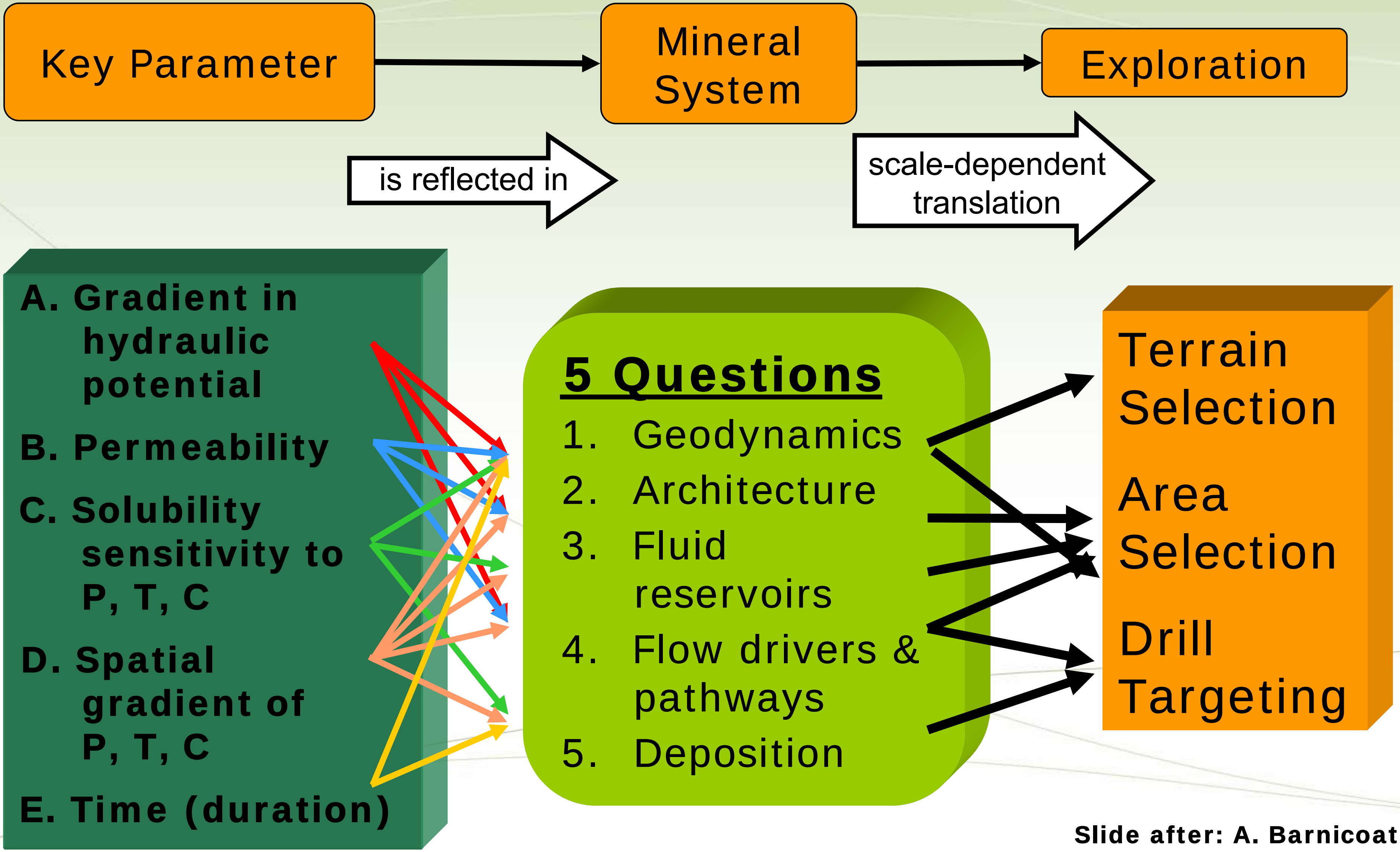
Enabling Technologies

Transport and Reaction Modelling



Slide after: A. Barnicoat

RT Modelling - Processes

$$\sum_m \nu_m^n \left(\phi U^m_{,t} + q_i U^m_{,i} - \left(D_{ij} U^m_{,j}\right)_{,i}\right) = \phi \rho^f \sum_n \nu_m^n R^m$$

permeability

$$\left(\frac{\rho^f k}{\mu} P_{,i}\right)_{,i} = \left(\frac{\rho^{f2} k}{\mu} g_i\right)_{,i}$$

porosity

density

pressure

HEAT

FLUID FLOW

DEFORMATION

CHEMICAL REACTION

chemistry

Specific heat

temperature

Thermal conductivity

$$\langle \rho C_p \rangle T_{,t} + \rho^f C_p^f q_i T_{,i} - \left(\langle\lambda\rangle T_{,i}\right)_{,i} = Q$$

$$\left(\phi U^m\right)_{,t} + \left(q_i U^m - D_{ij} U^m_{,j}\right)_{,i} = \phi\rho^f R^m$$

Slide after: J. Cleverley

Transport

Molecular diffusion is solute transport down concentration gradient (i.e. tea-bag in hot water).

Advection describes transport of solutes by movement of medium (e.g. fluid).

Dispersion describes the effect of an inhomogeneous flow field.

Diffusion

is solute transport down a concentration gradient (i.e. tea-bag in hot water)

The physical process driving molecular diffusion is the random motion of ions in solution.

Ions in a region of higher concentration will eventually mix with ions in a region of lower concentration to create an equal distribution in space.

Diffusion

concentration of
molecule or ion

coefficient of molecular diffusion

diffusive flux

$$q_d = -D_w \frac{dC}{dx}$$

distance along the length
of the diffusion gradient

FICK's first law

Diffusion

The diffusion coefficient (Dw) in Fick's law is expressed for pure and open water.

In the subsurface, diffusion (Dm) occurs within a porous medium. Tortuosity, *t* , of the flow path increases the distance over which the solute must travel to get from one point to another.

Tortuosity is a dimensionless measure of how the shape of the flow path. It is expressed as the average actual flow path divided by the length of a straight line between points.

Where n_e is the effective porosity, i.e. the pore space through which molecules can actually move continuously (no dead ends…)

$$D_m = \frac{n_e}{\tau} D_w$$

Advection

Concentration change governed by:

advection + diffusion / dispersion + reaction

Idealized transport conditions including simple chemical reactions (one dimensional form)

Chemical reactions

Huge crowd of molecules and ions in pores of granular material (on order of 107 – 1015)

Solutes generally surrounded by water molecules

Solute-solute collisions 109 times per second

Collision energetic enough and molecules oriented properly and prone of reaction

- rearrangement of bonds (essence of reaction)
- remove / add solutes from / to solution

Thermodynamic equilibrium – kinetic reactions

The higher solubility – the quicker the reaction

Chemical Equilibrium

At equilibrium, the potential energy, the Gibbs free energy, G, of the chemical system is minimized. The Gibbs free energy is related to

enthalpy H, representing thermal energy,

temperature, T, in Kelvin, and

entropy, S, representing disorder or randomness of a system

$$G = H - TS$$

Chemical Potential

The partial derivation of the Gibbs free energy with respect to the number of moles of a substance, n_i, corresponds to its chemical potential, μ_i.

$$\frac{\partial G}{\partial n_i} = \mu_i$$

Activity

Chemical potential is the driving force of chemical reactions and in turn depends on the dimensionless activity, a, of the dissolved solution species via the following equation, with the chemical potential at standard conditions (μ°) and the ideal gas constant, R.

$$\mu_i = \mu_i^\circ + RT \ln a$$

Kinetic Models

Mineral reactions fall into three groups:

(1) reaction rates may be so slow relative to the time period of interest that the reaction can be ignored altogether

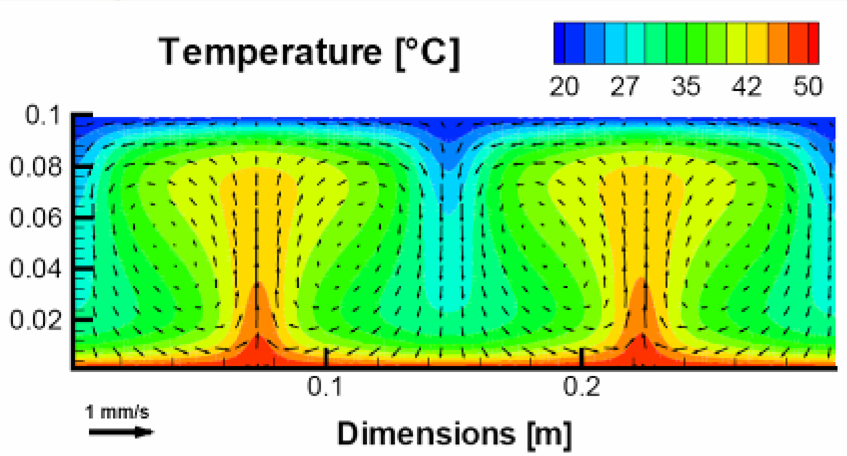
(2) those in which the rates are fast enough to maintain equilibrium

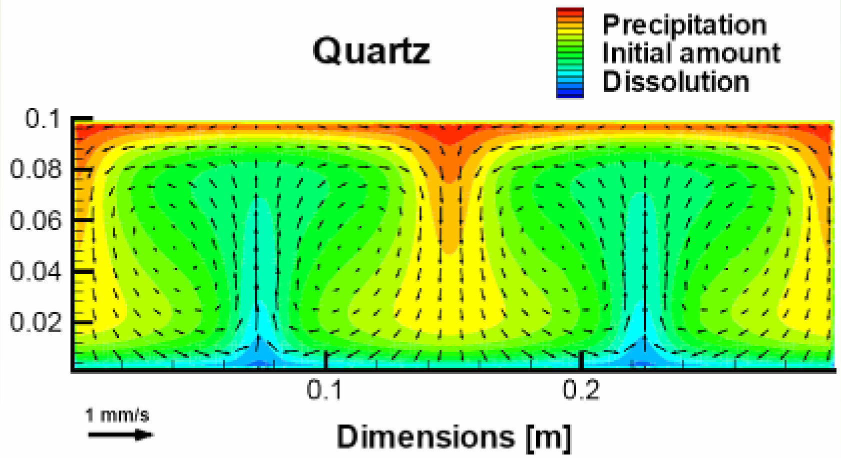
(3) the remaining reactions. Only those require a kinetic description

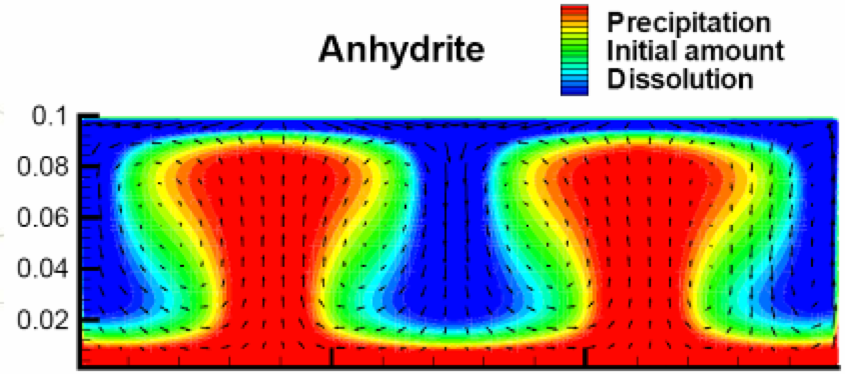
Table 3.3. Approximate ranges of reaction half times for different types of reaction taken from Langmuir and Mahoney (1984)

Type of Reaction	Typical Half Life
Solute - solute	Fraction of a second to minutes
Sorption - desorption	Fraction of a second to days
Gas-solute	Minutes to days
Crystalline solid - solute	Hours to millions of years

Reactions and thermal gradients

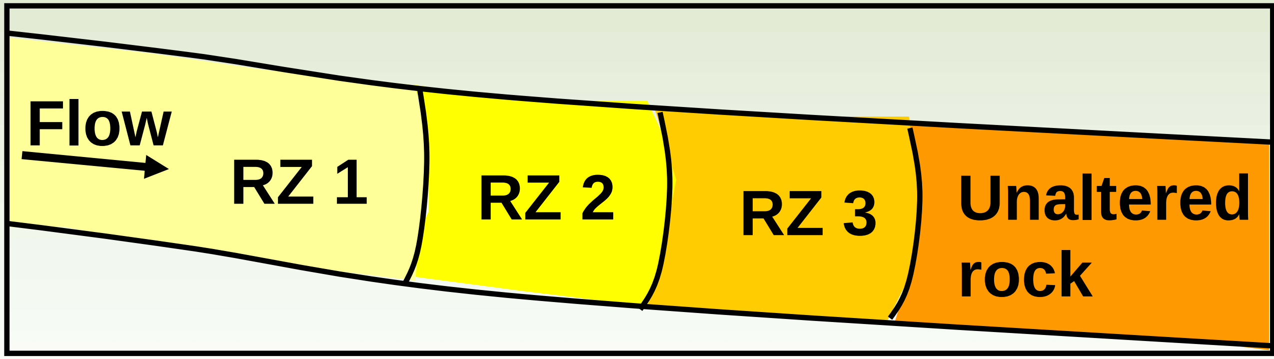




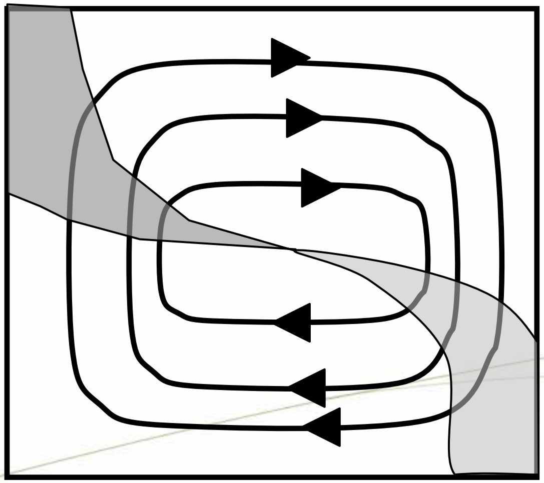


3 end-member types

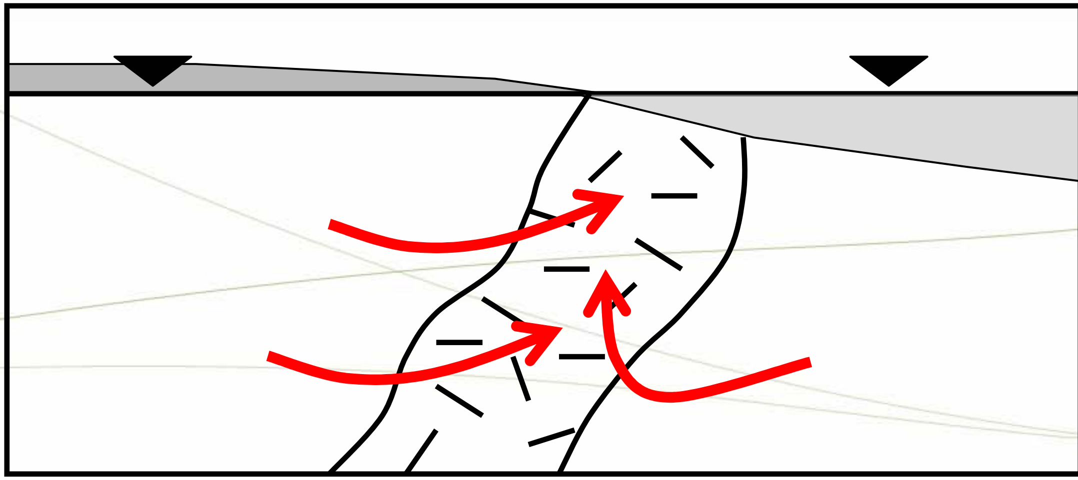
1) Isothermal reaction fronts



2) Gradient reactions



3) Mixing zone reactions



Why RT modelling?

RT processes important where there is a potential for fluid flow coexisting with spatial variations in the thermodynamic states of the system

Variations in:

- composition of the solid phase
- T or P
- composition of the aqueous phase

Variations may exist simultanously

Numerical methods

Numerical solutions necessary to preserve physical coupling of equations

Finite differences, finite element or finite volume methods applicable

In either approach simulated region discretized into finite number of nodes, blocks, or elements

Properties of elements specified

Workflow

initial model: specifies mineralogy, T, P, Poro, Perm

step 1: chemically equilibrate initial mineralogy according to thermodynamic principles

step 2: transport fluid within the model

series of transport steps until transport stage is completed

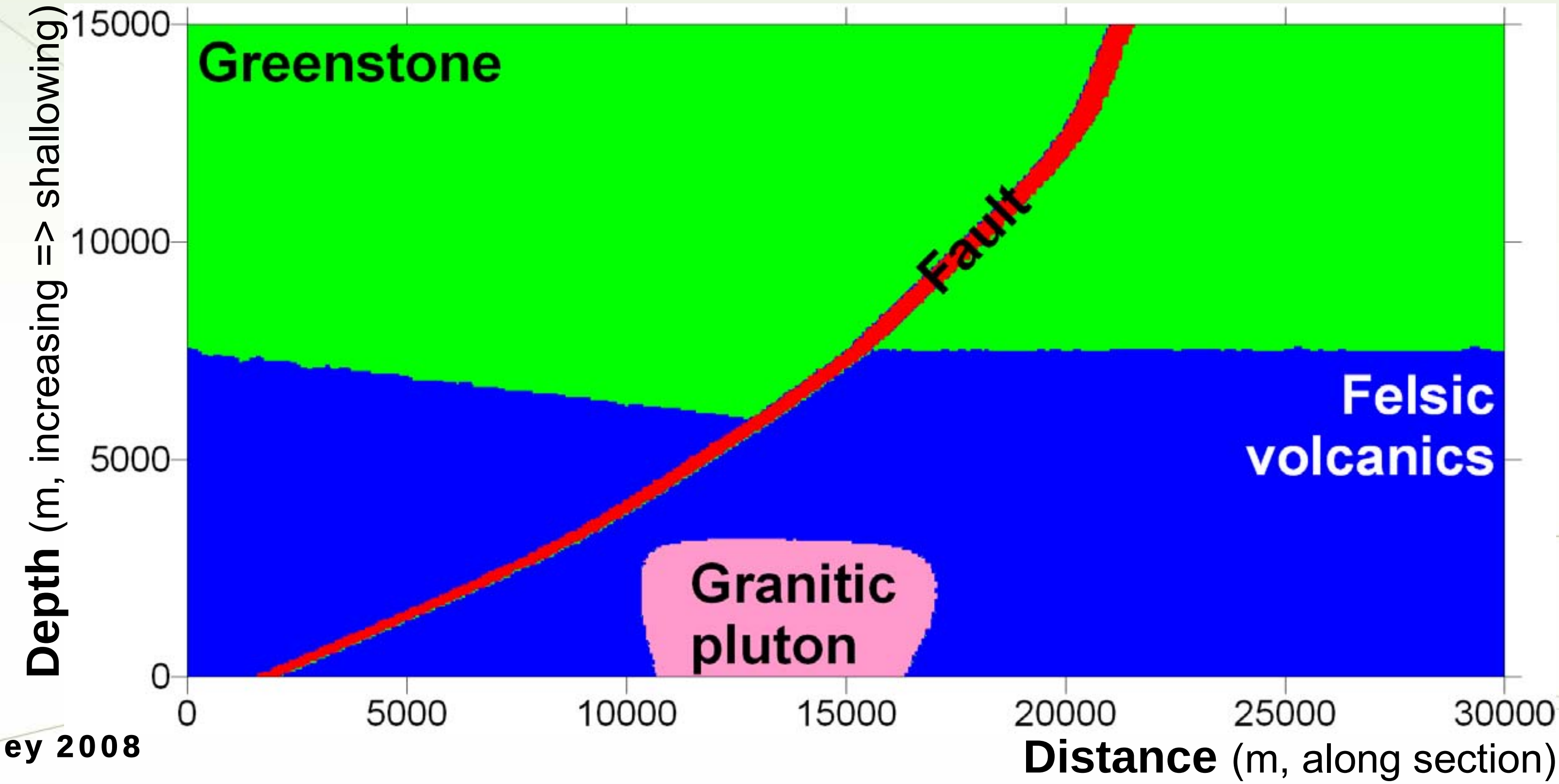
chemical equilibrate again to complete the first timestep of the model

RT model then continues to perform additional time-steps
- first transporting fluid
- then calculating chemical reactions

RT model runs over a set period of geological time (1-10 My)

Example: RT Gold model

Simple reactive transport model to simulate gold forming along a listric fault, with fluids driven from a cooling granite.



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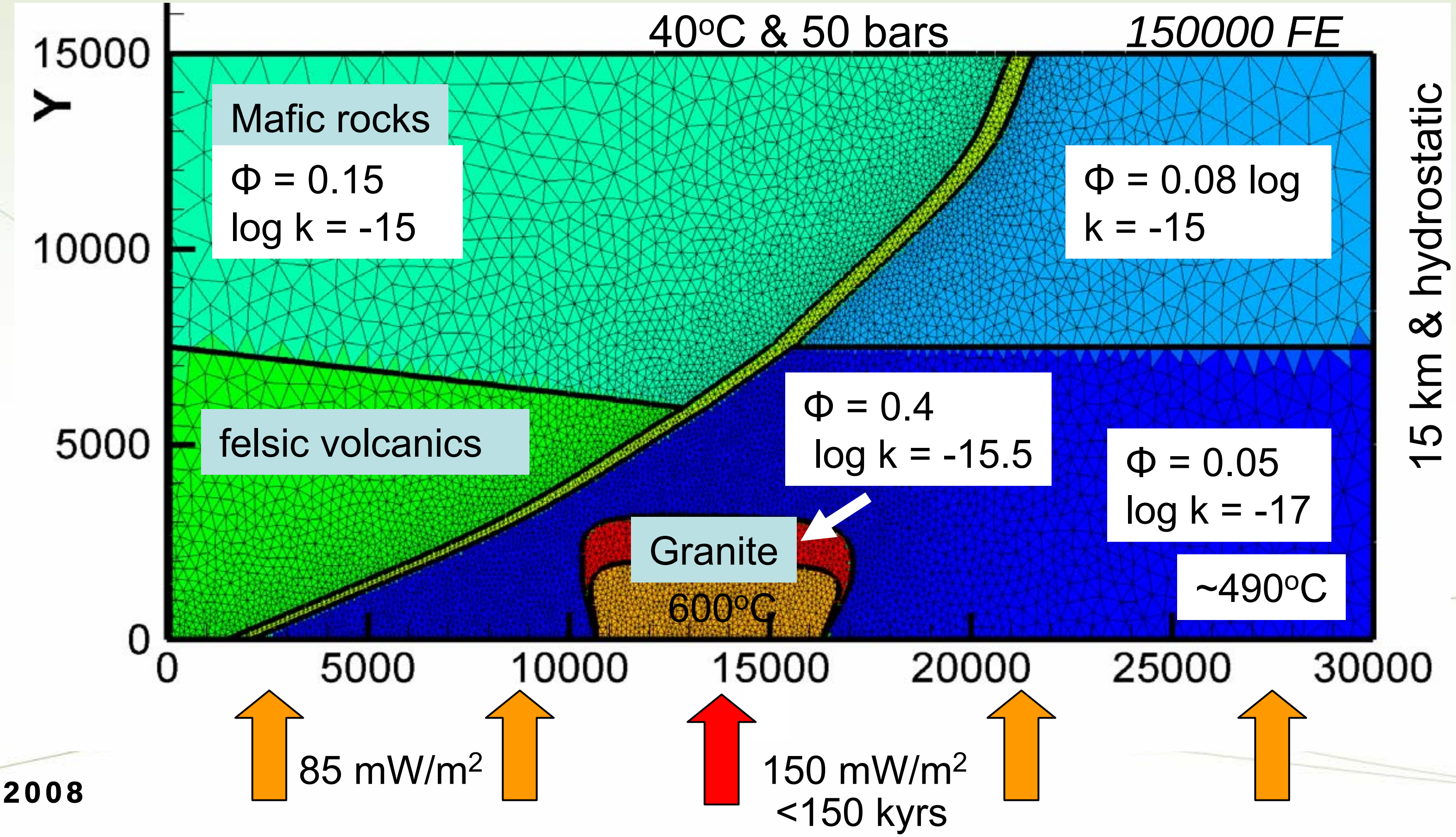
Example: RT Gold model

LFG Model Mesh & Geology



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Example: RT Gold model

Transport & Heat & Chemistry

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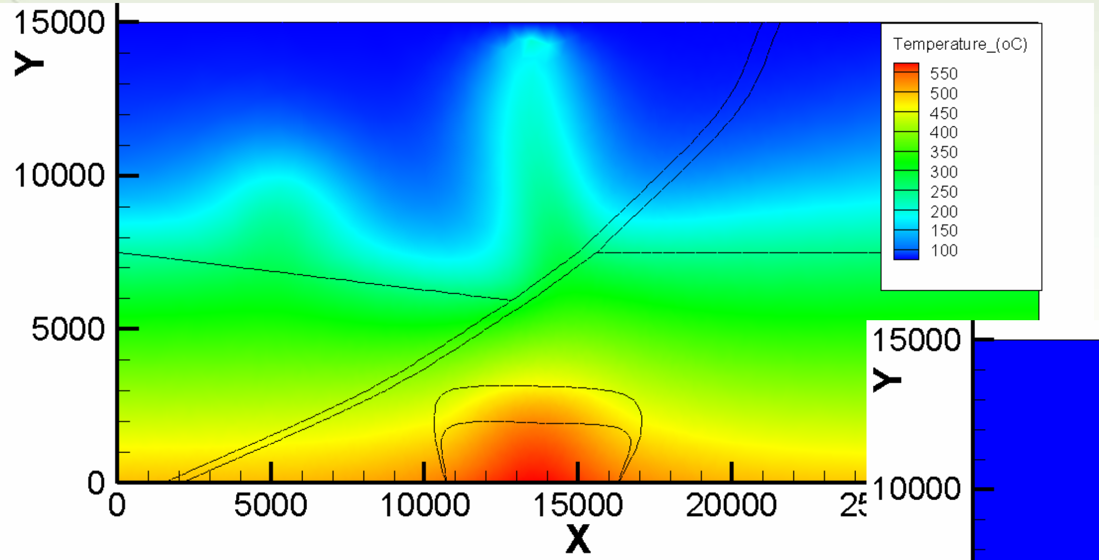

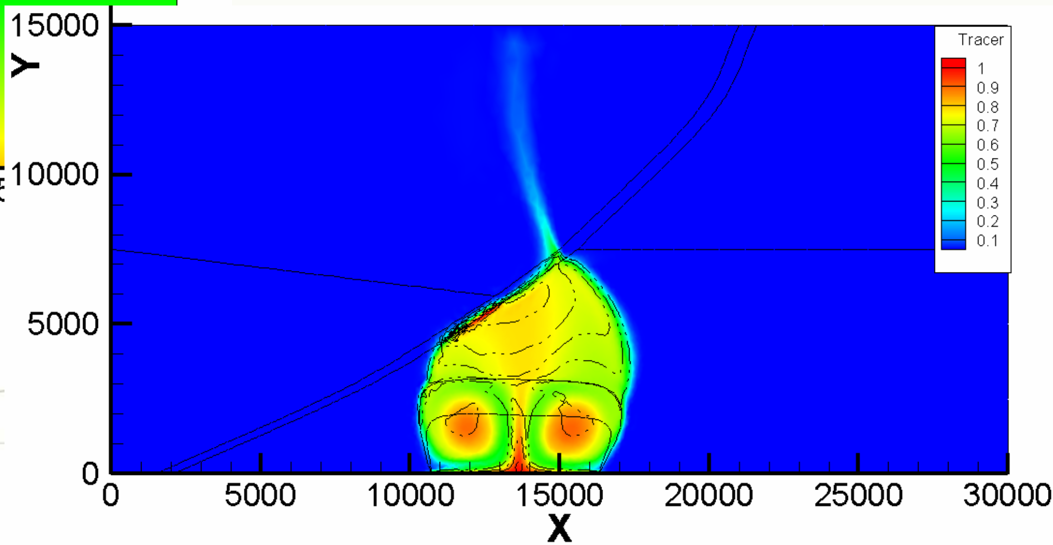

Example: RT Gold model

Heat & Transport only

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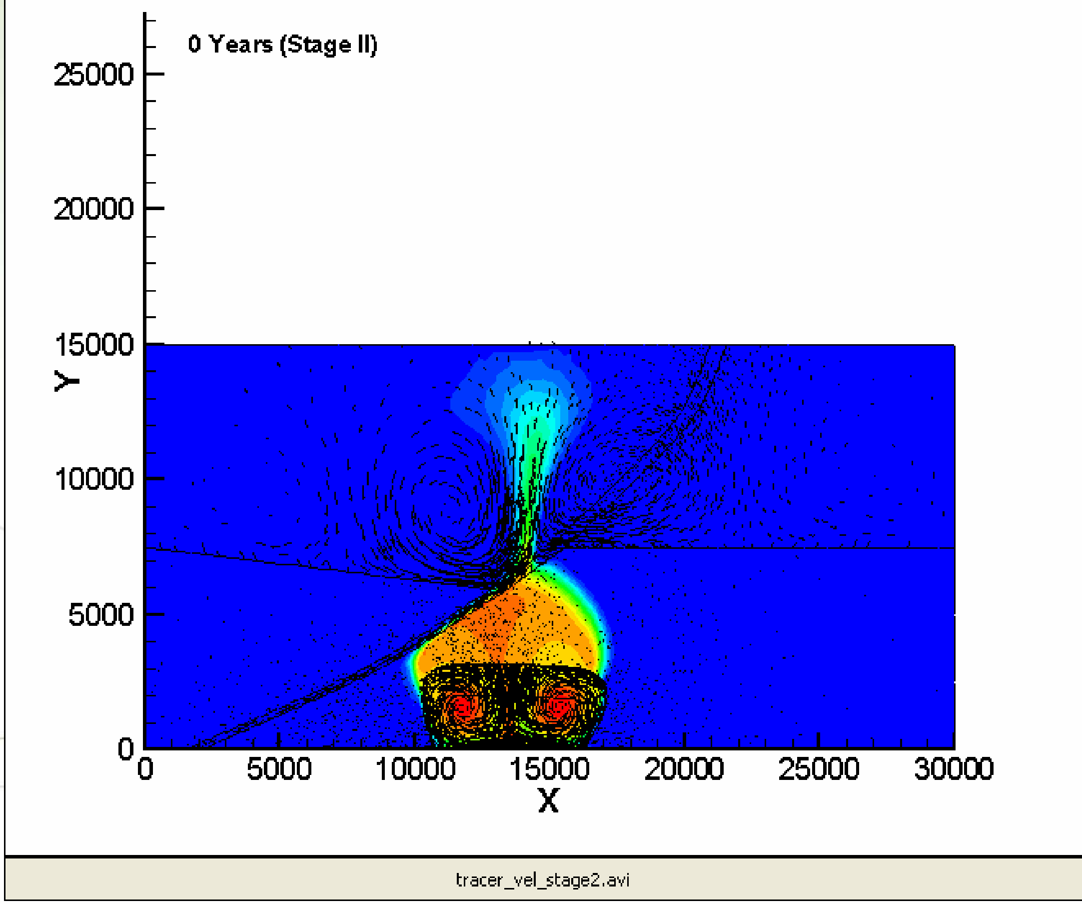
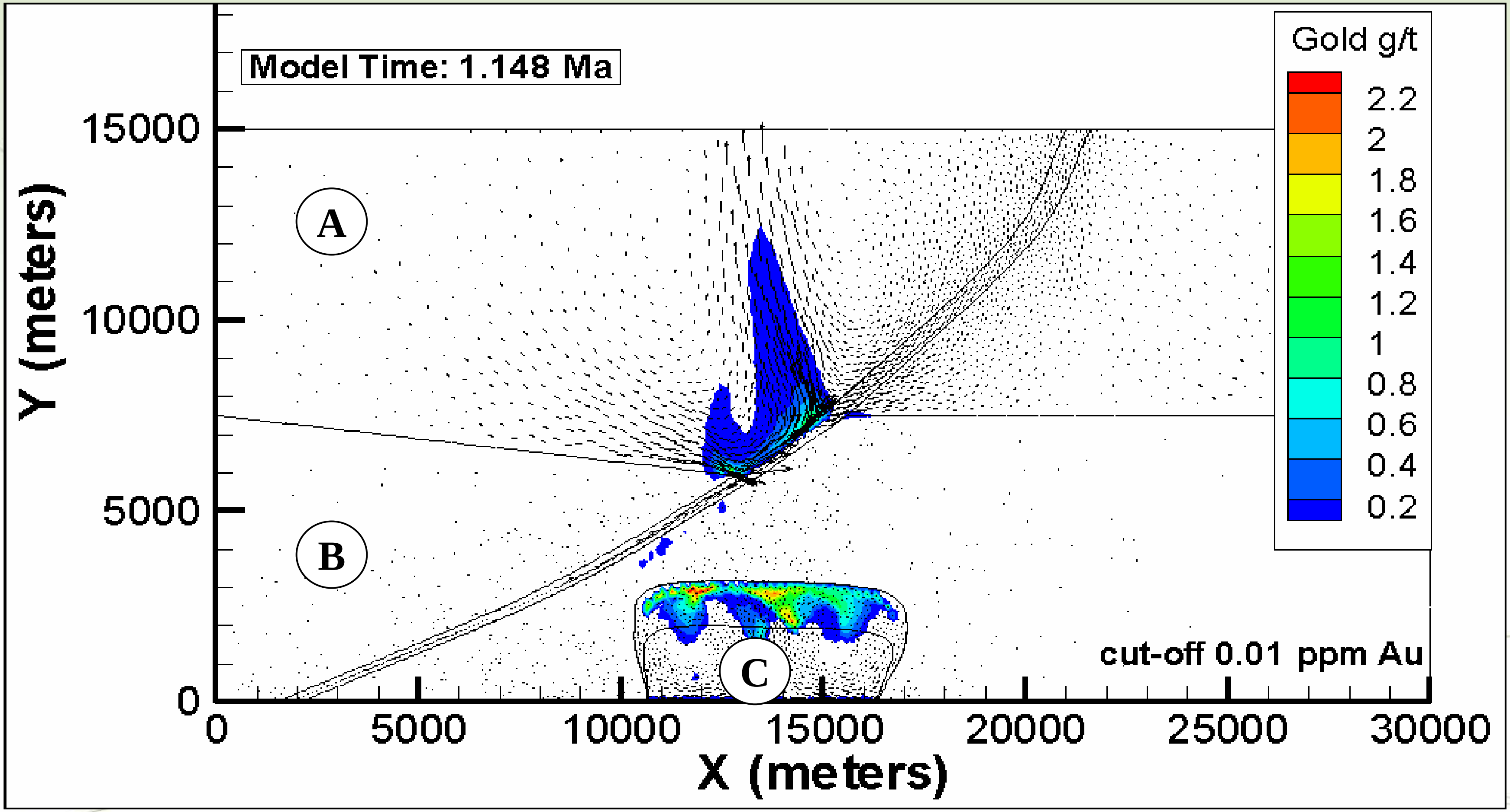


Granite up flow kicks off convection in the upper unit.

Thermal regime would cause convection in upper unit.

Example: RT Gold model



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Example: RT Gold model

Time evolution of gold precipitation

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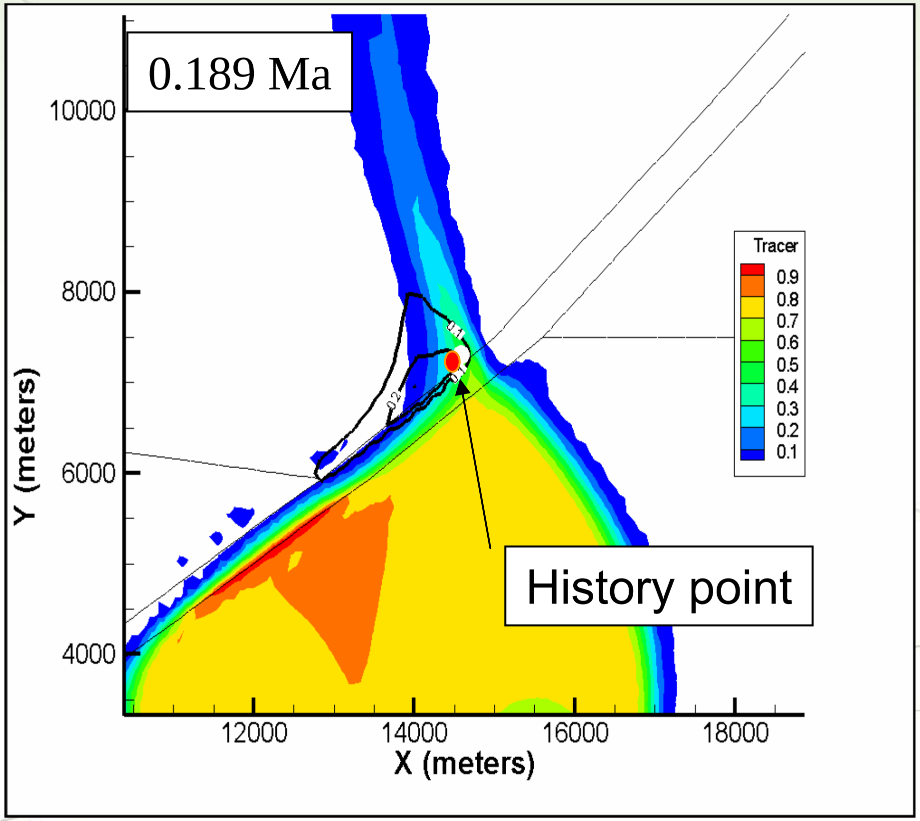
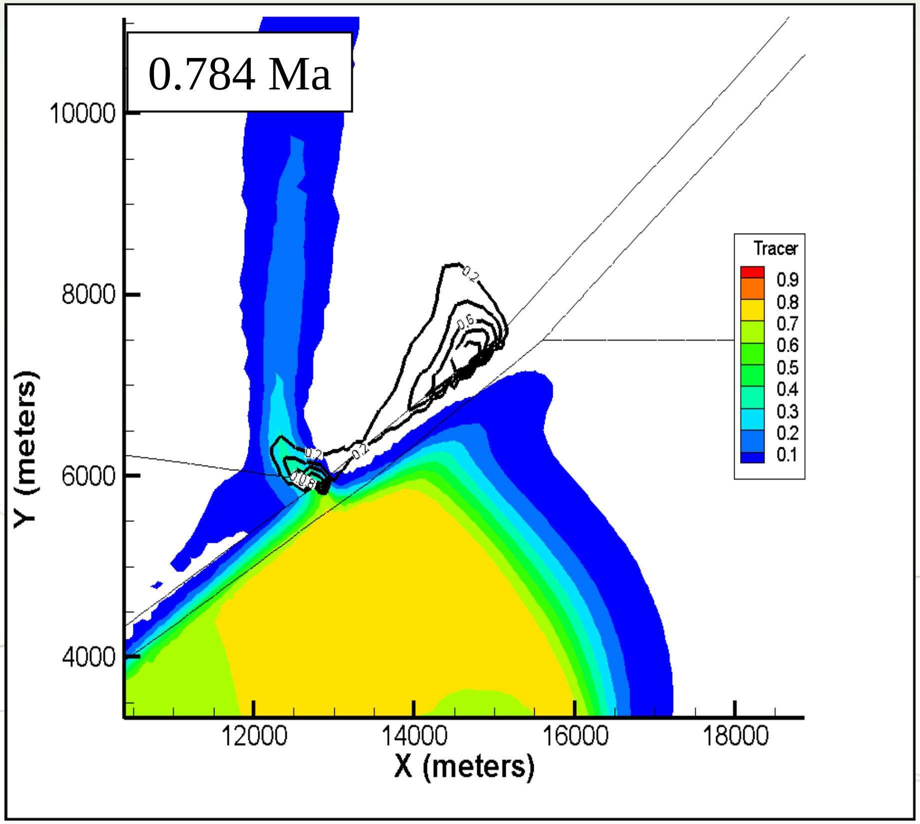
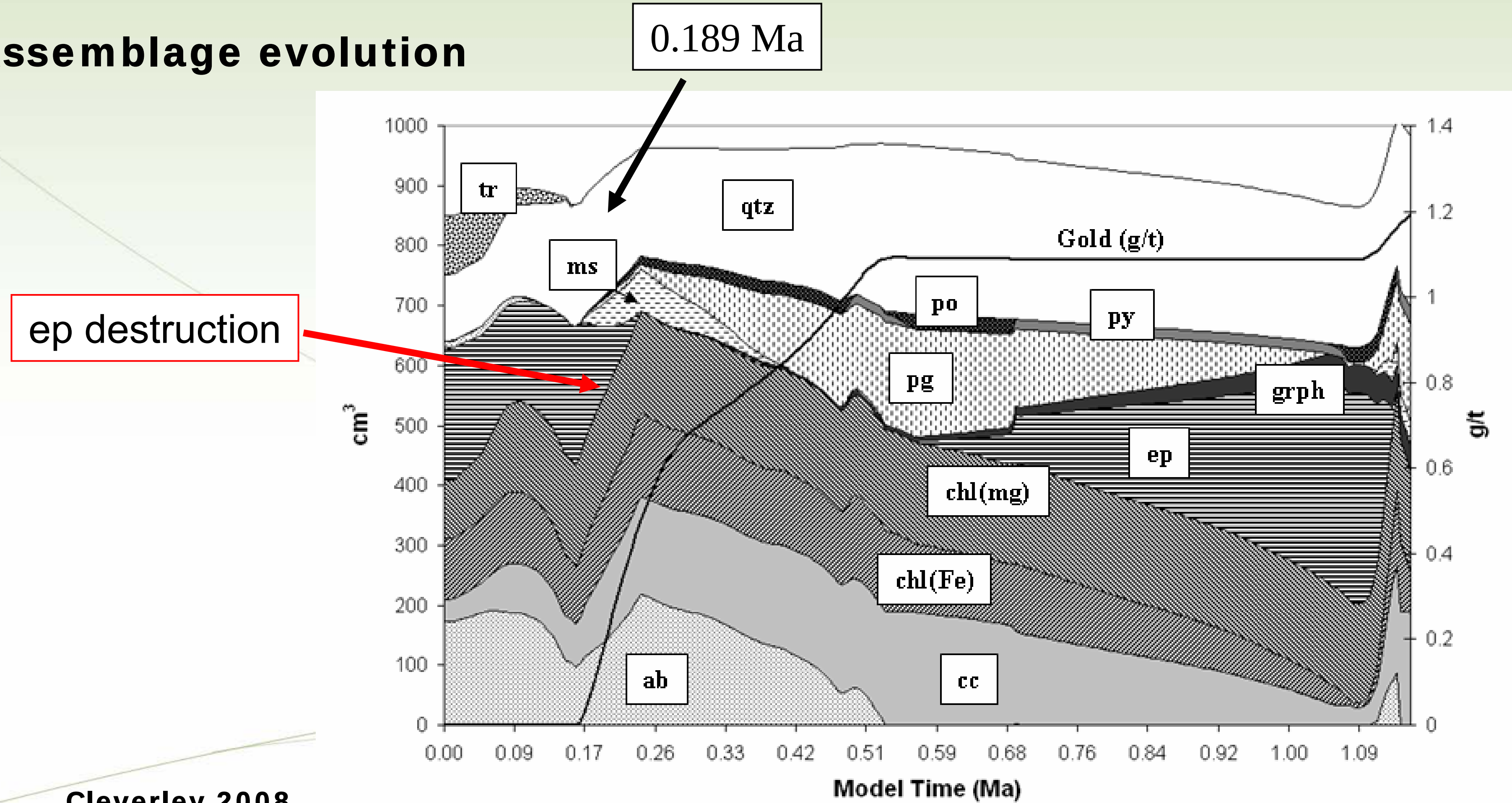




Example: RT Gold model

Assemblage evolution



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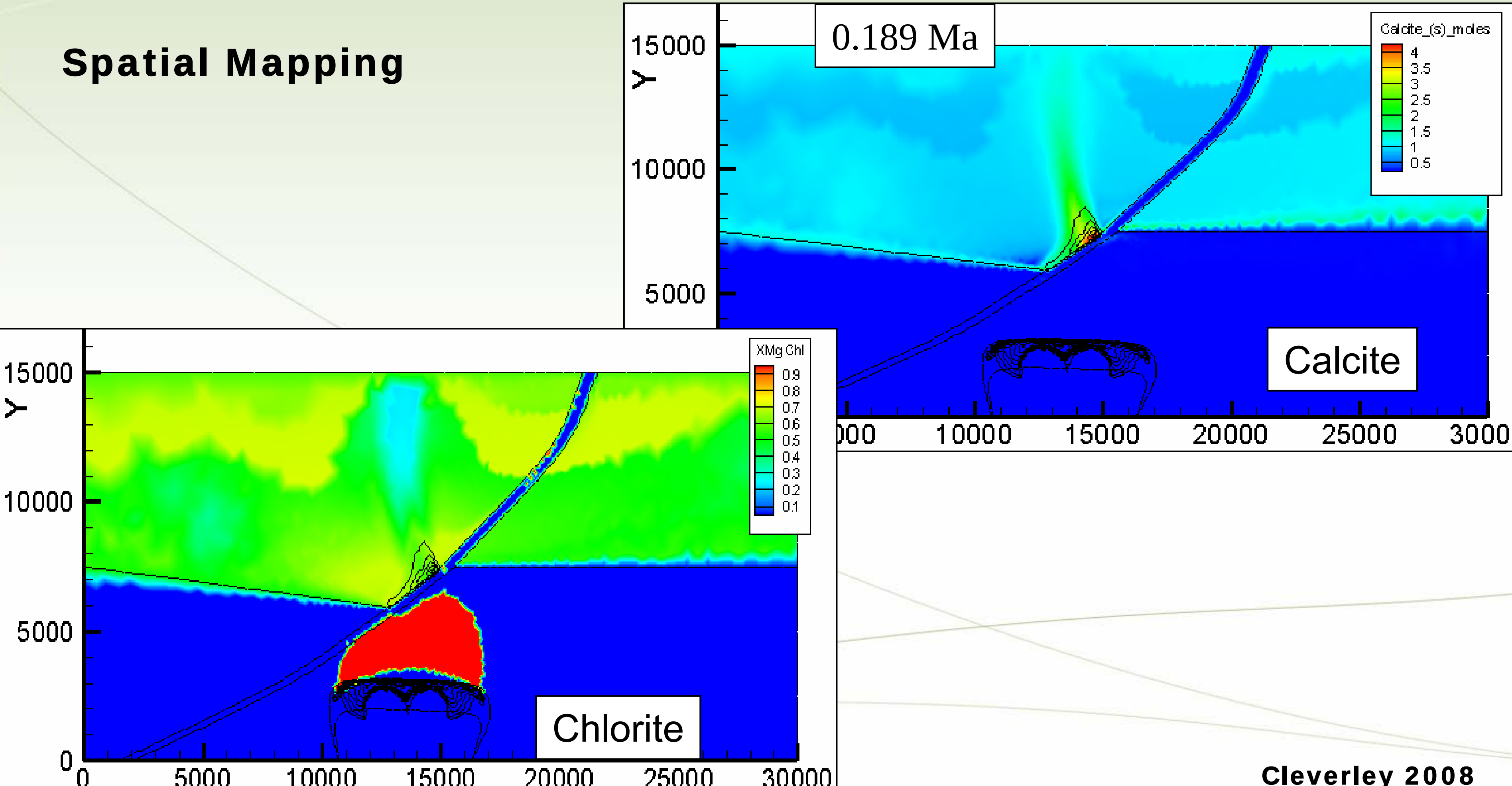
Example: RT Gold model

Spatial Mapping



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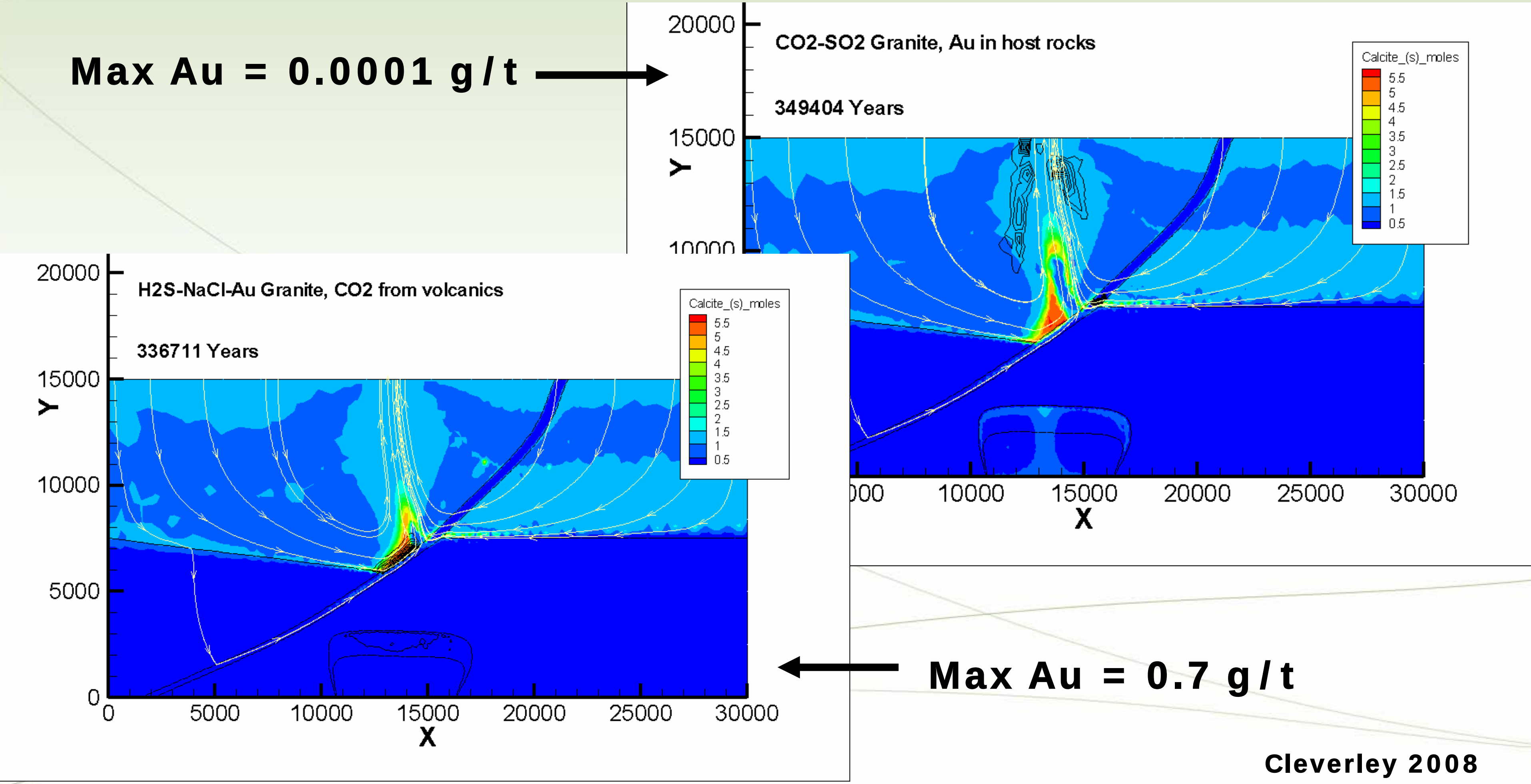
Example: RT Gold model

Max Au = 0.0001 g/t



Max Au = 0.7 g/t

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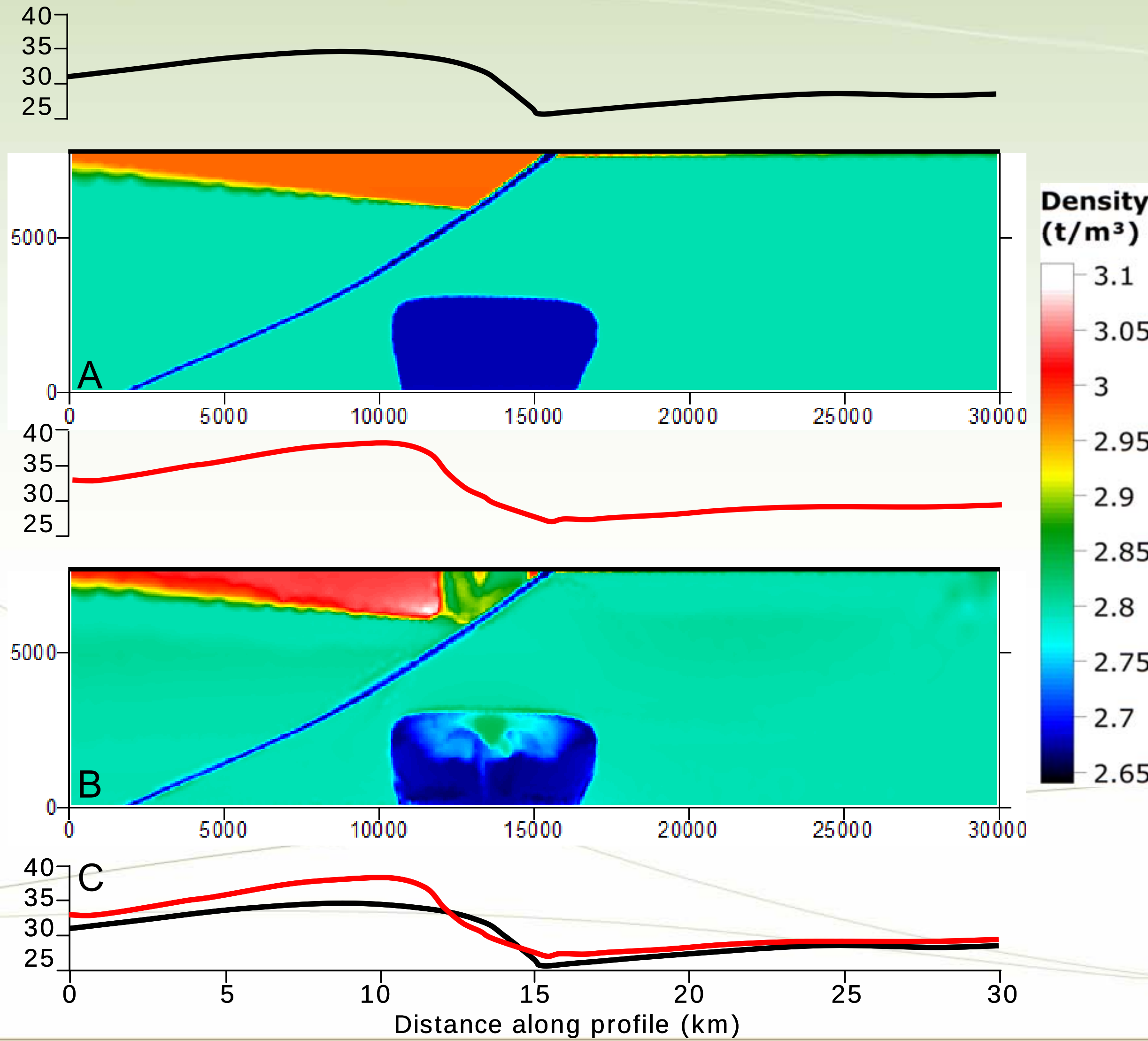
Example:
RT Gold model

Coupling Geophysical Forward Modelling



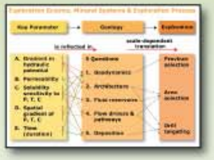
Chopping et al 2008

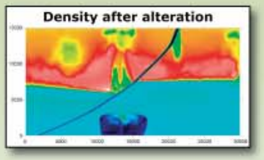
Implications for exploration

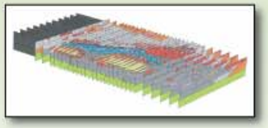
RT models can be used to simulate geophysical responses, allowing direct targeting from chemical models

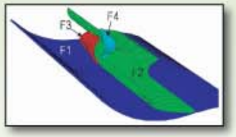
Simulation of key ore forming processes such as chemical reactions and fluid flow *predictive mineral discovery*Cooperative Research Centre*

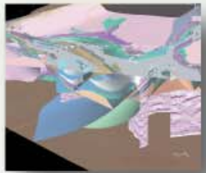
A legacy for mineral exploration science

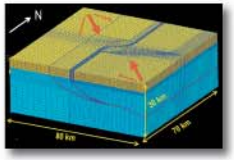


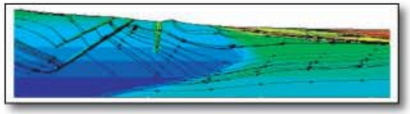


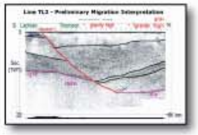












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*pmd*CRC* research areas

*pmd*CRC* research nodes

*pmd*CRC* working with State/Territory Surveys

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References

Chopping, R., Cleverley, J.S., Henson, P.A., and Roy, I.G. (2008). