



*pmd*RT: Coupled fluid, heat and chemical modelling*

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Project F6-M9

Why Reactive Transport Models

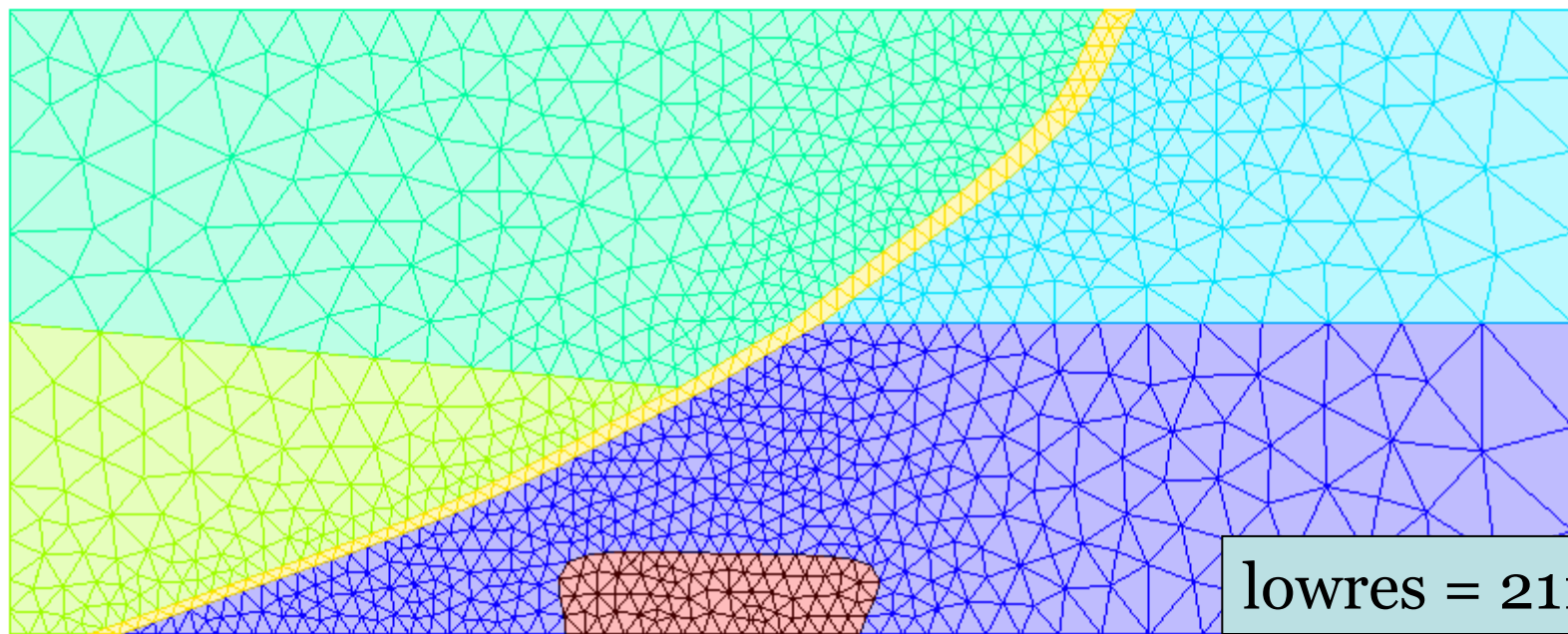
- RT Modelling simulates coupled fluid-flow, heat-chemical transfer, and fluid-rock reaction
- Modelling to understand the feedback, interaction and outcomes of coupled physical processes
- Progress towards modelling natural processes in 3D
 - predictive 3D boxes!

Summary

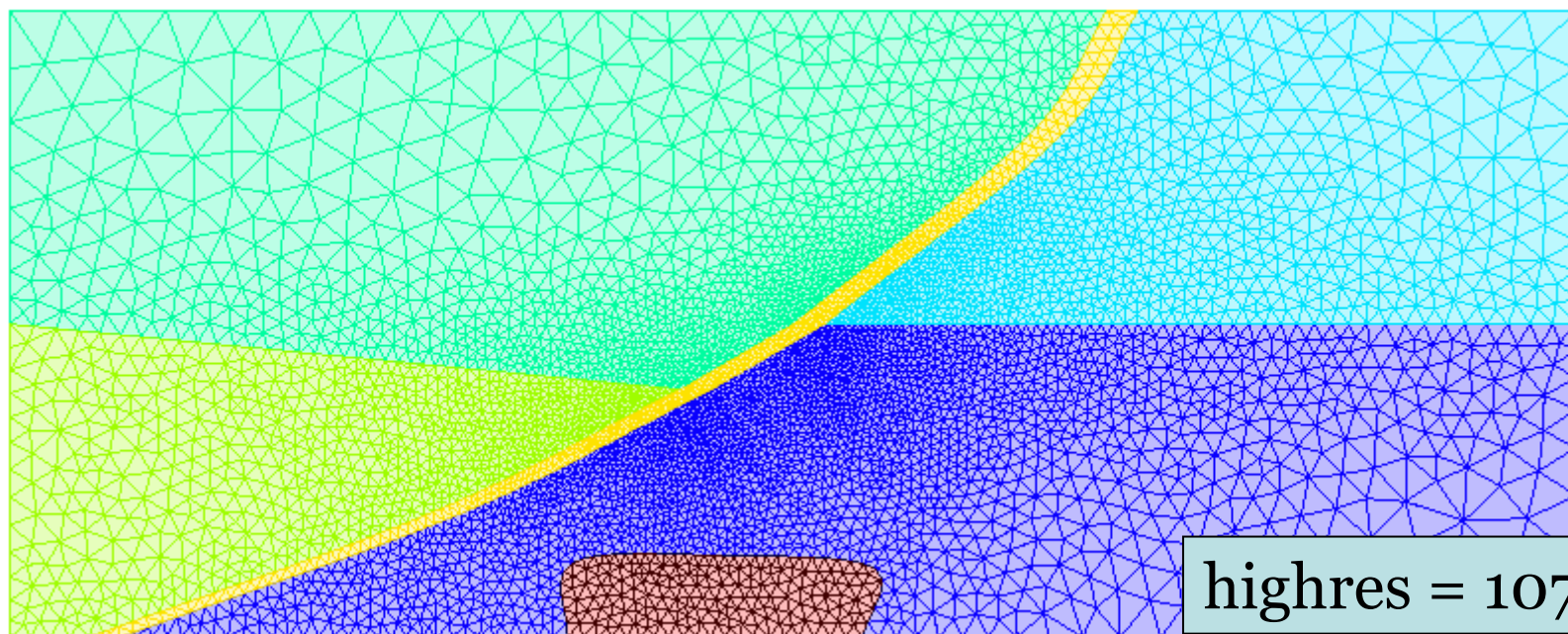
- pmd*^{CRC} now has a usable reactive transport code
- Applied development stage at the moment
 - Some issues to be sorted but very serious progress being made
 - Benchmarking started
- GUI being developed (Chook-RT?)

*pmd*RT?*

- **pmdCRC developed reactive transport code**
 - Couples heat, fluid and chemical transport and chemical reaction – Mechanics being currently being considered!
 - Uses finite element – non-uniform mesh
 - Uses FastFlo4 to solve PDE's coupling of external modules (i.e. EOS)
- **Running in windows environment**
 - JCU Cluster – Win64 on multiprocessor AMD opteron 2.6 (20% quicker than P4 3.2HT)
- **Chemical Solving**
 - Currently via the WinGibbs solver used in HCh
 - Log K solver capability being developed
- **Easy to add extra functionality via Python**



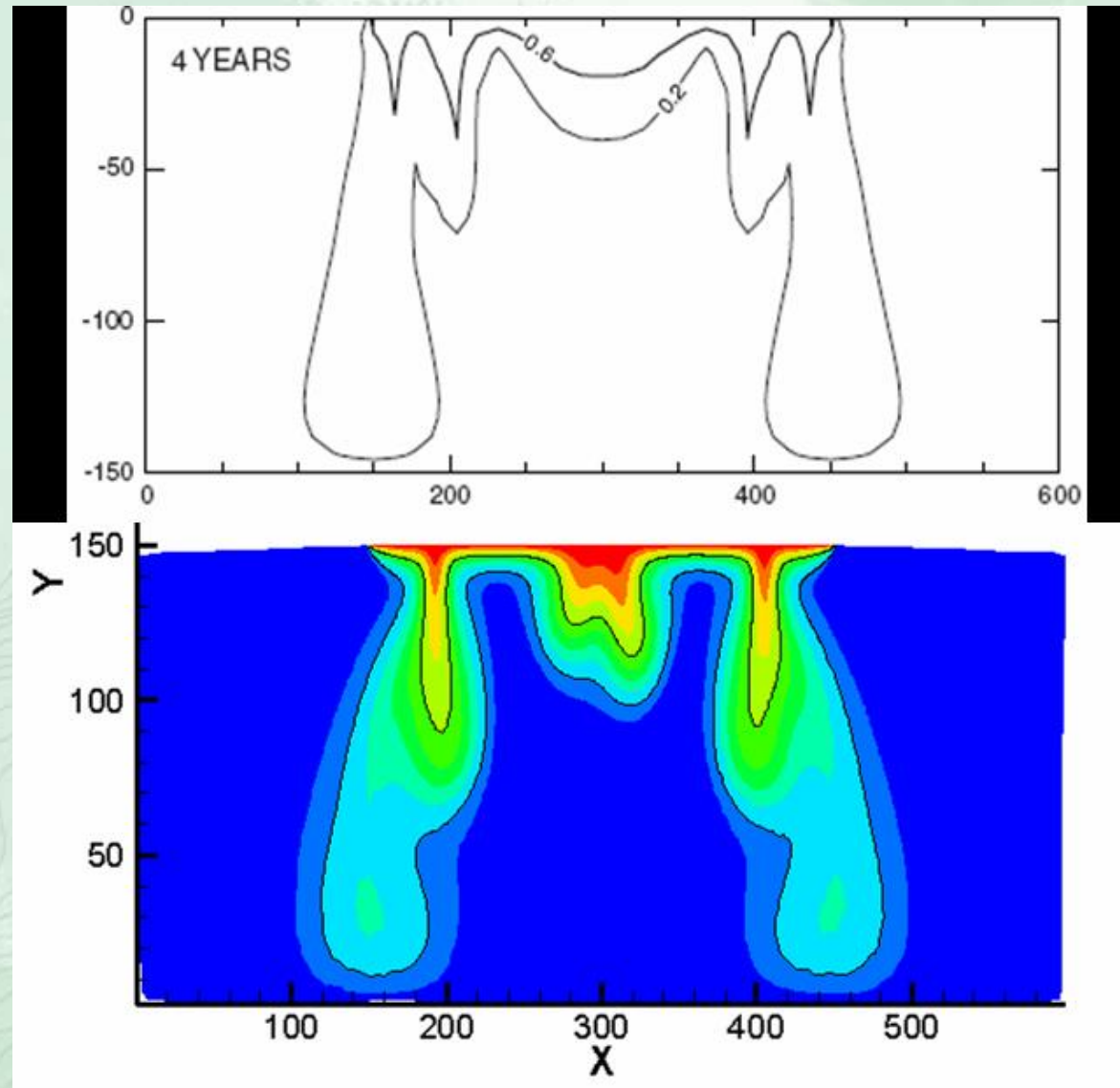
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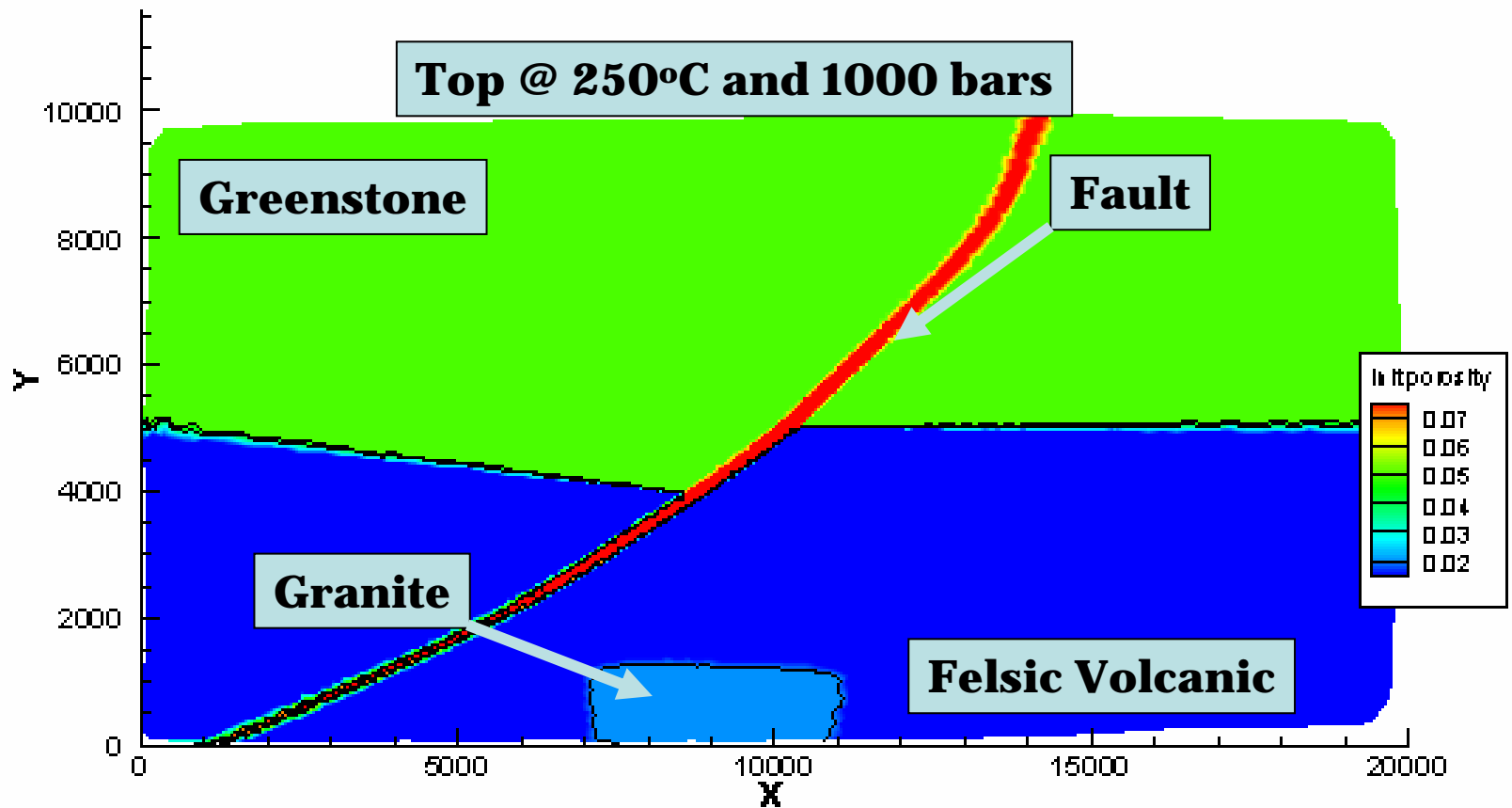
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Benchmarking

Comparison of
modified Elder
problem with
HST3D (USGS
benchmark
hydrological code)



Application and Testing



