{86}Sr$

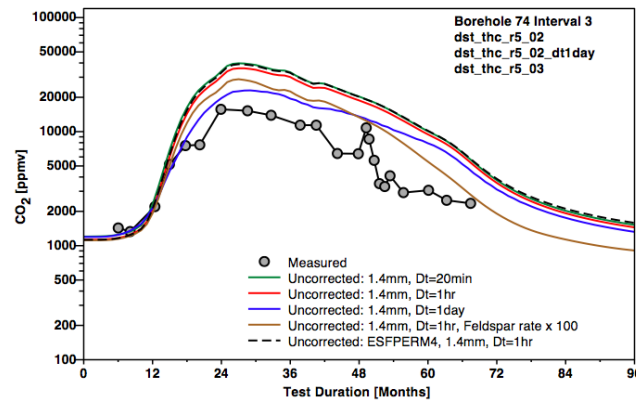
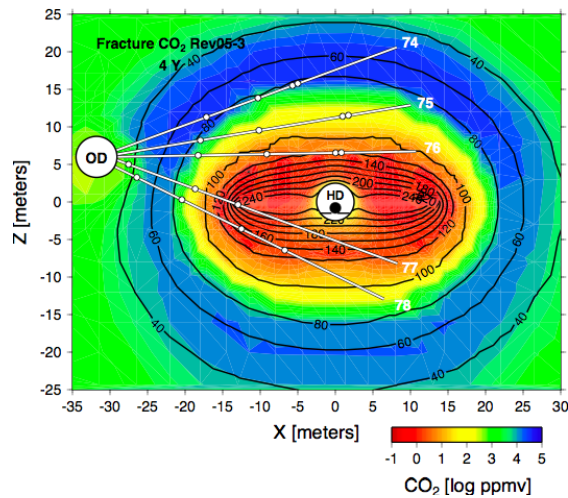
**Gas Species:**  $H_2O$ , air,  $CO_2$ ,  $H_2^{18}O$ ,  $H_2^{16}O$

> 200°C

**Minerals:** Calcite, cristobalite, tridymite, quartz, amorphous silica, feldspars, clays, zeolites, hematite, gypsum, fluorite, salt phases



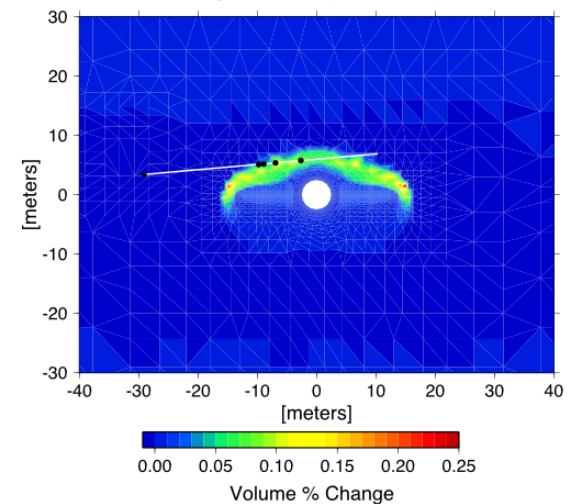
## Dual-Permeability Modeled and Measured $CO_2$ in Gas Phase



$CO_2$  fugacity sensitive to feldspar reaction rates and effective gas species diffusivities

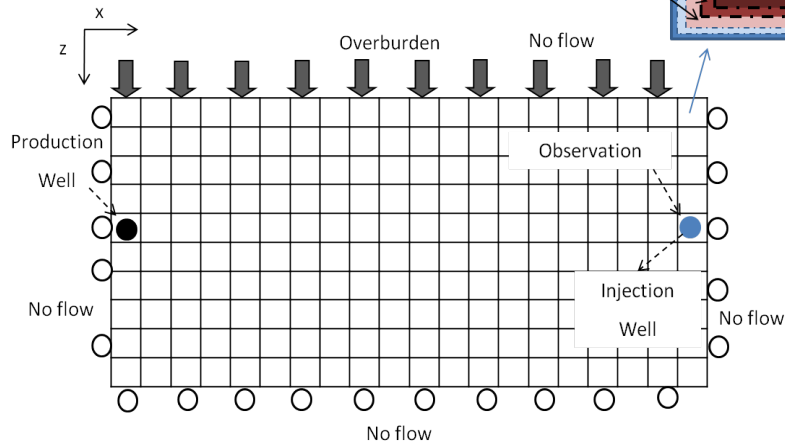
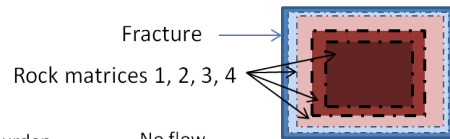
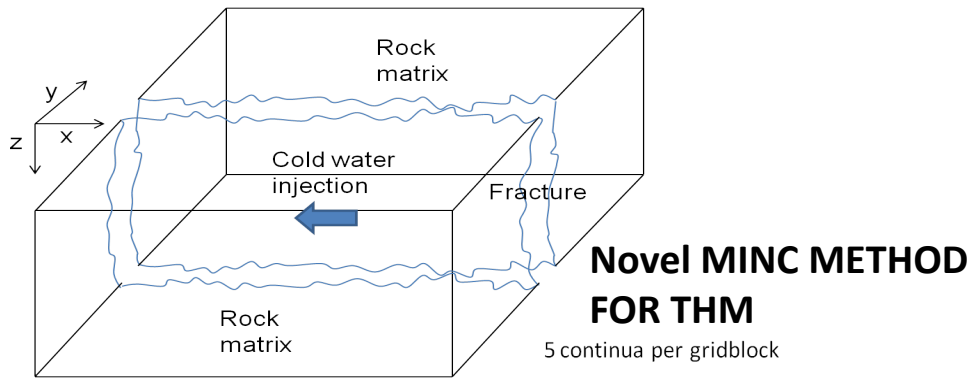
## Amorphous Silica Cap predicted: Boiling, reflux and precipitation

Modeled Fracture Amorphous Silica (Nov. 2000)  
Borehole 54 Side Wall Core Samples - Observed Amorphous Silica (filled circles)

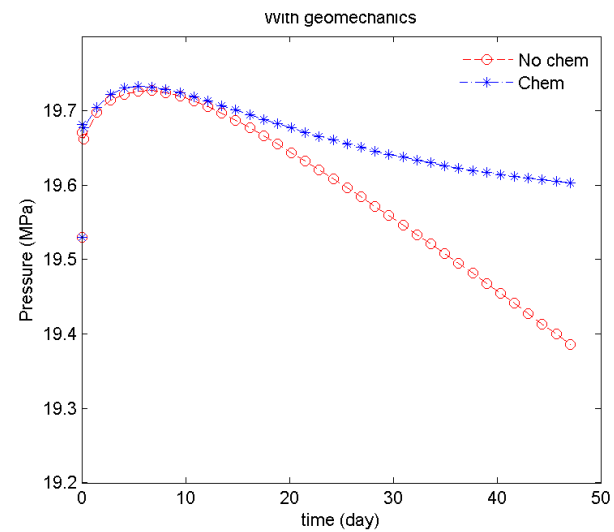
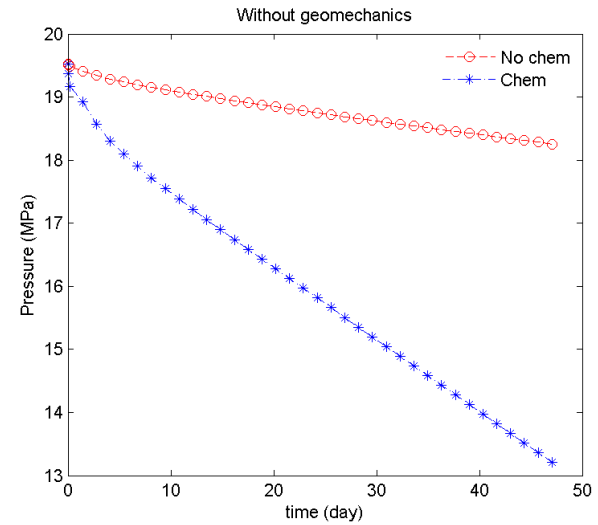


*Sonnenthal et al., 2005*

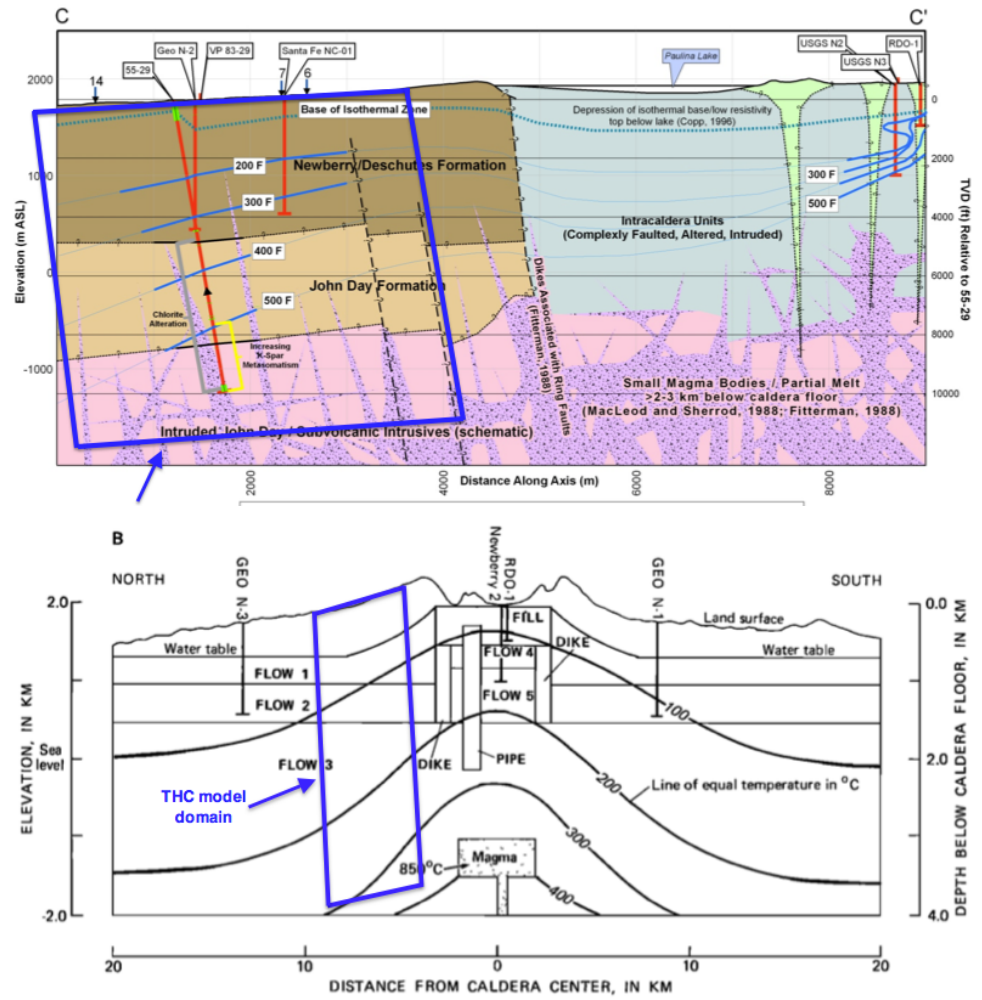
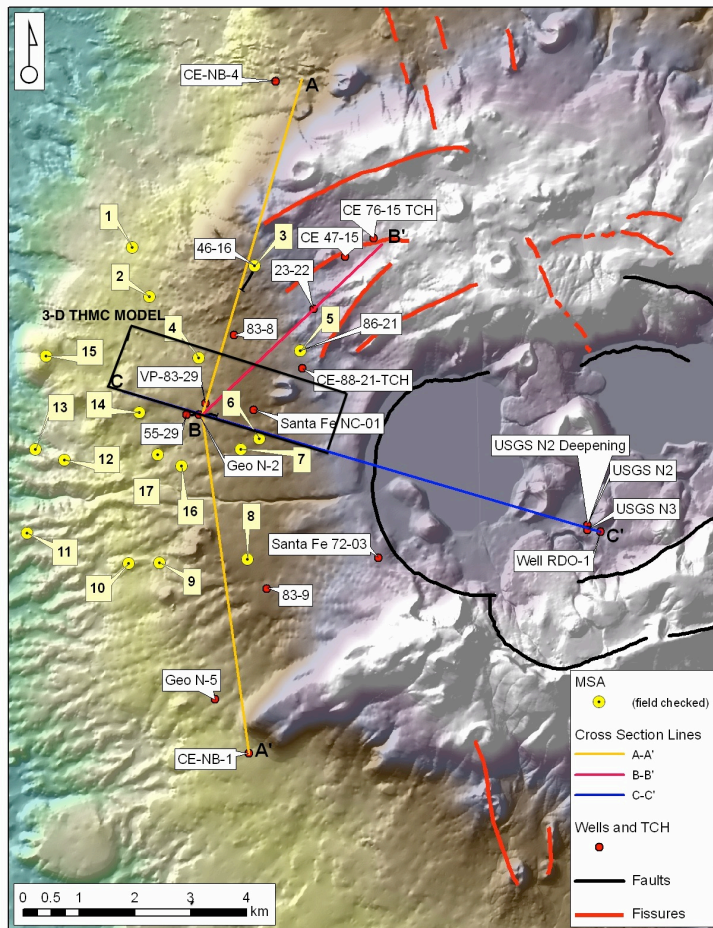
# Chemo-Thermo-Poro-Mechanics in Single Fracture



Kim et al., 2012, 2015

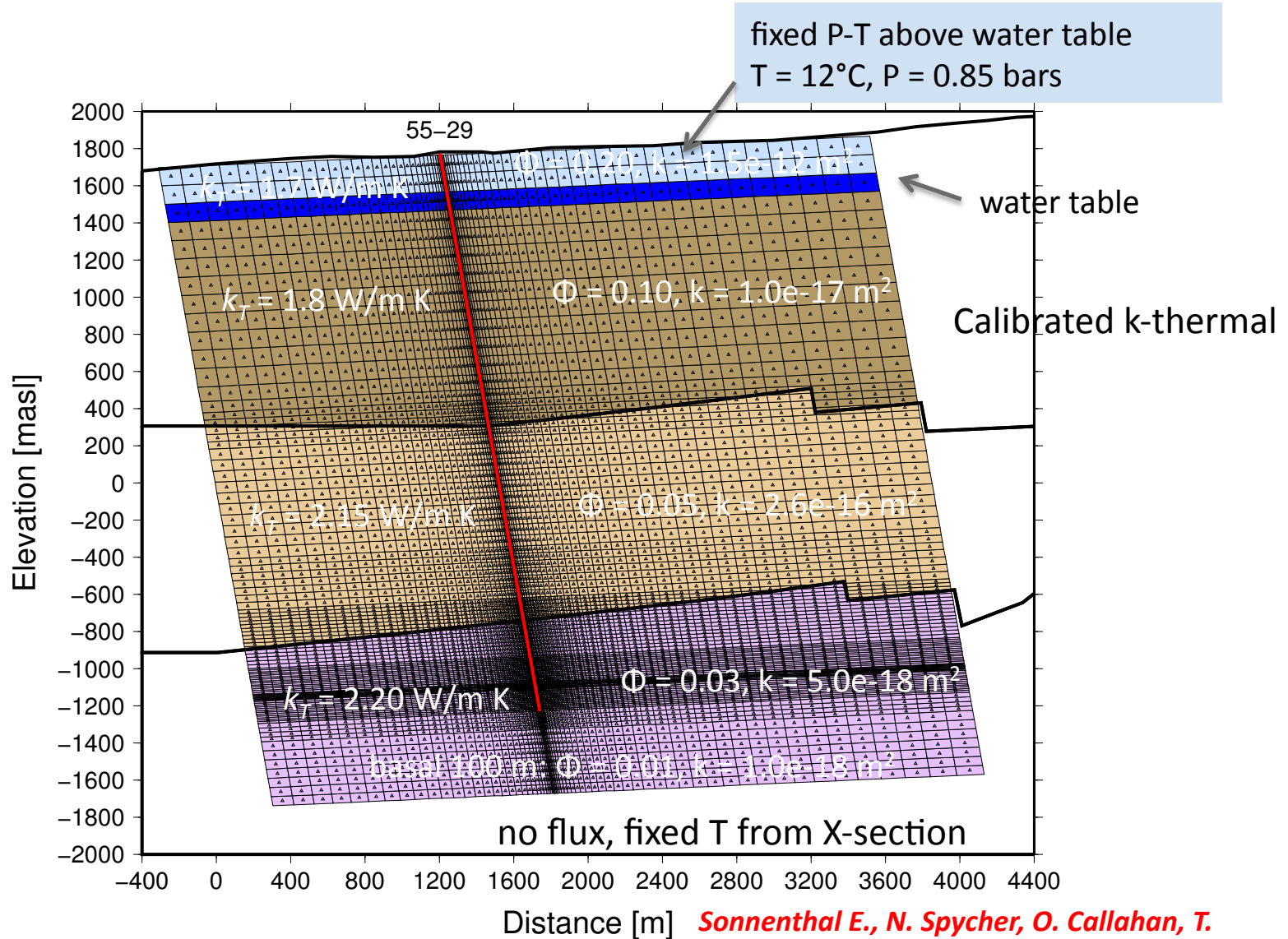


# Newberry Volcano EGS Demonstration Project 3-D THMC Model



Sammel et al. (1988). A conductive cooling model assuming intrusion of an 850°C rhyolitic magma was used to generate the isotherms.

# NEWBERRY VOLCANO 3-D MODEL GRID

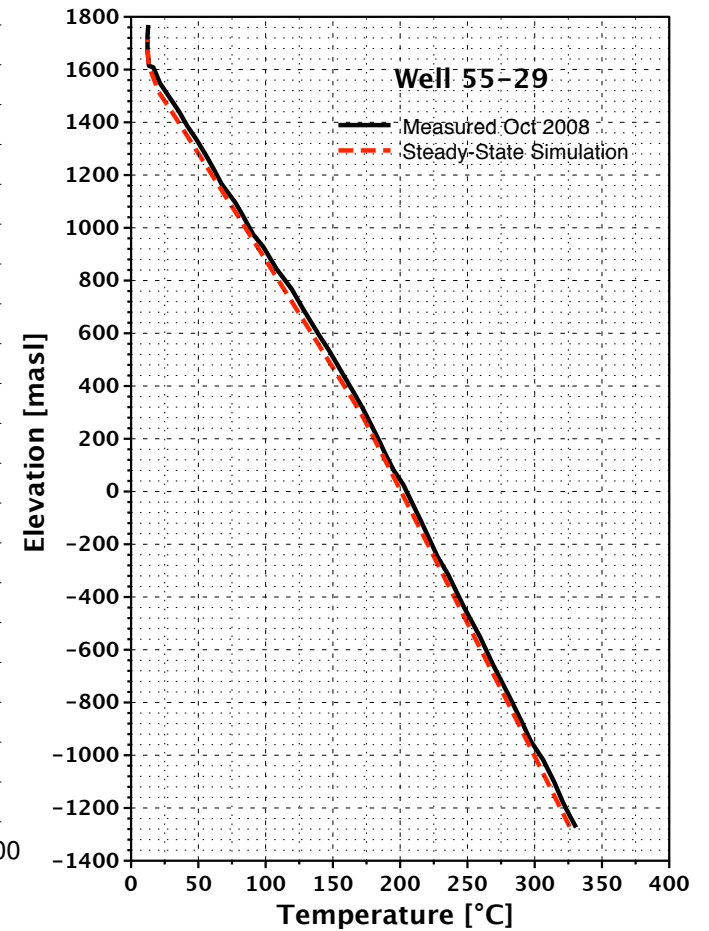
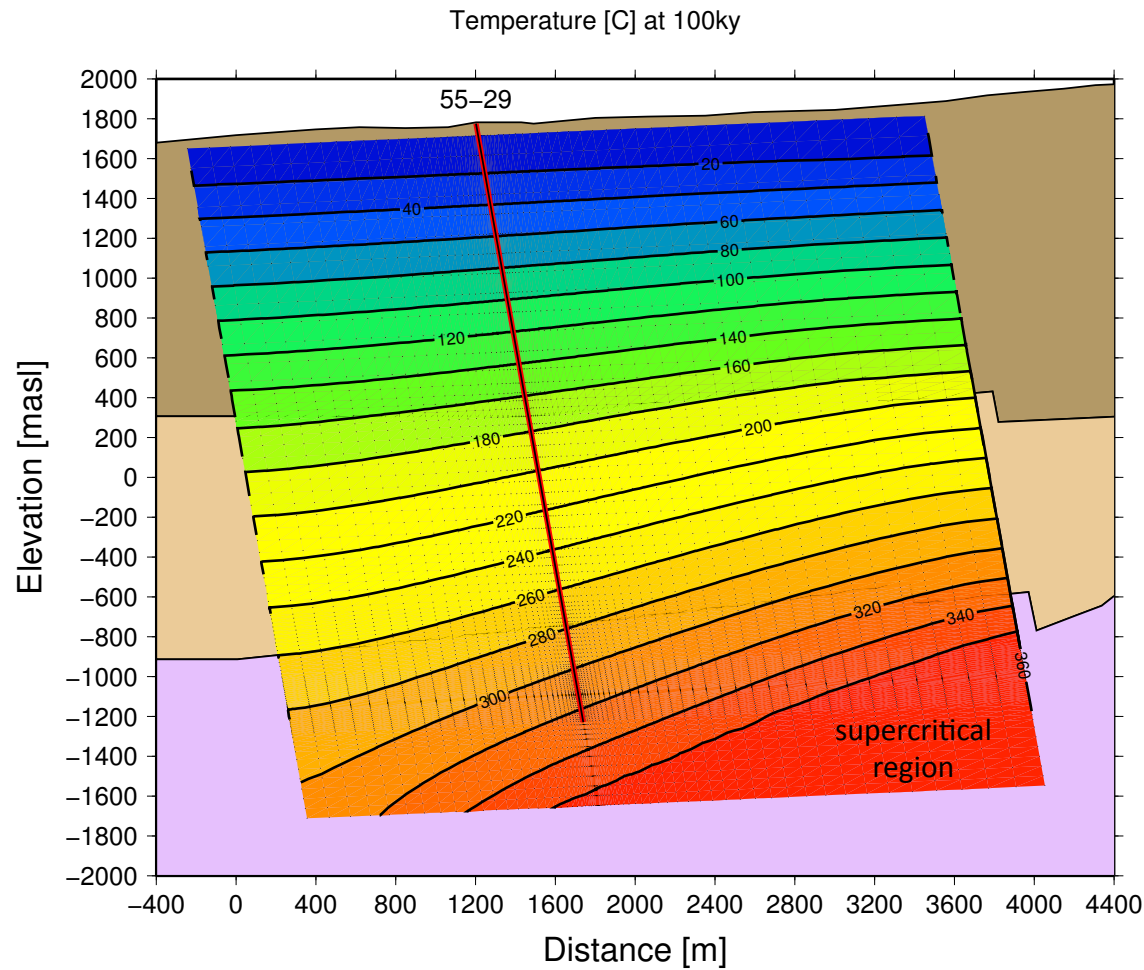


*Sonnenthal E., N. Spycher, O. Callahan, T. Cladouhos, and S. Petty, 2012.*

# Steady-State P-T Simulations

- Created initial and boundary conditions by projecting C-C' temperature contours to boundaries
- **Thermal properties** initially from Sammel et al (1988) or estimated (**density, heat capacity, thermal conductivity**)
- Set supercritical region to constant temperature (365°C)
- **Permeabilities**: Spielman and Finger (1998) and Sammel et al. (1988)
- Simulated steady-state hydrostatic P-T variations using Toughreact V2 (Xu et al. 2011)
- Calibrated thermal conductivities to temperatures in NWG 55-29
- Temperature-pressure simulated using supercritical AUTOUGH2 (Croucher & O' Sullivan, 2008)

# Steady-State Temperature Field



# Water-Gas Chemistry and Mineralogy

## Water

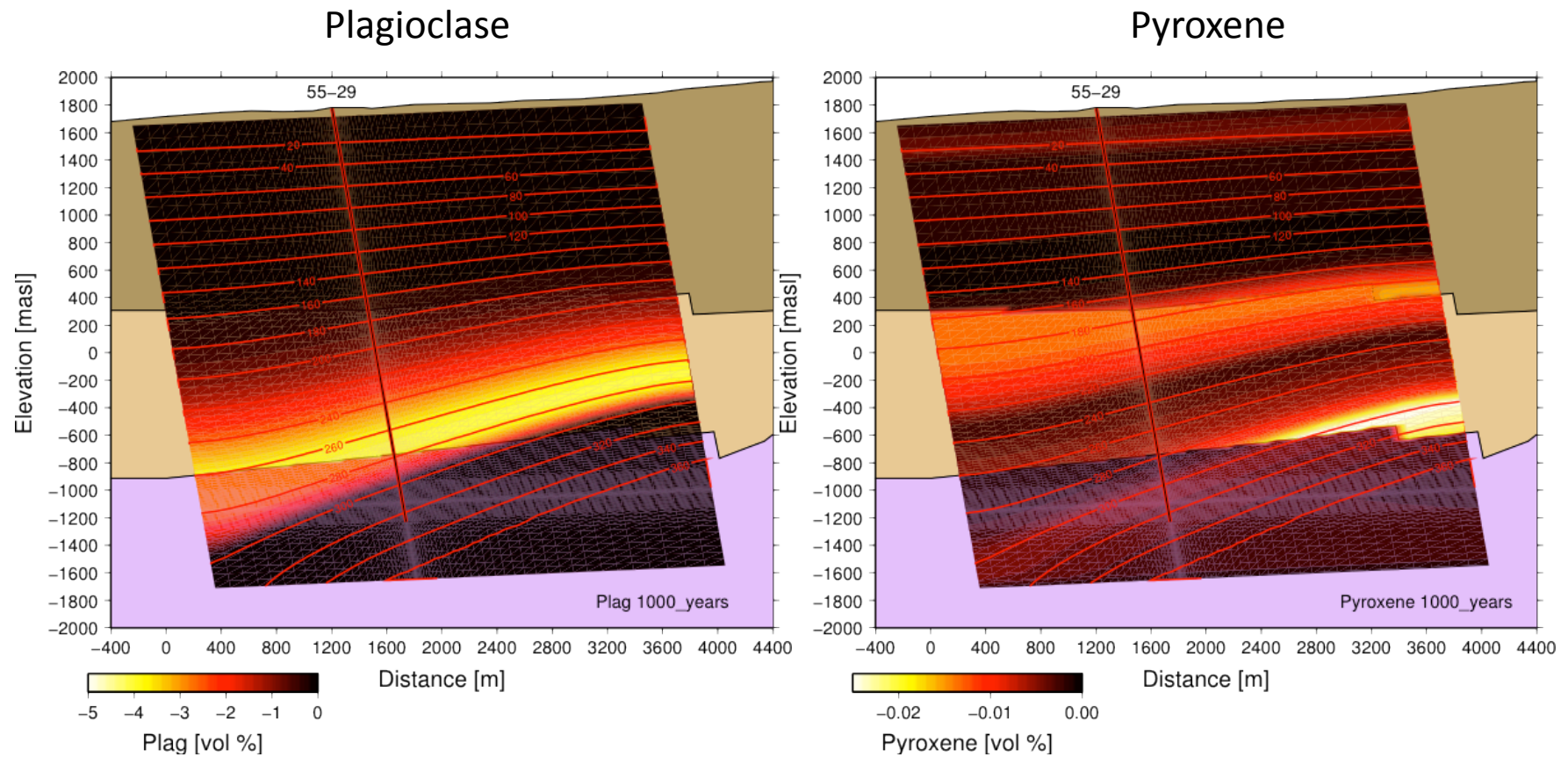
Component (mg/kg)	Pad S-29	WW2	NWG 55-29 Weir Box	East Lake Hot Spr. 5B
pH (lab)	7.97	7.85	8.3	6.3
Na	42.	45.7	1360	54
K	5.	4.72	120	8.3
Ca	19.	20	15.3	72
Mg	24.	24.9	3.36	34
Li	nd	< 0.1	nd	33
Sr	0.08	< 0.1	nd	360
Ba	0.008	0.064	2.62	
Rb	0.012	nd	nd	
B	0.55	0.57	247	1200
Al	bd	nd	nd	
Fe	bd	<0.05	7.98	4
Mn	bd	0.0089	1.14	
F	0.5	0.582	7.75	
Cl	3.0	13.8	646	1
SO <sub>4</sub>	2.5	2.58	233	10
P	0.2	nd	nd	
Si	60.	54.7	99.4	471
Ar	nd	0.034	3.96	
Total Alk	230	296	2930	
CO <sub>3</sub> <sup>2-</sup>	nd	< 2.00	235	
Alk (HCO <sub>3</sub> <sup>-</sup> )	230.	296	1350	
NH <sub>3</sub>	nd	< 0.255	12	

## Gas

Noncondensable Gases		
Well	NWG 55-29	NWG 55-29
Sample	#2	#3
Date/Time	7.19.08 0:00	7.19.08 0:36
	Dry gas % by vol	Dry gas % by vol
H <sub>2</sub> O vapor	none measured	none measured
CO <sub>2</sub>	99.2	99.2
H <sub>2</sub> S	0.0589	0.0601
NH <sub>3</sub>	<.0274	<.0144
Ar	0.00138	0.00151
N <sub>2</sub>	0.622	0.562
CH <sub>4</sub>	0.042	0.0408
H <sub>2</sub>	0.113	0.106
%air	0.117	0.014

Primary Minerals	Potential Secondary Minerals
Albite	Calcite
Anorthite	Siderite
Microcline	Ankerite
Sanidine	Dolomite
Diopside	Anhydrite
Hedenbergite	Chalcedony
Phlogopite	Quartz
Annite	Microcline
Muscovite	Muscovite
Quartz	Paragonite
Cristobalite	Illite
Magnetite	Nontronite-Ca
	Nontronite-Mg
	Nontronite-Na
	Nontronite-K
	Kaolinite
	Epidote
	Daphnite
	Clinocllore
	Heulandite
	Laumontite
	Analcite
	Magnetite
	Hematite
	Goethite
	Pyrite
	Pyrrhotite

# Results: Primary Mineral Dissolution

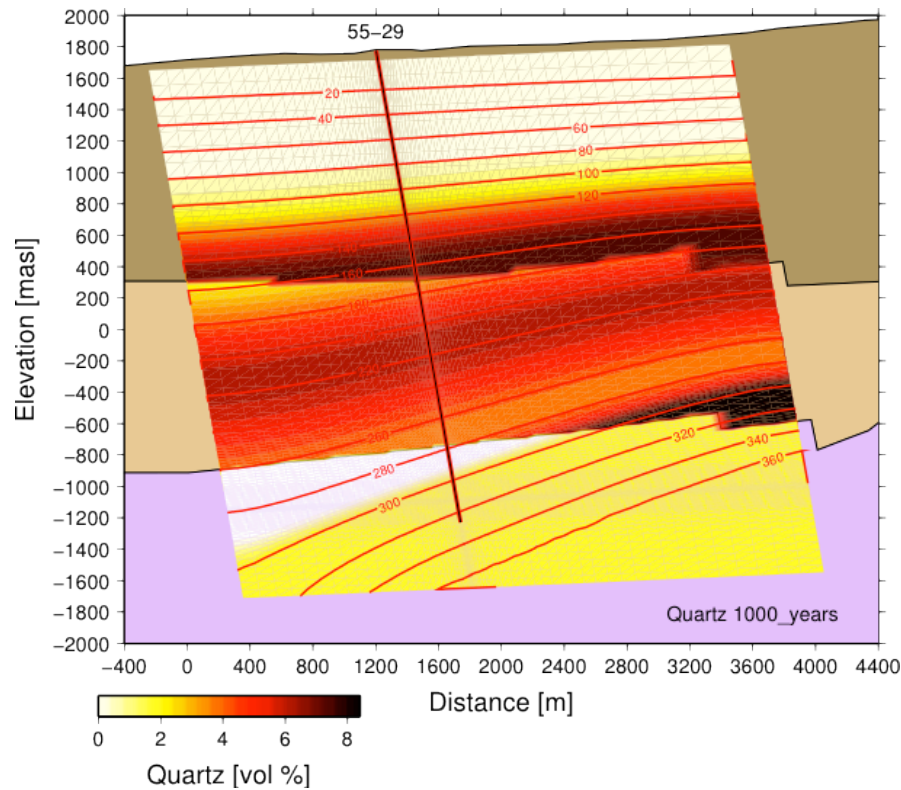


Primary igneous plagioclase, pyroxenes, cristobalite unstable as expected  
Dependent on temperature, initial abundance, water-rock ratio



# Precipitating Secondary Phases

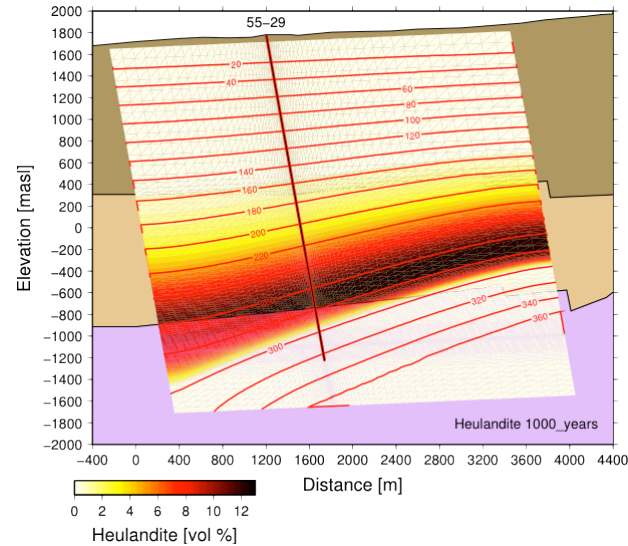
## Quartz



Quartz common in fractures at depth and as silicification (aided by cristobalite dissolution)

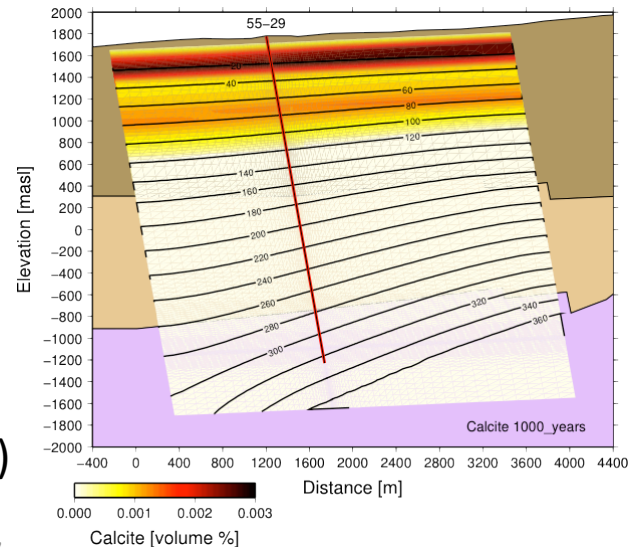
## Heulandite

\*Not common



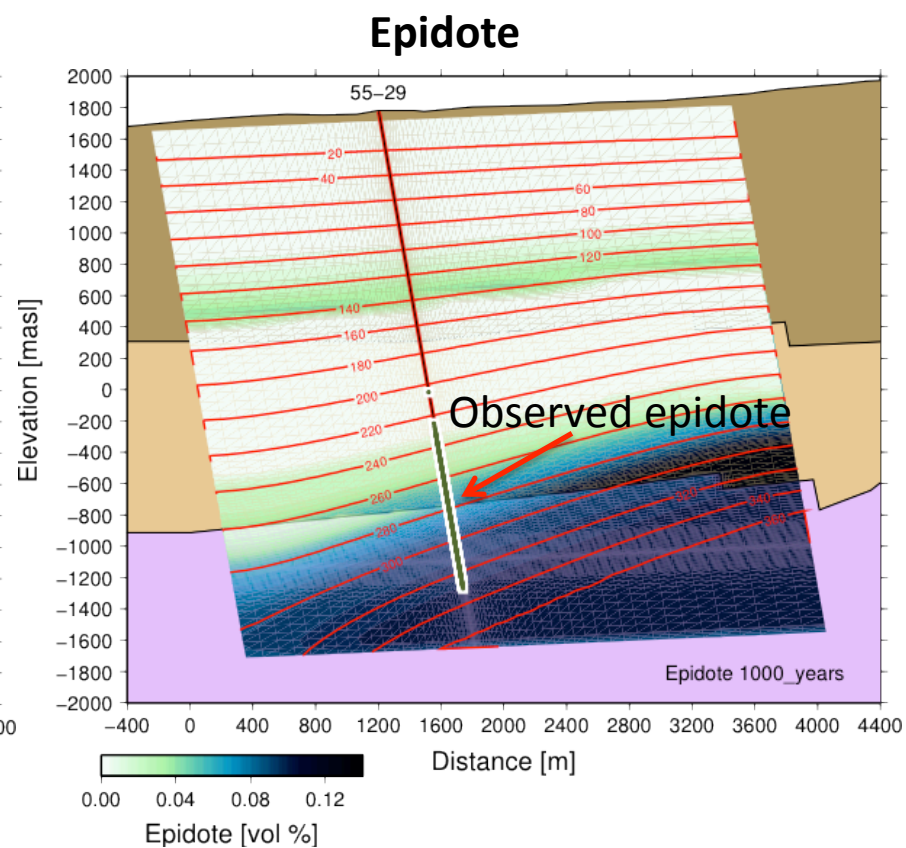
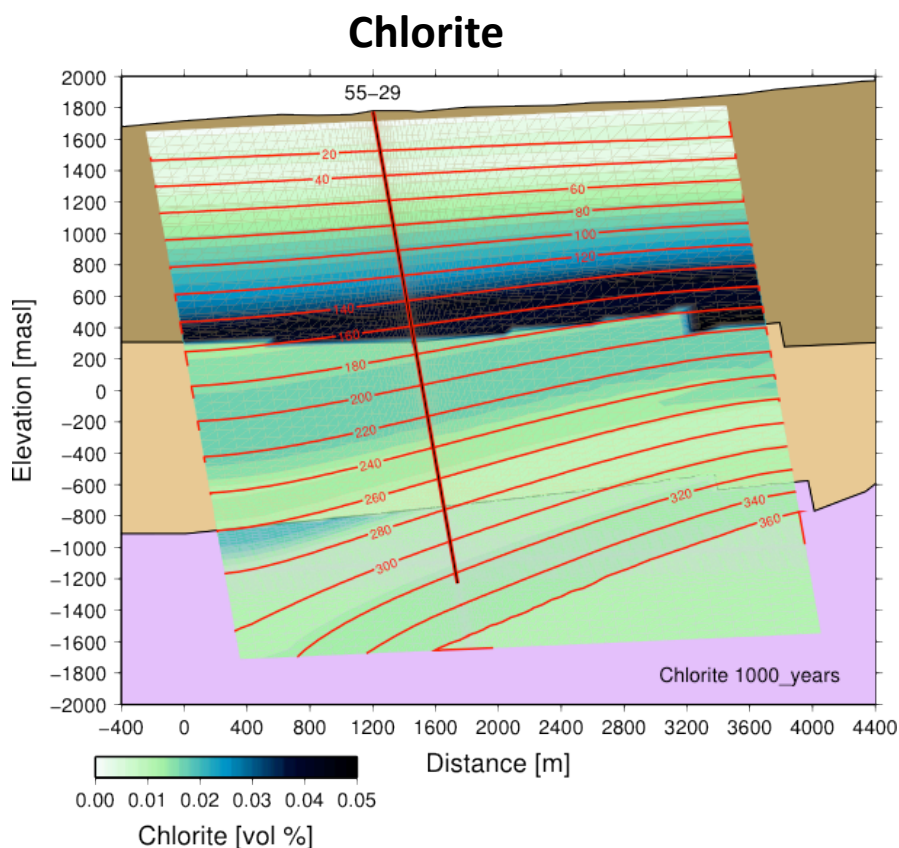
## Calcite

\*Common in fractures at depth



Pyrite also common, but not in model

# Chlorite and Epidote Distributions



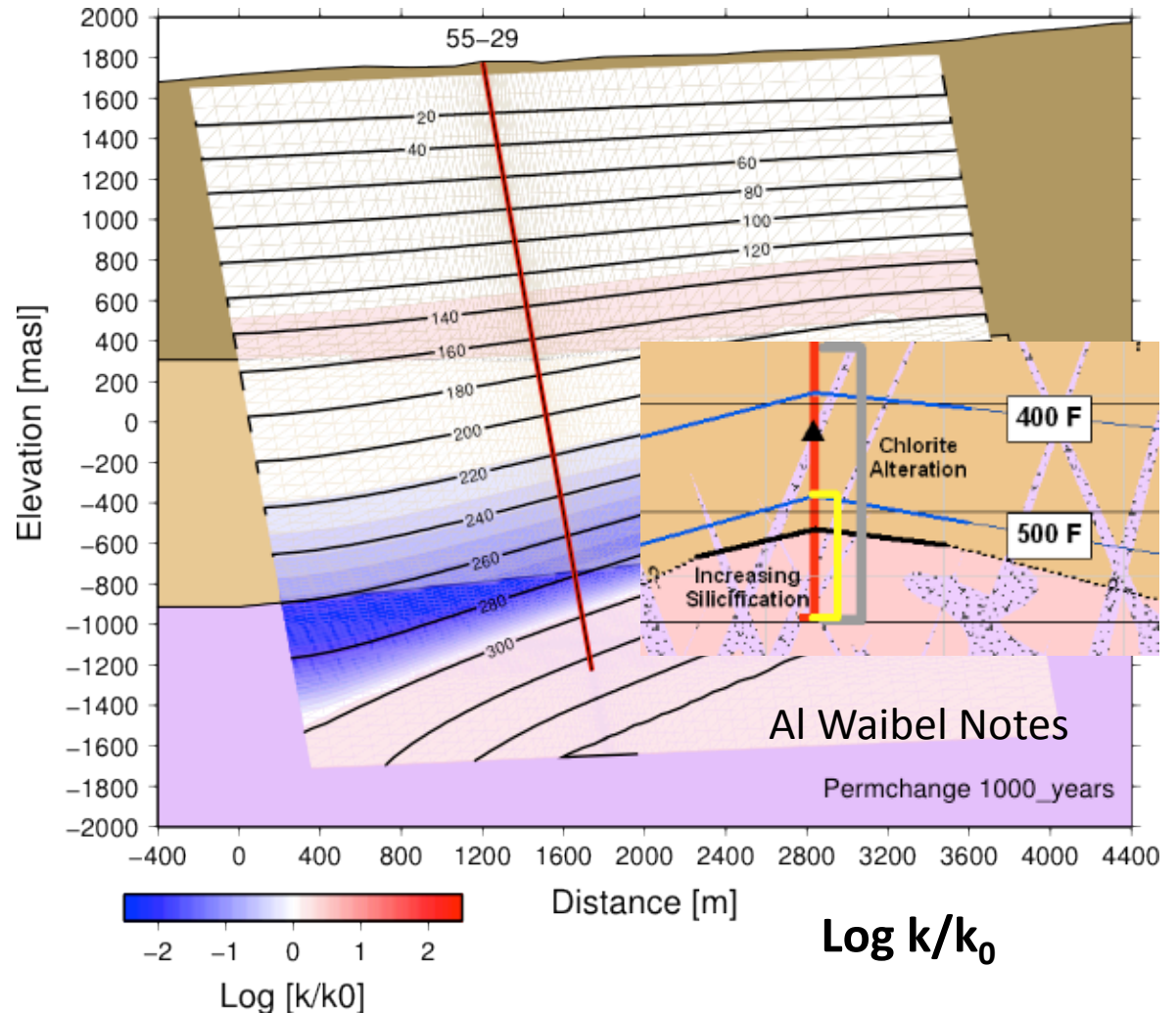
Chlorite-smectite and chlorite are commonly observed alteration minerals over most depths

Epidote observed below 207°C in green shaded zone  
 Except for shallow metastable epidote in the simulation, modeled distribution is close to observed  
 -> Temperatures never much hotter than at present

# PERMEABILITY EVOLUTION

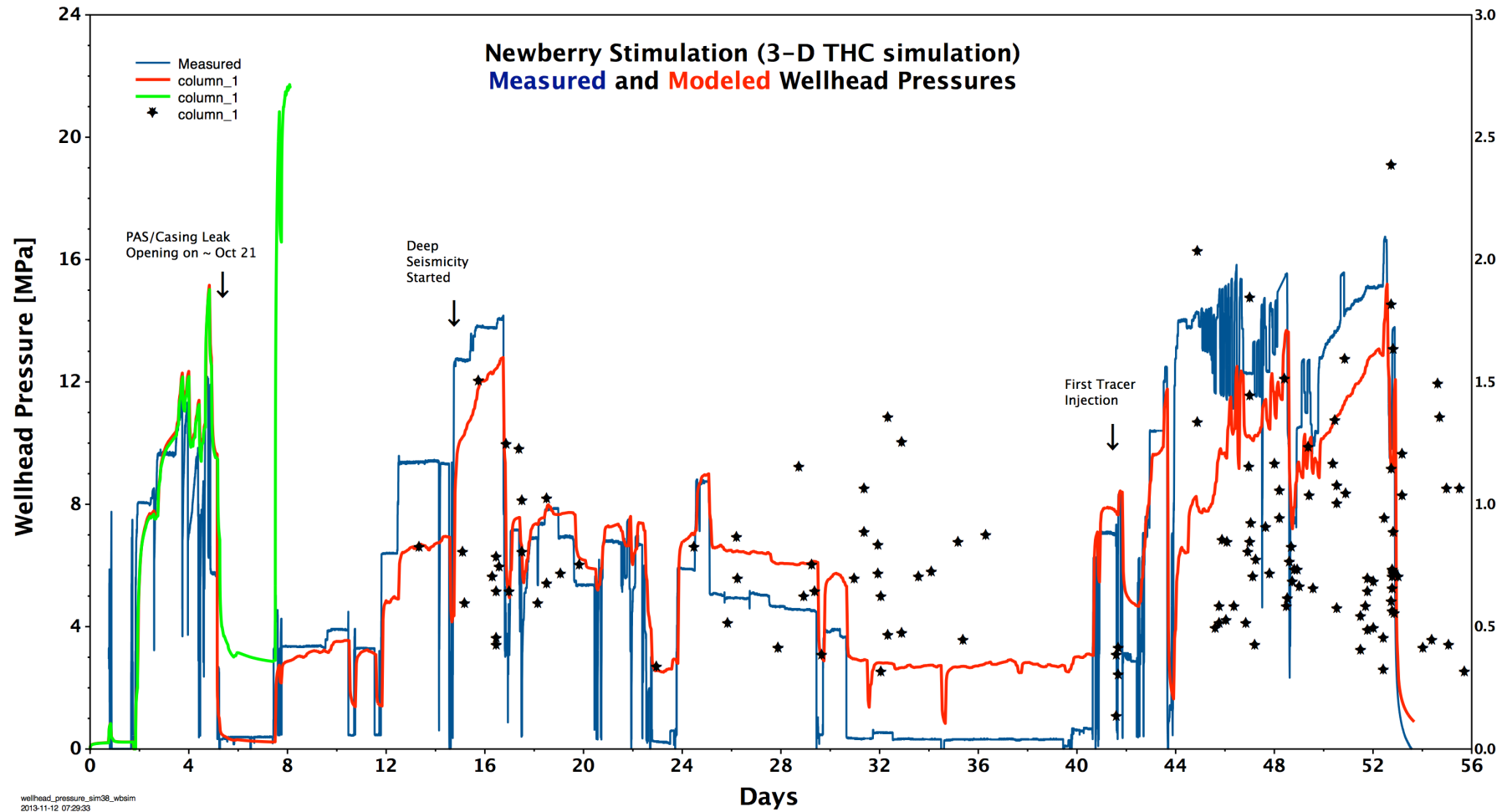
Permeability Evolution (1000 yrs)

- Objective: Find regions most likely to have either lower or higher permeability than expected
- Reaction-induced permeability changes related to lithology, temperature, fluid fluxes and composition, porosity & permeability, fracture properties, pressure
- Evaluate permeability structure for siting EGS, design of wells, long-term operation



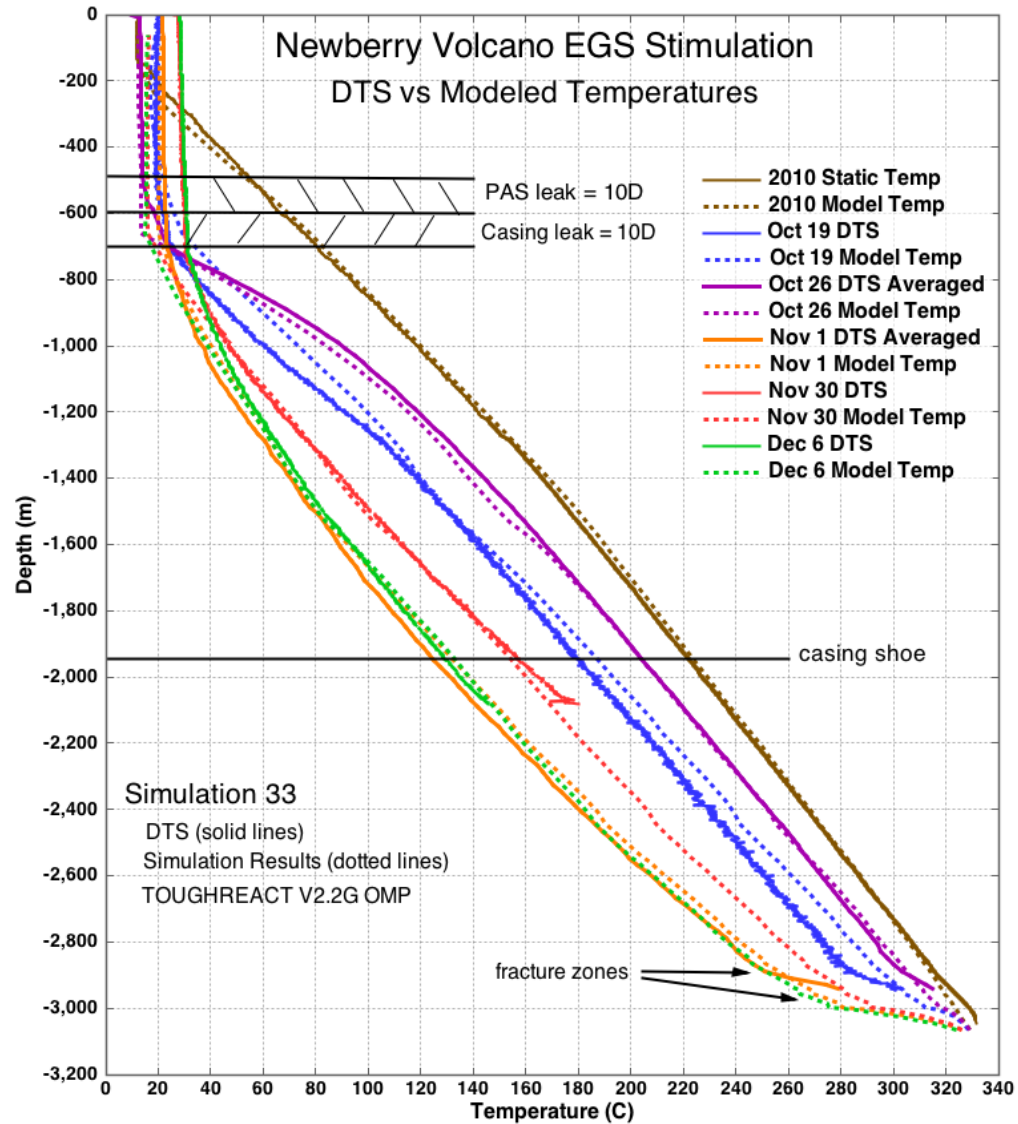
# NEWBERRY VOLCANO EGS 2012 STIMULATION

## Wellhead Pressure and Microearthquakes



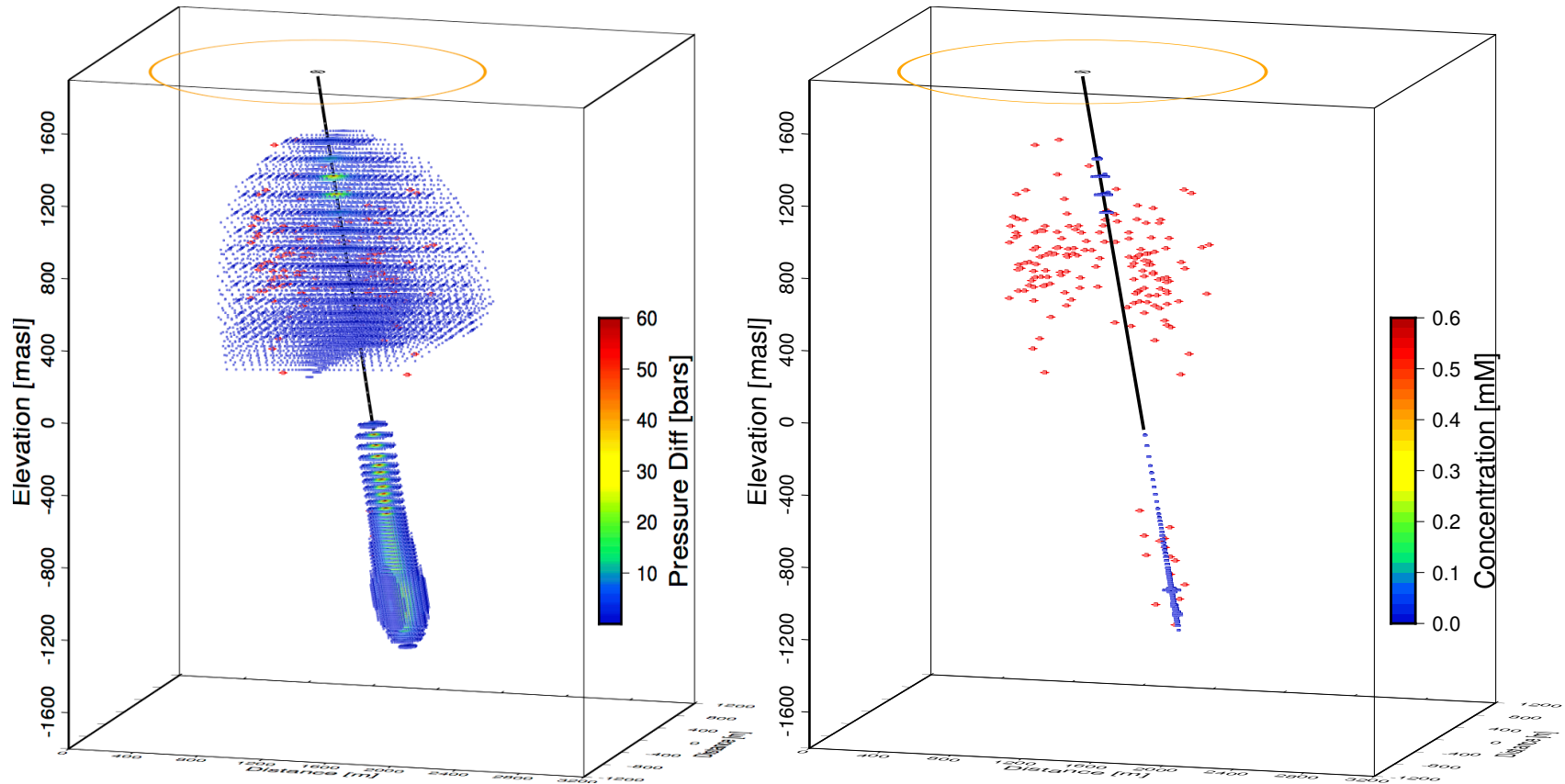
# NEWBERRY VOLCANO EGS 2012 STIMULATION

## Temperatures Changes During Stimulation



Measured temperatures:  
AltaRock Energy

# Newberry Volcano EGS Stimulation MEQs and Modeled Pressure and Thermal Tracer

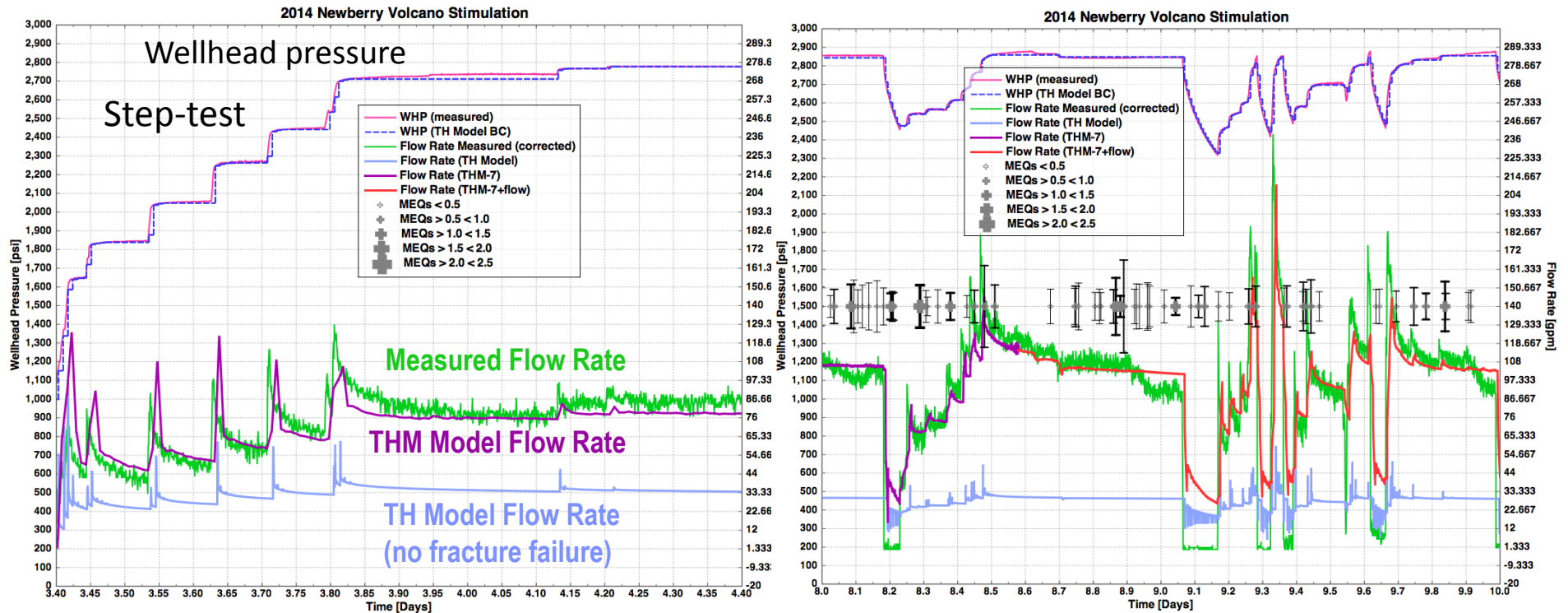


Pressure differential (left;  $P_{\text{total}} - P_{\text{hydrostatic}} > 0.05 \text{ MPa}$ ) and thermally-degrading tracer (right) plotted at 50 days (close to the end of stimulation). Yellow circle outlines a region having a 1 km radius from the wellhead (black circle at top). Cased interval is in black. Red symbols are relocated MEQs (Cladouhos et al., 2013).

# 2014 Newberry Stimulation Wellhead Pressure and Flow Rates Compared to 3-D THM Model Results

9/26-9/27/2014

10/1-10/3/2014



## THM Model Parameters:

2 degree MC dilation angle

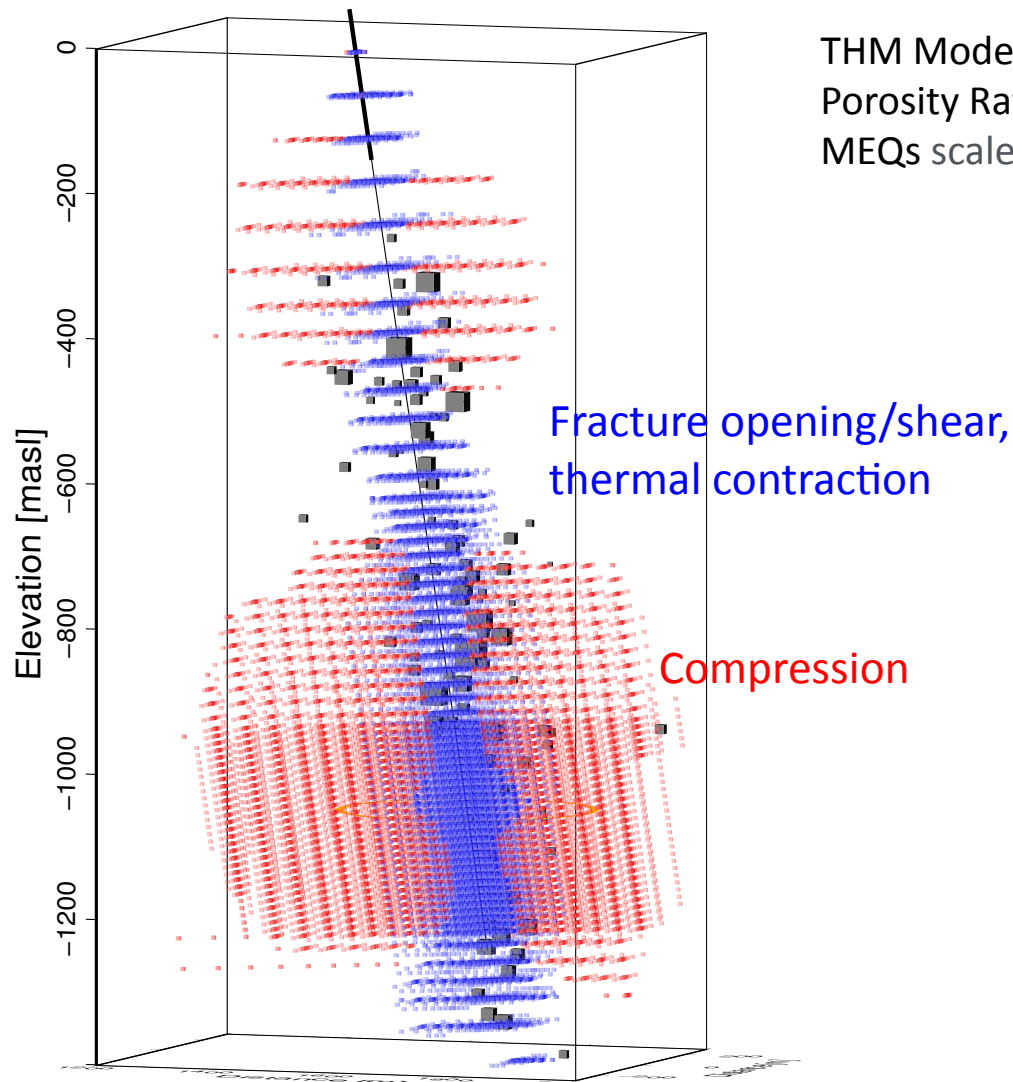
Fracture Porosity = 0.001

Cohesion: 2 MPa

Stress Model: (Cladouhos et al., 2012)

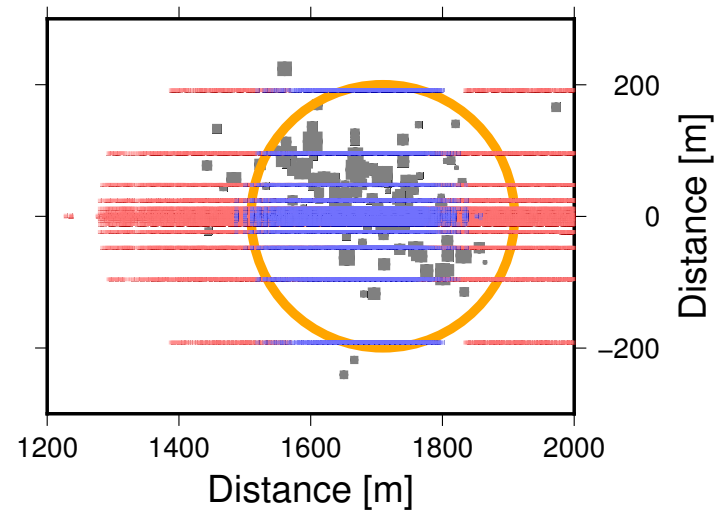
- TH Model (no failure) predicts only ~32 gpm (~2 kg/s) flow rate
- Early shear+tensile failure increases permeability ~10-100x and captures increased flow rate to ~120 gpm
- Restarting TH model (no failure; red curve) with permeabilities kept constant from THM model matches flow rates throughout the rest of the injection period, indicating no near-wellbore improvement after 9 days

# Simulated Thermal-Hydro-Mechanical Changes in Porosity and Observed Microearthquakes (MEQs)



THM Model at 9 Days  
Porosity Ratio ( $\varphi/\varphi_0$ ) Blue  $> 1$  Red  $< 1$   
MEQs scaled by magnitude

Surface Plan View (yellow circle is 200m radius around wellhead)

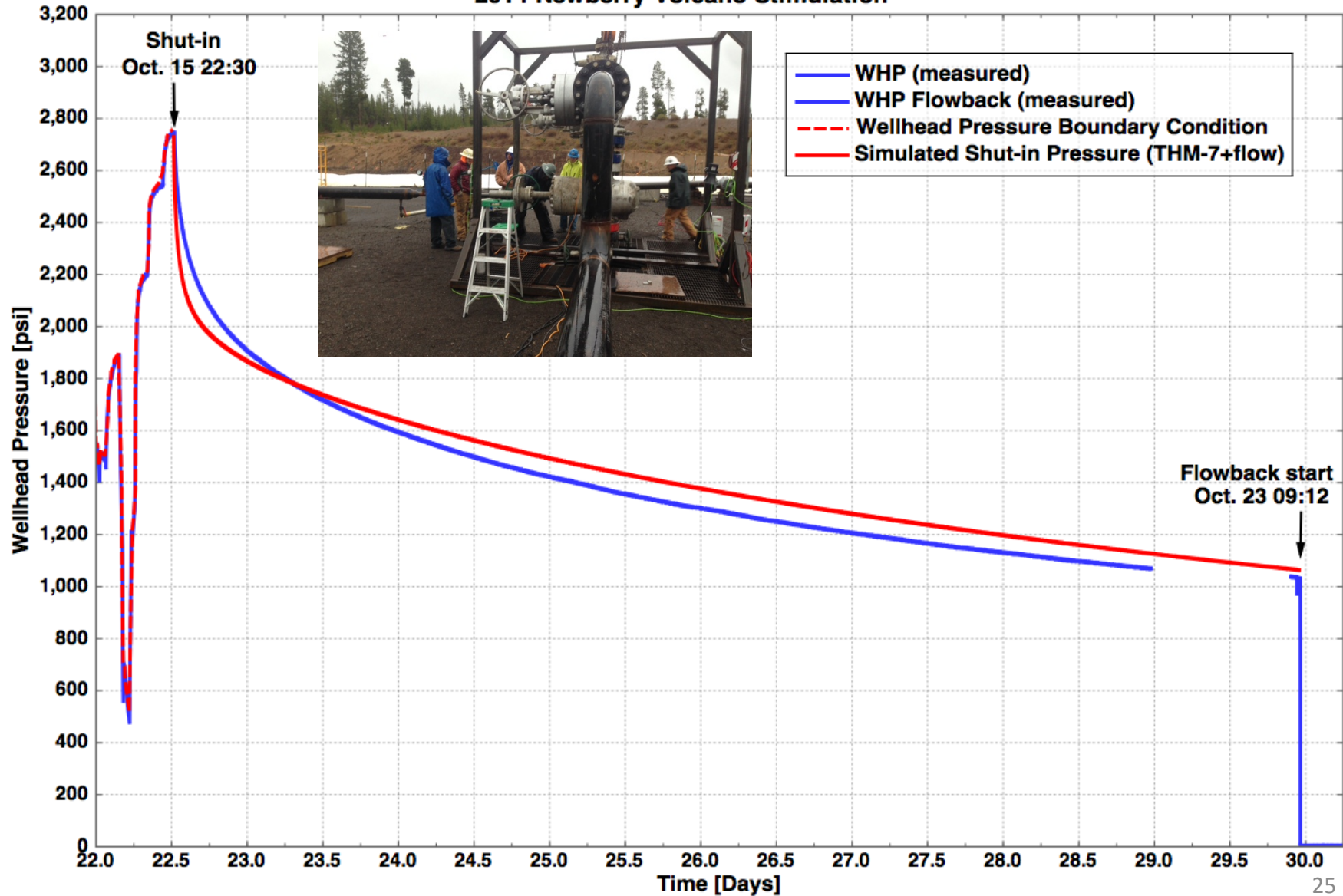


Sonnenthal et al., 2015; Smith et al., 2015  
Cladouhos et al., submitted

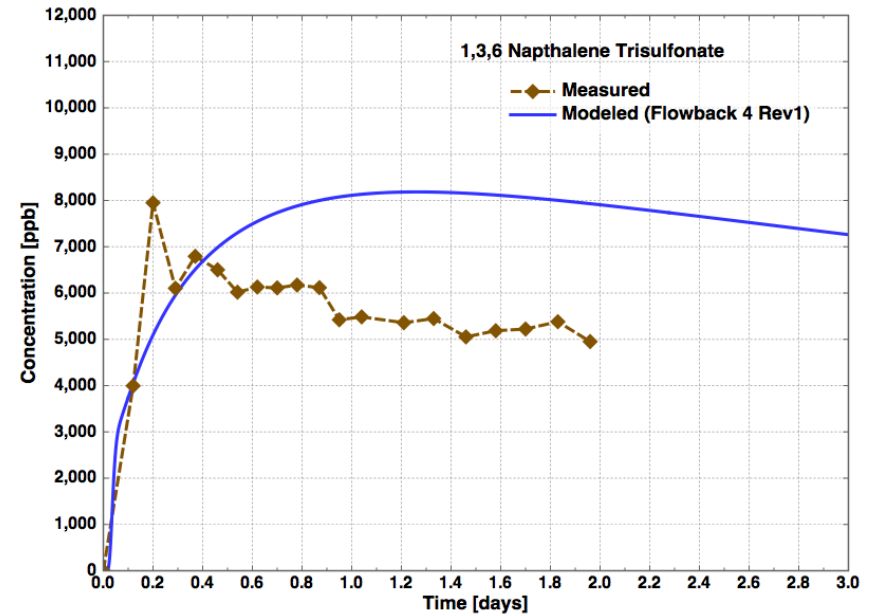
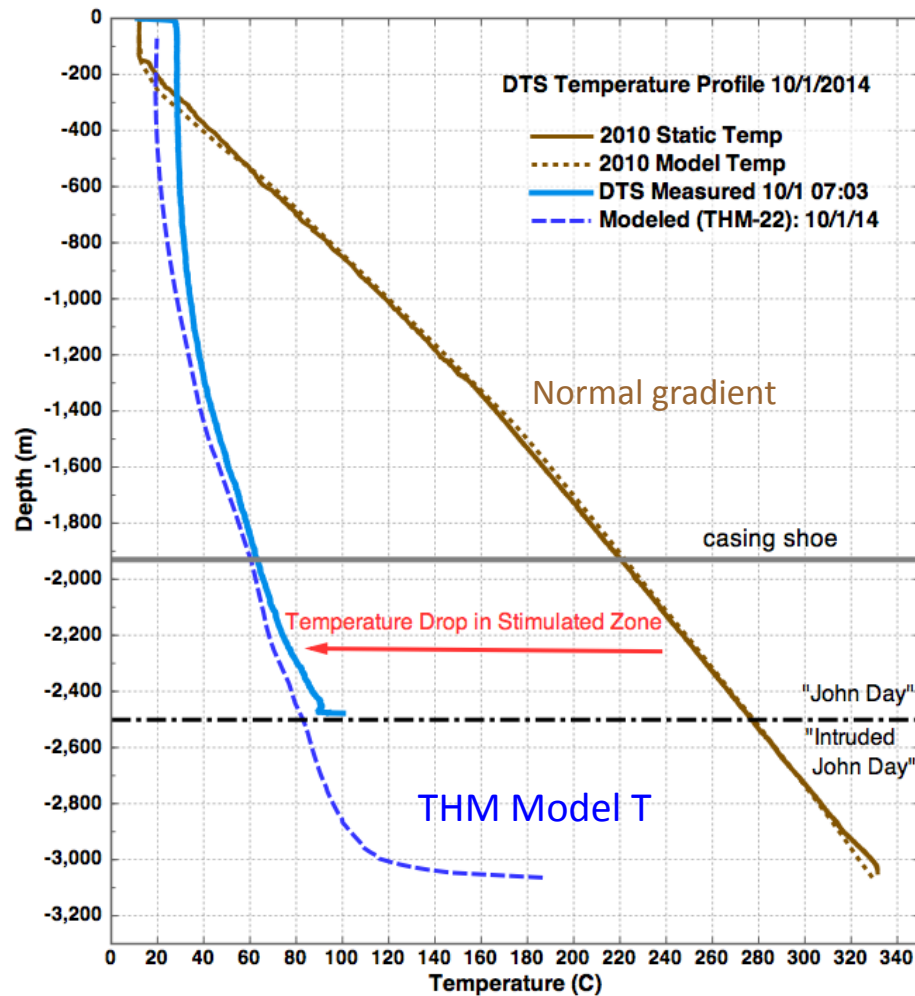


# Wellhead Shut-In Pressure 10/15/2014 – 10/23/2014

2014 Newberry Volcano Stimulation



# Measured/Modeled Wellbore Temperatures and Naphthalene-Trisulfonate 1,3,6 Tracer Concentrations



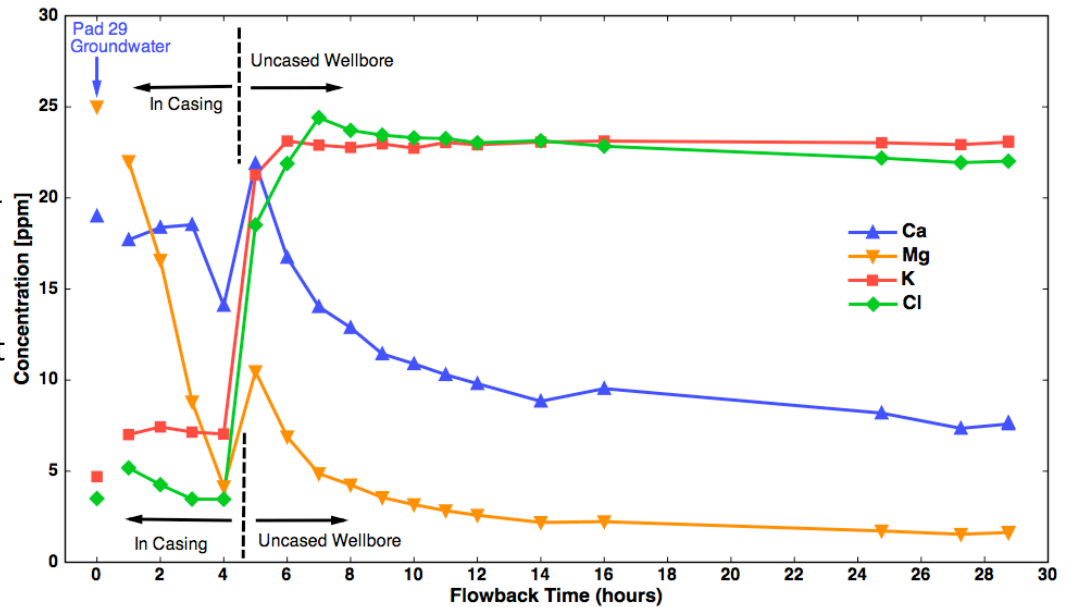
- Tracer recovery greater in THMC model likely owing to plugging by chemical diverter in field test

- Temperature range of open hole from 220 – 330°C
- Wellbore temperatures at maximum flow rates are depressed by ~180°C in the reservoir center (2400 m below surface) during stimulation

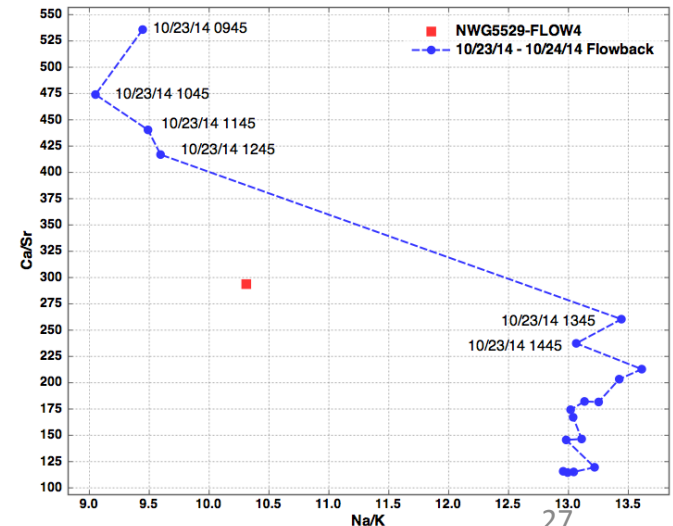
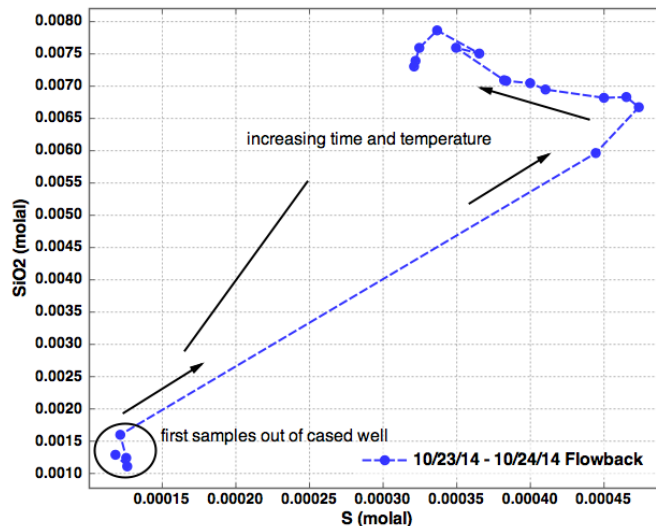
*Sonnenthal et al., 2015*

# Flowback Water Chemistry: Oct. 23-24, 2014

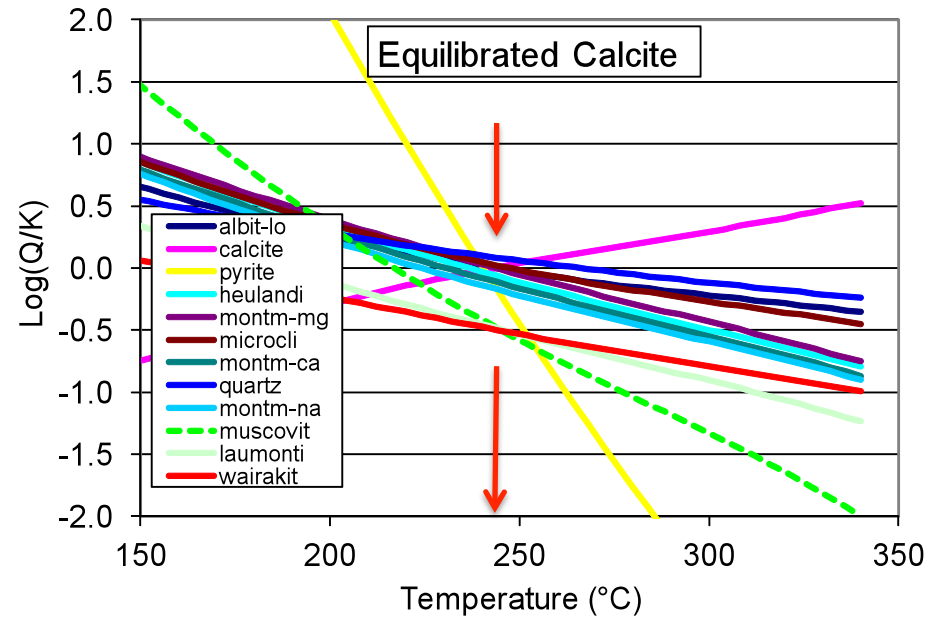
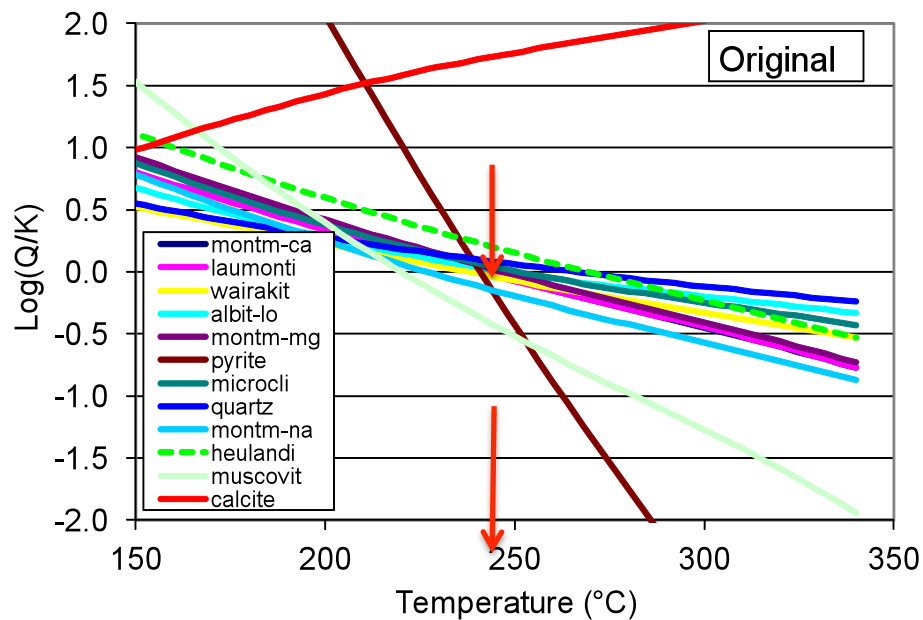
- > Flowback waters show systematic trends from heated groundwater in the cased interval to water-rock reaction and mixing with hydrothermal waters
- > Sharp increase in Cl indicates mixing of injected groundwater with a small amount of more saline *in-situ* geothermal/magmatic fluid (He R/Ra ~ 8)
- > Increase in K indicates reactions with feldspars
- > Increases in Ca, followed by a sharp decline reflect calcite dissolution and precipitation at higher temperatures
- > Mg declines owing to Mg-silicate precipitation during groundwater heating in casing, precipitation of chlorite in rock, followed by redissolution in casing during flowback



- Silica increases owing to reactions with quartz and feldspars
- Total sulfur increases due to reactions with pyrite & sulfides but then decreases
- Ca/Sr vs Na/K show trends due to calcite dissolution/precipitation and feldspar reactions in the rock



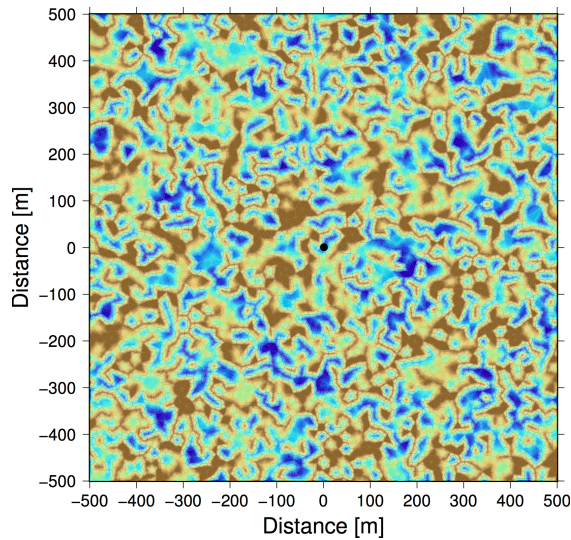
# Multicomponent Geothermometry on Flowback Waters



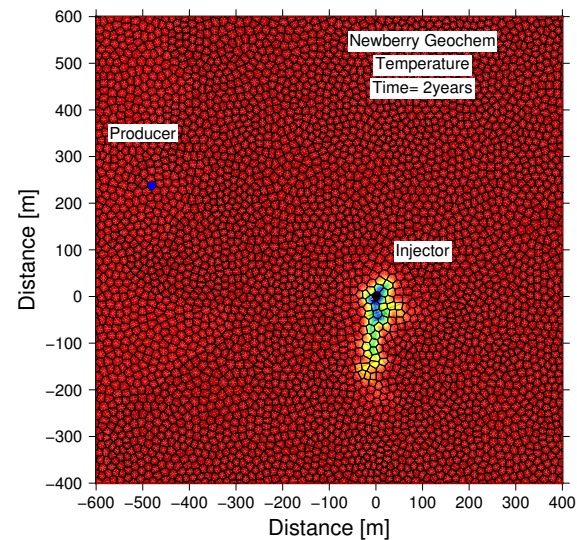
- Multicomponent Geothermometry using GeoT (Spycher et al., 2011; 2014)
- Sample from end of first flowback ( $T \sim 90^\circ\text{C}$  at wellhead)
- Estimated  $T$  around  $240\text{-}250^\circ\text{C}$  using realistic minerals - *where curves cross  $\log(Q/K) = 0.0$*
- Large supersaturation wrt calcite (chlorite also hugely above saturation)

# THC Predictions of Mineral Dissolution-Precipitation in a Stimulated Fracture System with Injector-Producer wells

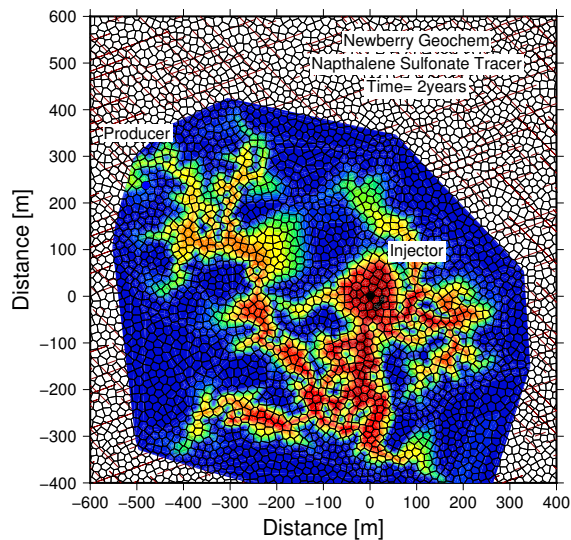
Permeability field – plan view



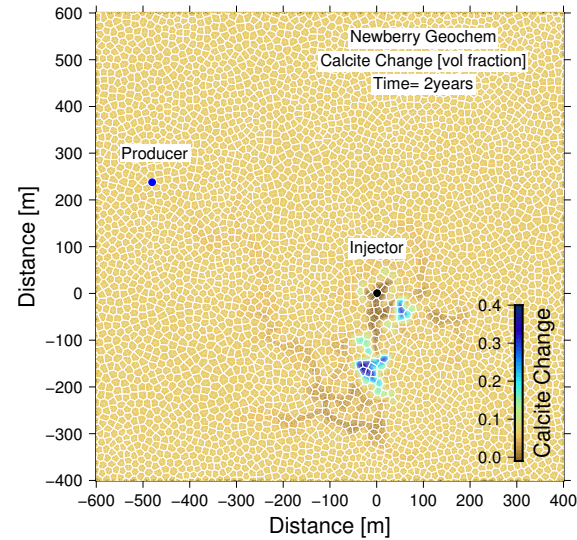
Temperature Drop after 2 years



NTS concentration after 2 years

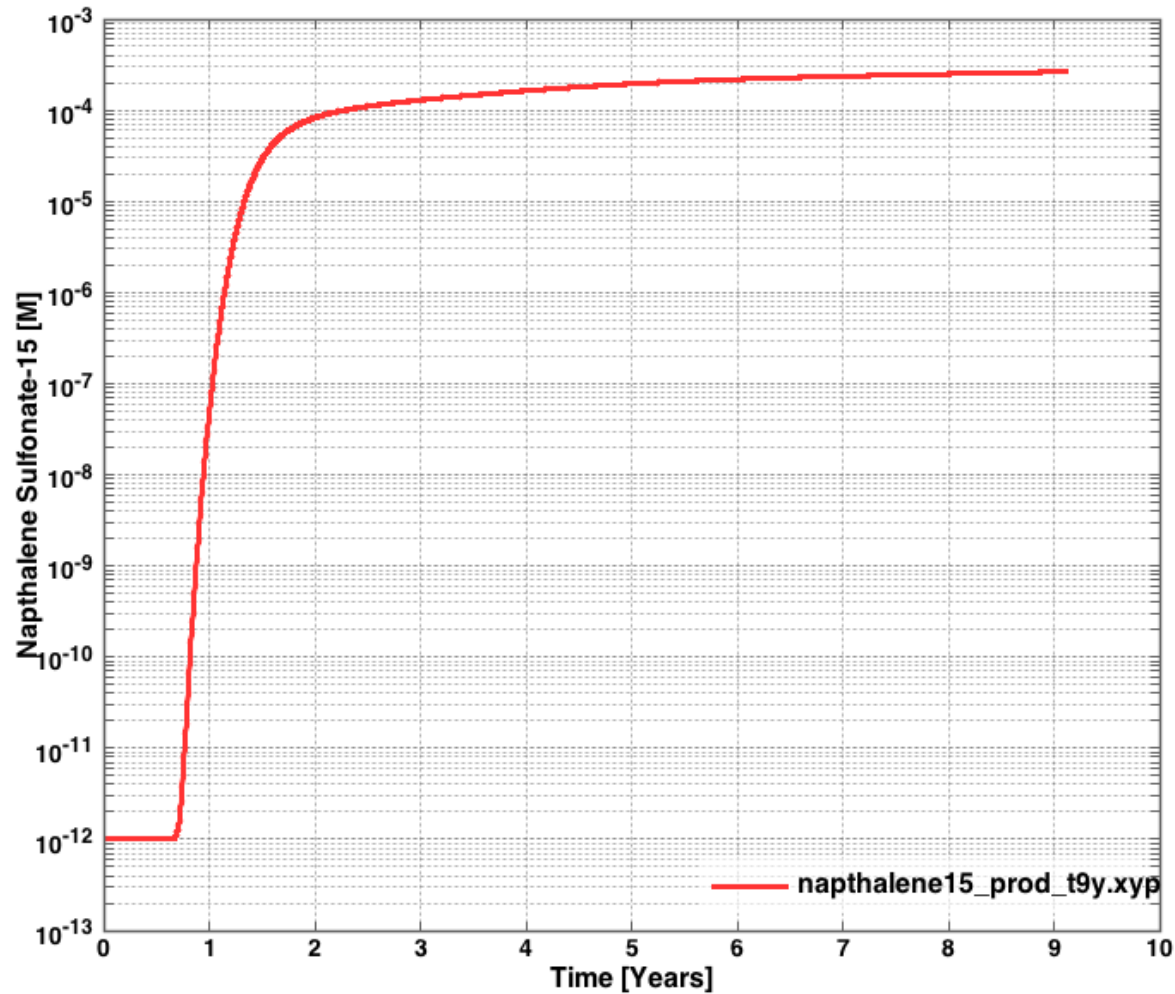


Calcite diss/prec after 2 years



Injection = 80 kg/s per 1 km interval

# Tracer Concentrations at Producing Well



~ 9 Years

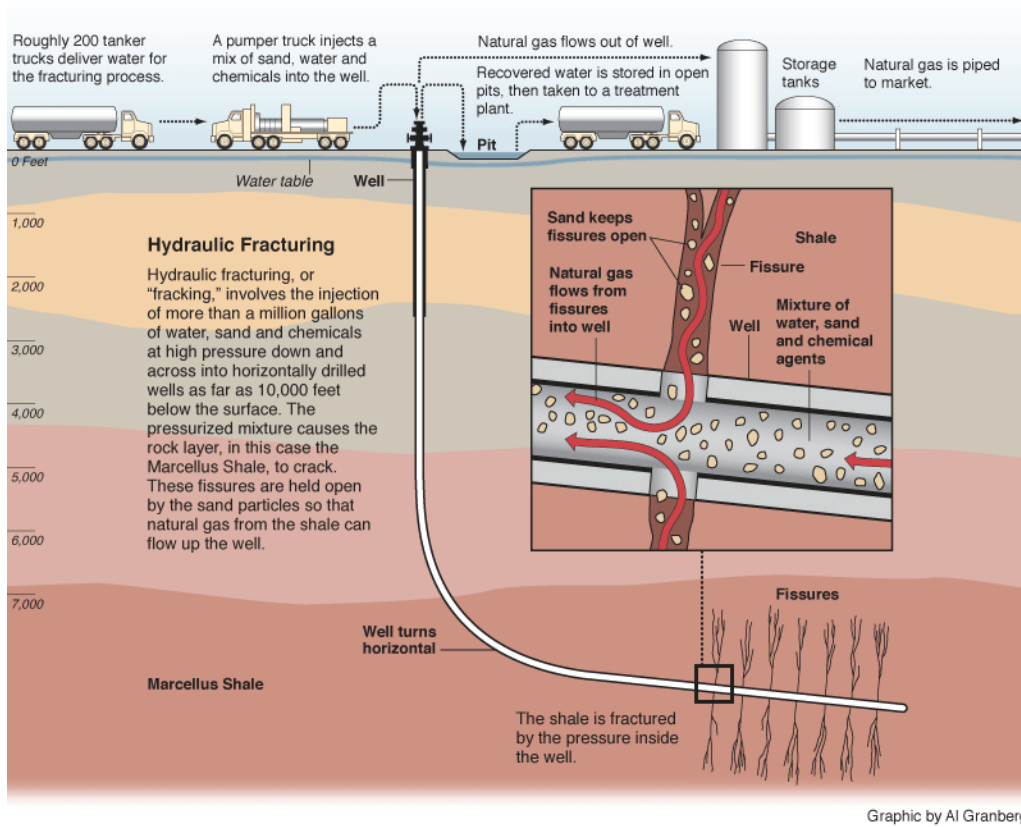
Newberry Geochemistry

Injection = 80 kg/s per 1 km interval

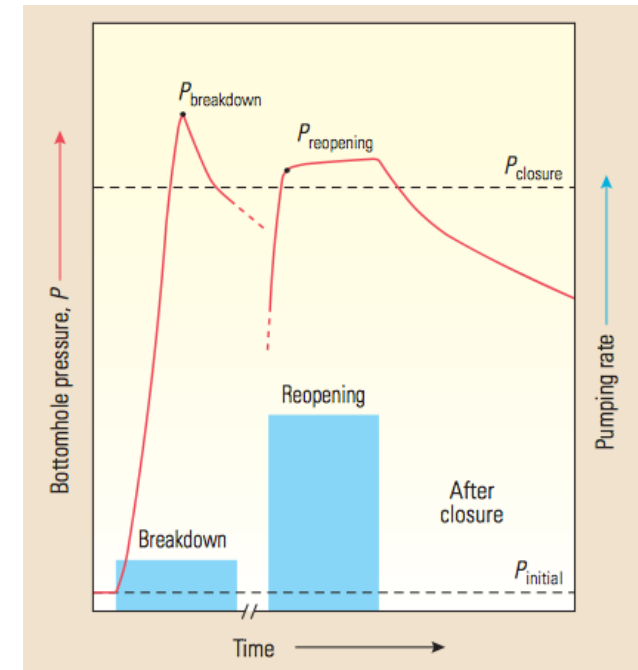
Production = 80 kg/s per 1 km interval

# Hydraulic Fracturing: A THMC Problem

- Injection of fluids, multiple chemicals at high pressure into the deep subsurface is inherently a THMC problem
- Understanding the processes and predicting the results is important for improved resource recovery and to address environmental concerns



<https://www.propublica.org/special/hydraulic-fracturing-national>



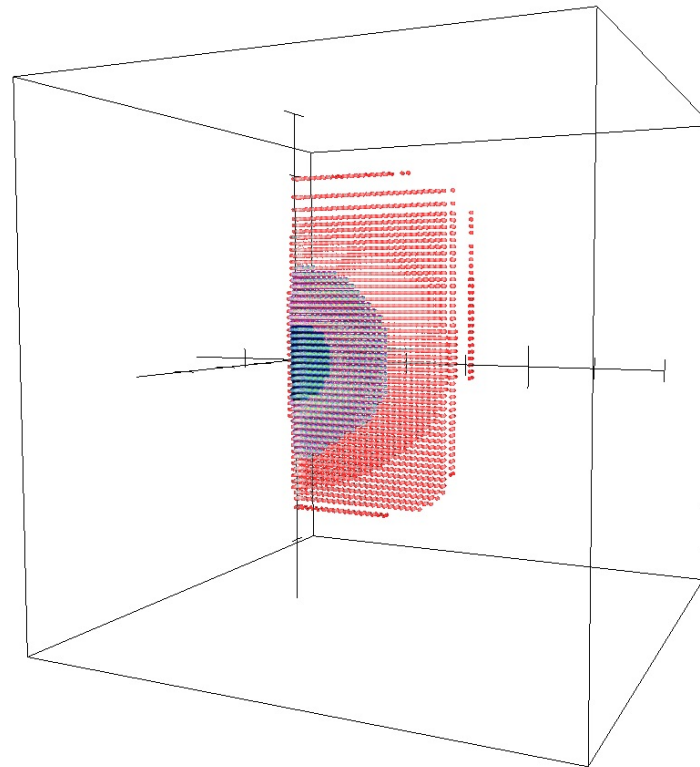
[http://www.slb.com/~media/Files/resources/oilfield\\_review/ors13/sum13/defining\\_hydraulics.pdf](http://www.slb.com/~media/Files/resources/oilfield_review/ors13/sum13/defining_hydraulics.pdf)

# Thermal-Hydrological-Mechanical Modeling of Hydrofracture Growth

## TOUGHREACT-ROCMECH THMC CODE

- Single plane, two plane and simultaneous three plane, tensile, shear, and mixed tensile/shear failure
- Simultaneous triple failure predominant in hydrofracture
- Single plane, simultaneous two plane shearing predominant in shear halo

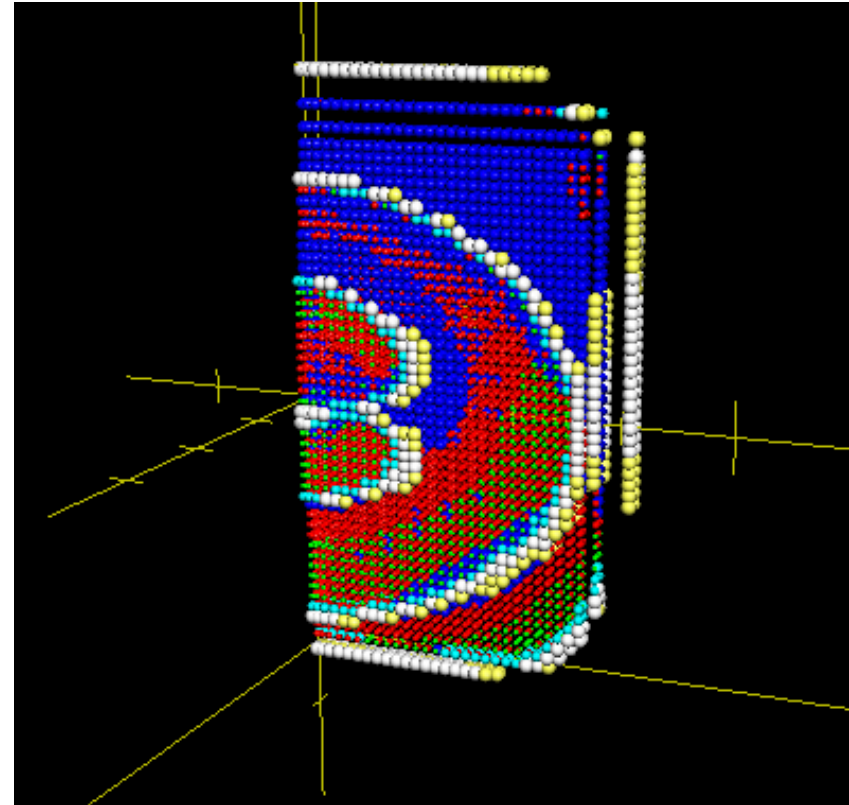
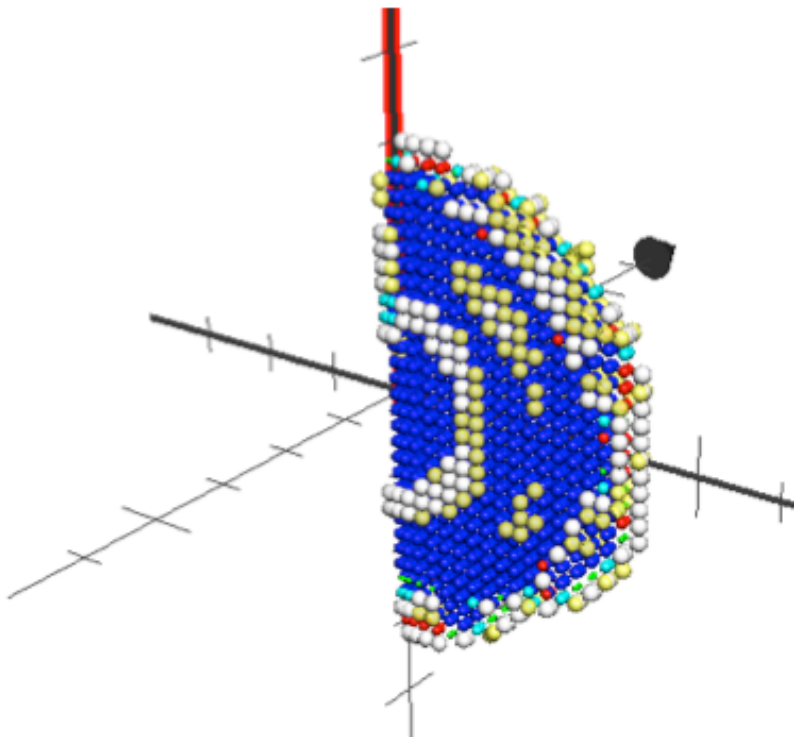
### Generic Fracture Propagation over time



Fracture half-space



# Permeability Structure in Simulated Generic Hydrofracture in Uniform Rock



blue > red > cyan > white > yellow

# Conclusions

- Reactive-Transport – THMC models/codes can provide valuable insights into conceptual models and reservoir models from the native-state, to reservoir development, to long-term production
- During the 2-month Stimulation Test at Newberry Volcano, permeability increases owing to shear stimulation took place as evidenced by 3-4x increase in flow rates and several hundred MEQs
- Modeled permeability increases owing to THM effects allow for a close match to increased flow rates, decreased wellbore temperatures, and shut-in pressures, and tracer returns
- THMC models combined with geochemical and isotopic data on fluids and gases provide strong constraints on the extent of fracture surface area contacted by fluids, reservoir hydrological properties, reservoir development strategies, and long term sustainability
- Simulating THMC effects of hydraulic fracturing is a challenging problem that needs to be addressed for improved resource recovery and to quantitatively address environmental issues

Thanks !!