Physical Properties

Rock Unit	~mineralogy	Log permeability	porosity	ini gold in fluid (molal)
<i>Greenstone</i>	qtz calcite albite tremolite chlorite pyrrhotite	-16	0.05	1×10^{-9}
<i>Felsic Volc</i>	qtz pyrite albite muscovite k-feldspar	-17	0.01	1×10^{-9}
<i>Fault Zone</i>	qtz albite muscovite calcite pyrite pyrrhotite	-15	0.08	-
<i>Granite</i>	qtz muscovite k-feldspar plagioclase (ab-an) pyrite magnetite biotite	-16	0.02	1×10^{-6}

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granite:

'NaCl (aq)' : 0.89,
'KCl (aq)' : 0.28,
'CaCl₂ (aq)' : 0.02,
'FeCl₂ (aq)' : 0.40,
'H₂S (aq)' : 1e-3,
'Au+ (aq)' : 1e-6

fault_zone :

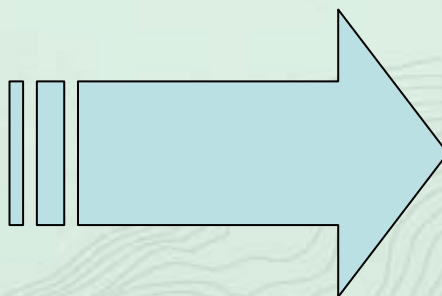
'NaCl (aq)' : 1,
'KCl (aq)' : 1

felsic volcanic:

'NaCl (aq)' : 1.32,
'KCl (aq)' : 0.40,
'CaCl₂ (aq)' : 0.12,
'CO₂ (aq)' : 4.7,
'H₂S (aq)' : 2.86e-2,
'SO₄-- (aq)' : 1e-5,
'Au+ (aq)' : 1e-9

greenstone :

'NaCl (aq)' : 0.78,
'KCl (aq)' : 0.16,
'CaCl₂ (aq)' : 0.75,
'CO₂ (aq)' : 0.05,
'H₂S (aq)' : 5.6e-4,
'Au+ (aq)' : 1e-9



1) Aqueous components
added to rock and fluid
(vol by porosity)

2)

-> Equilibrium step 0

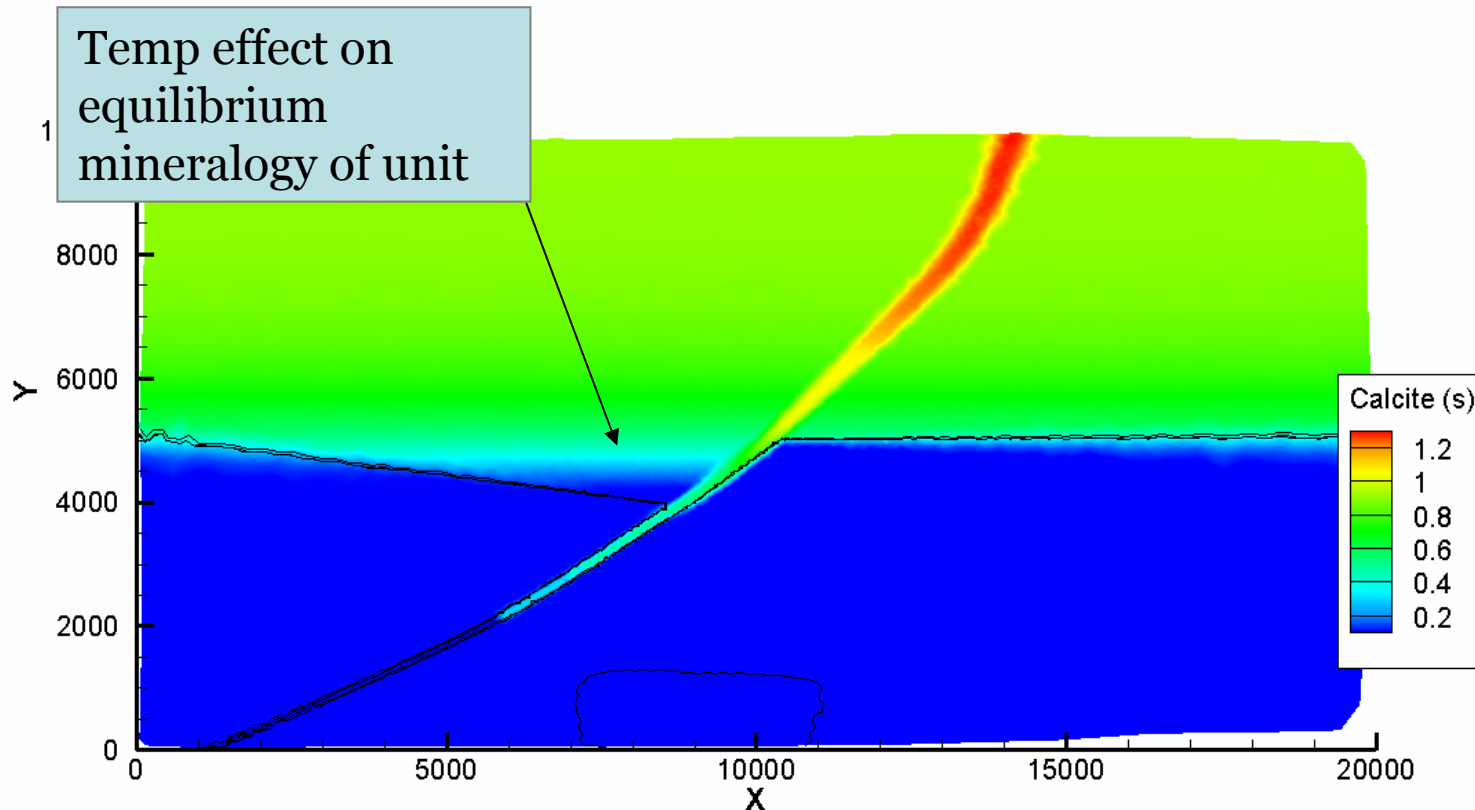
-> Equilibrium step 1



Initialised Fluid-Rock System

Initialisation of Chemistry

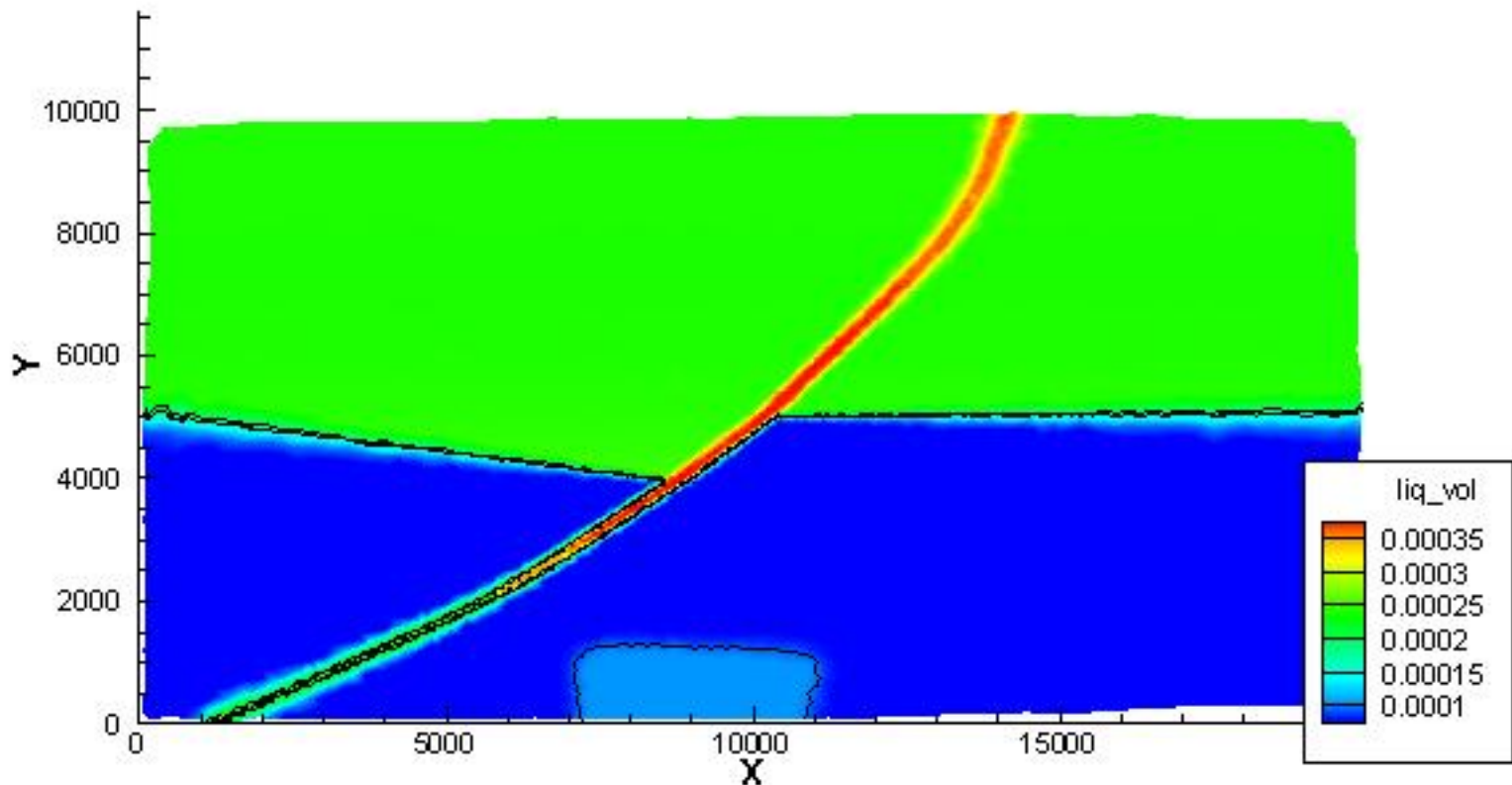
Frame 001 | 10 Feb 2006 | LFG_RT01_CPor_c_hrm at Time 10.00 years



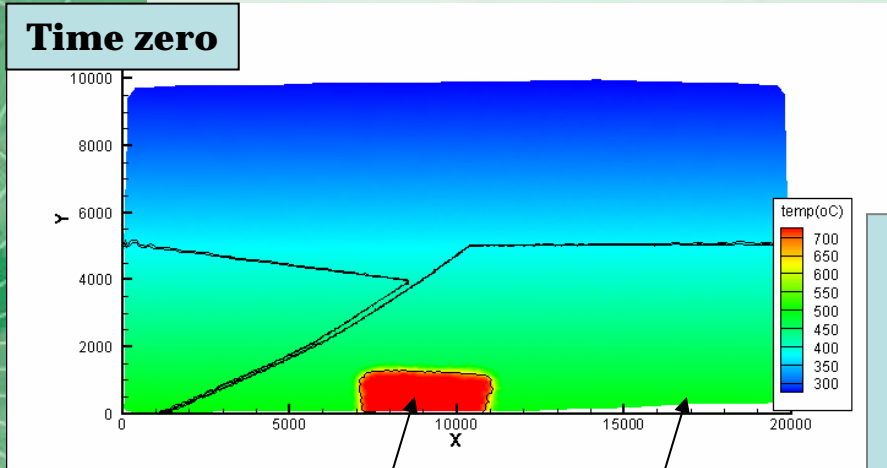
Liquid_volume @ step 0

Frame 001 | 28 Feb 2006 | LFG_RT01_CPor_c_hmat Time 0 years

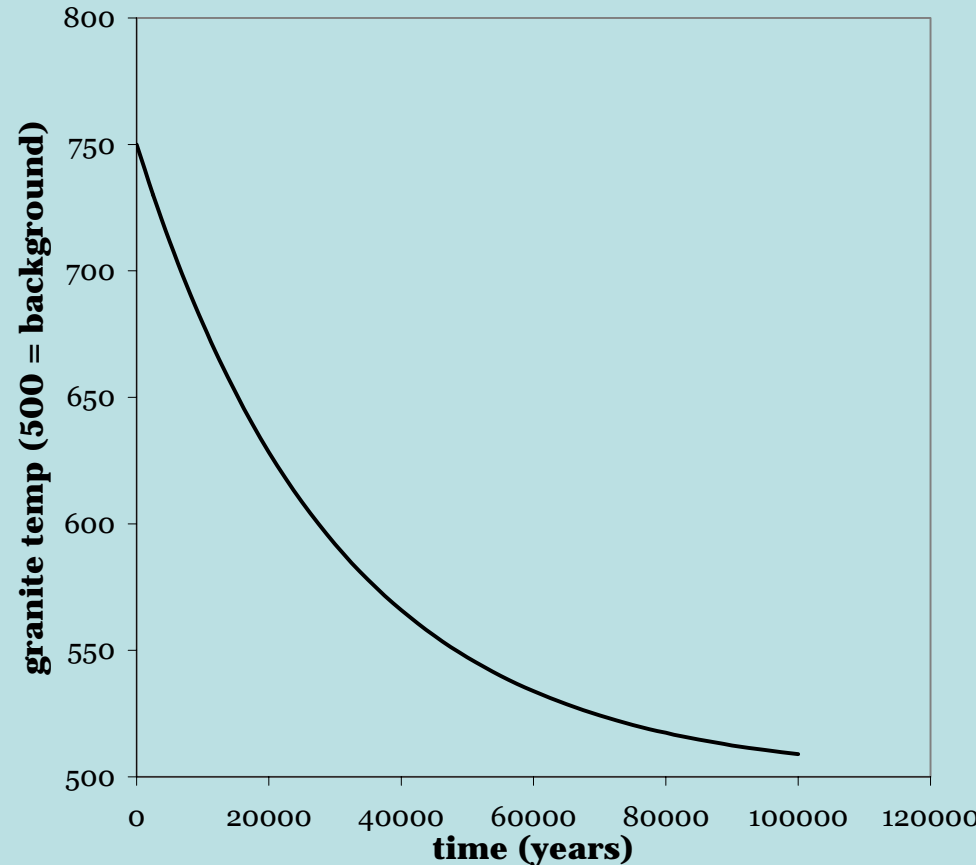
Liquid_volume from
FFPCU.phaseVolume



Granite



Uses a dynamic boundary condition that allows the fluid to cool the granite further.



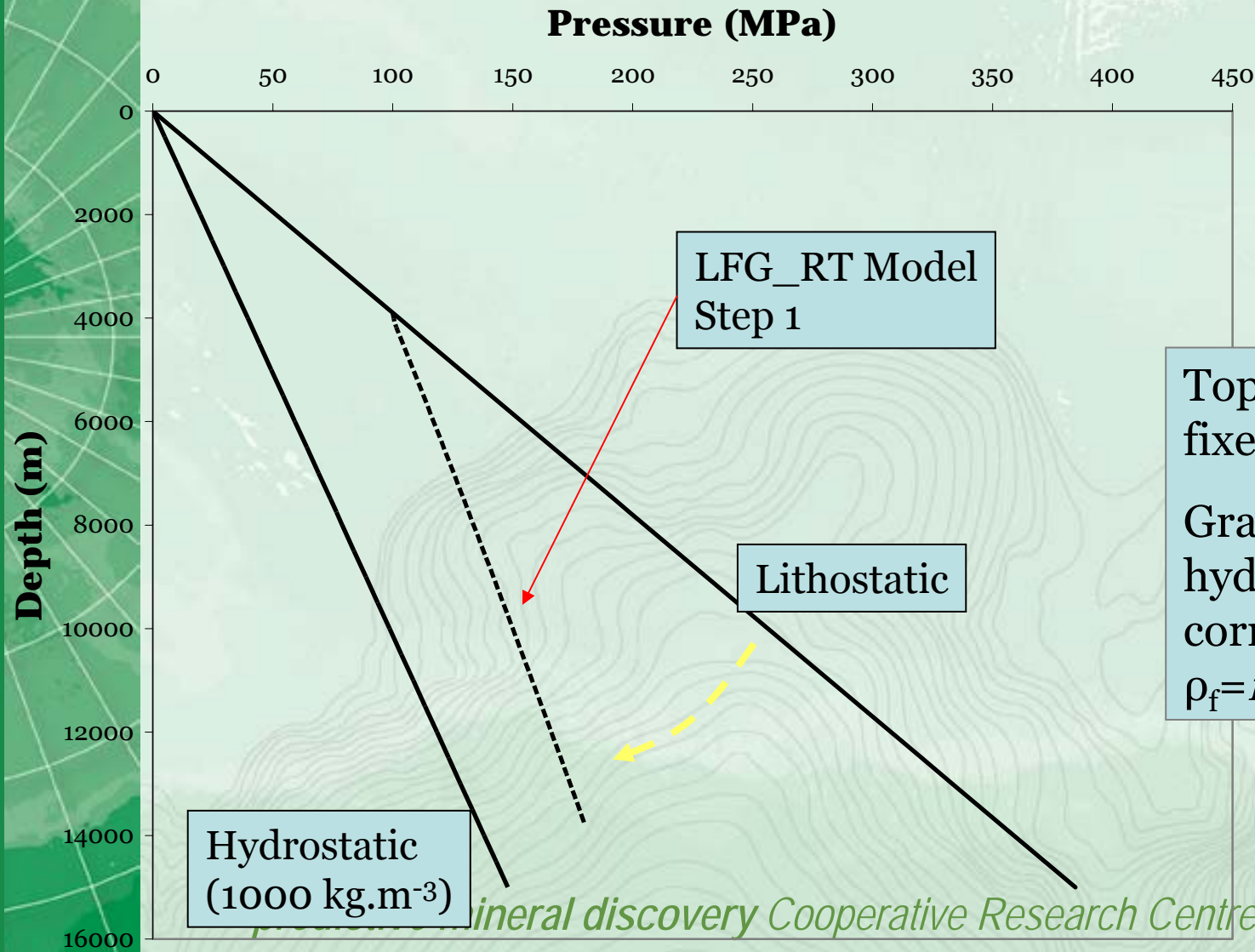
Granite cools by:

$$\text{excess_t} * e^{(-\text{time}/\text{event_length})}$$

$$\text{event_length} = 30,000$$

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Pore Pressure



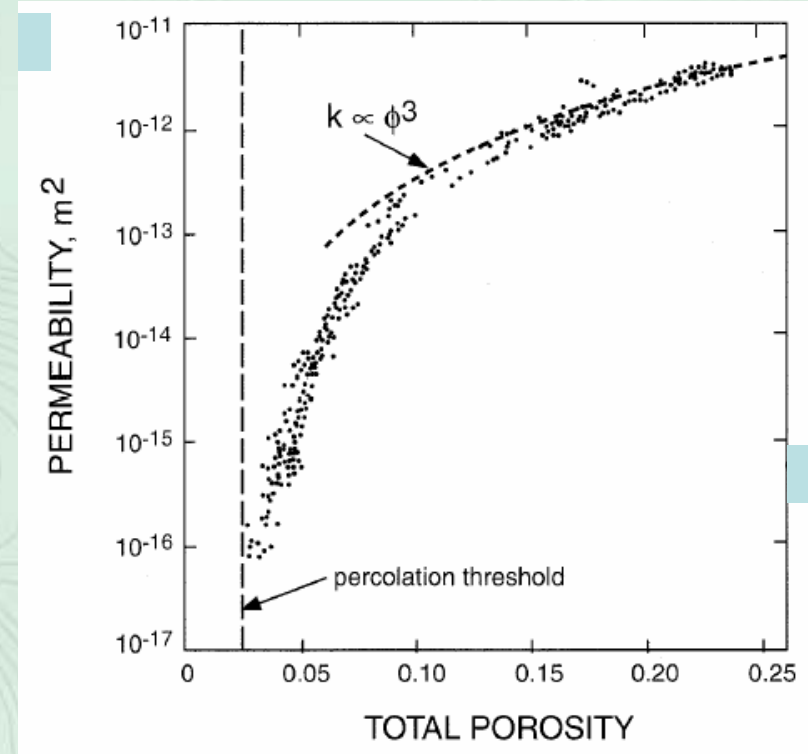
Movie

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Dynamic Porosity-Permeability

- Chemical reactions will dissolve or precipitate mass
 - Porosity increases or decreases
 - Permeability will change based on some relationship to porosity



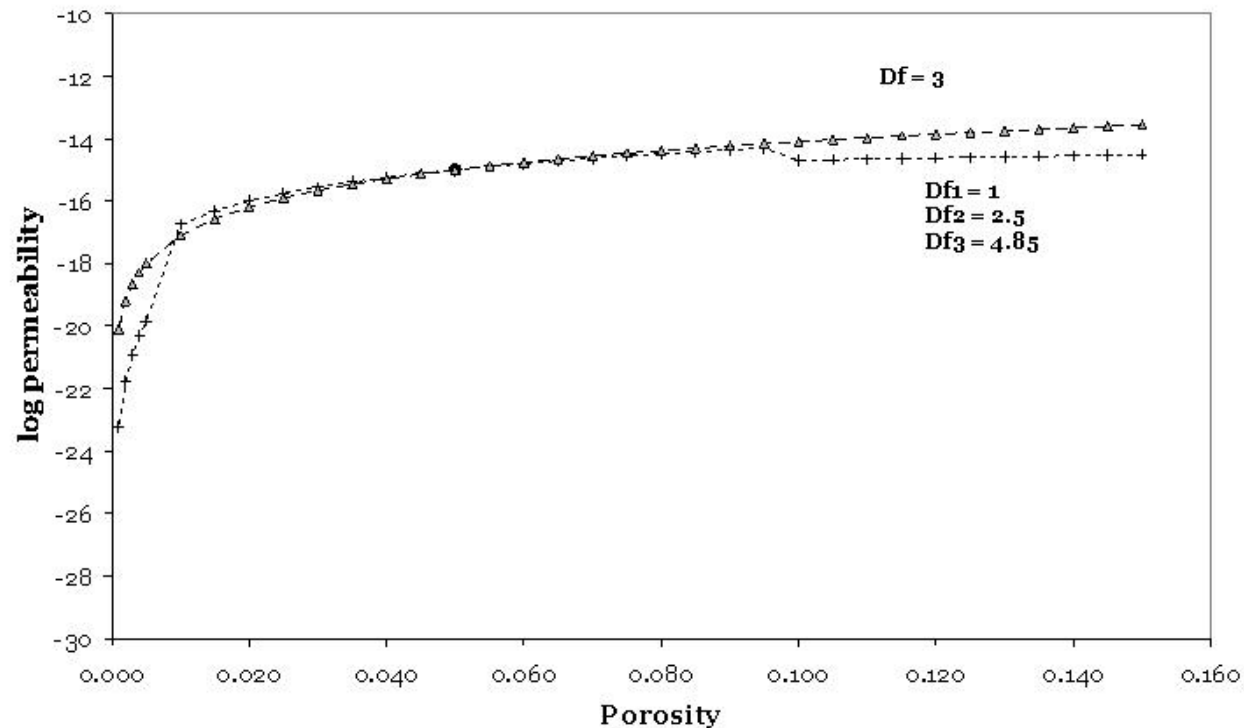
Cox et al., 2000

Dynamic Porosity-Permeability

FFPyChemUtils.phaseVolume

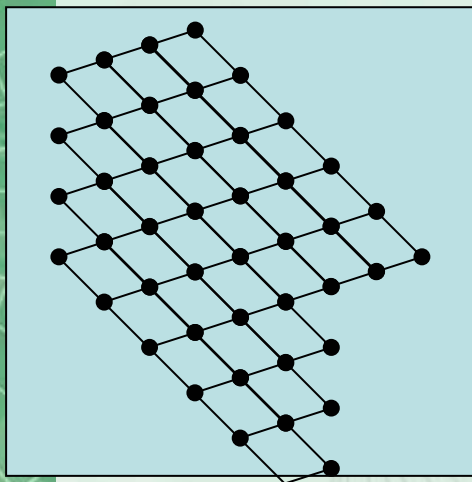
$$\phi = V_f$$

$$K = K_0 \left(\frac{\phi}{\phi_0} \right)^n$$

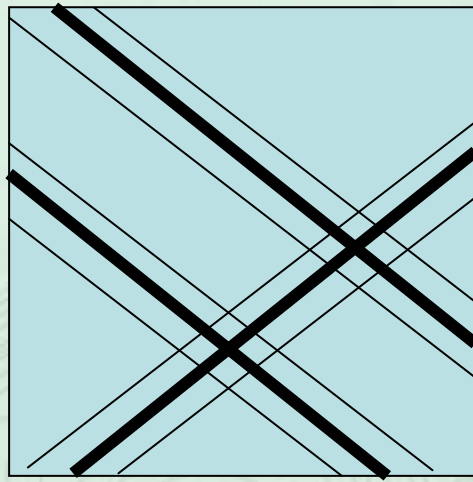


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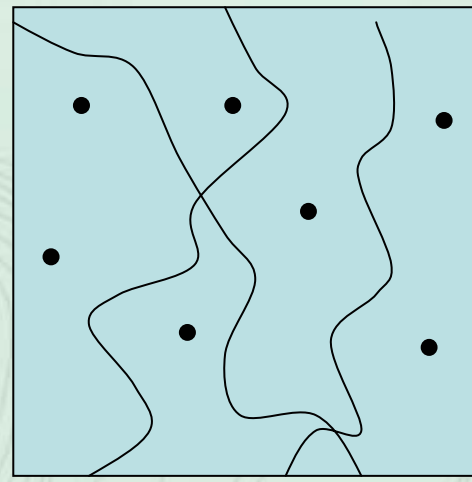
How much rock does my fluid know about?



Distributed effective porosity



Fracture porosity and percolation limited alteration



Limited effective porosity

unreactive solid fraction = changes the chemical f/r

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Dynamic Chem Por-Perm

$$\phi_c = \frac{\phi}{(1 - \omega)}$$

$\omega = \text{unreactive_sol_fraction}$

$$\phi = (\Delta\phi_c)\phi$$


If por = 0.08, $\omega = 0.80$ then por_chem = 0.4


Equivalent to fracture porosity

The model stores two dynamically linked porosities

Thank-you
Reminder ..

More details about dynamic
porosity-permeability in poster!





Coupled dynamic porosity-permeability with chemical reaction

James S. Cleverley, Project F6

1. Introduction

Reactive transport modelling is used to investigate the coupling between physical processes such as fluid flow and chemical reaction. One of the key coupled processes is the feedback between chemical reaction and changes in the porosity of the rock as minerals dissolve or precipitate. This in turn changes the permeability of the rock volume and thus there is direct feedback between this process and the Darcy flow velocity.

In this poster we explore the mathematical implementation of dynamic porosity-permeability in the pmd*RT (FastRT) reactive transport code and its subsequent effect on the results of Yilgarn-type models.

2. Linking Reaction and Flow

Changes in the porosity caused by chemical reaction are calculated using the liquid phase volume (V_l) of the finite volume where:

$$V_l = V_r - 1 \text{ and,}$$

$$\dot{V}_l = \dot{V}_r$$

During mineral precipitation and dissolution mass is transferred between the liquid and solid phase. Because the liquid mass is transported through the model the total porosity of a model volume can increase or decrease.

The flux of fluid through the model is controlled by the Darcy flux:

$$v = -\frac{k}{\mu} (\nabla P + g\rho)$$

Where k is the permeability, μ the viscosity, ∇P the pressure gradient and, $g\rho$ is the body force (gravity and the liquid density).

While the chemical reaction modifies porosity we need to link this to the expected changes in permeability in order to feed back to the calculated flow rates. There are a large number of empirical and measured relationships between porosity and permeability and these will be incorporated in the pmd*RT code. For this work we used the Carman-Kozeny relationship:

$$k = k_0 \left(\frac{\phi}{\phi_0} \right)^n$$

where the subscript 0 denotes the reference or initialised value and n is the fractal exponent that varies for different rock types. For the test case model a fractal value of 2 was applied. These equations are solved at each time step to dynamically link the changes in rock properties by reaction with fluid flow.

3. The Chemical Porosity Concept

Porosity in rocks is often considered in the context of the pore space between grain crystals, however in crystalline rocks much of the measured porosity could be via fracture or grain boundary spaces (Fig. 1). In this case the fluid only considers a fraction of the total rock volume. In order to approximate this behaviour pmd*RT incorporates a separate chemical porosity that is dynamically linked to changes in physical porosity.

The chemical porosity (ϕ_c) is defined by:

$$\phi_c = \frac{\phi}{(1 - \phi_0) + \phi_0}$$

where ϕ_0 is the volume fraction of unreactive rock in the total volume. The chemical and physical porosity values are linked by:

$$\phi_c = \phi$$

$$\Delta \phi_c = \frac{\phi_c}{\phi} \Delta \phi$$

$$\dot{\phi} = \Delta \phi_c \dot{\phi}_c$$


where i is the step number and 0 is the reference or initialisation value (step 0).

4. Example: Listic Fault & Granite Model

Parameter	Value
Temperature	Isotaxium 750°C at time 0, cooling with time
Pressure	Hydrostatic 250°C top and 300°C/bm 100 MPa at top
Permeability	0.001-0.01 (by region)
Porosity	10-100 (by region)
Chemical porosity	10-100 (by region)
Current porosity	250

Figure 1: Schematic of fluid infiltrating rock where the primary porosity is controlled by different physical factors in the rock: (a) pore space, (b) fracture, and (c) grain boundaries.

Figure 2: Plot of the porosity and Darcy flux for a granite model with dynamic porosity-permeability. The model time is 10,000 years and $\mu = 0.001$ Pa.s after the granite has cooled. However the flow of magmatic fluid initially spreads but permeability in the upper half is high so there is a combined preferential flow. The lower diagram shows the variation in permeability across the model depth line, upper figure illustrating the total permeability changes that impact of flow paths. The log plot in the lower diagram represents the 'half' - the permeability was calculated at a constant value in the regions of time 0.



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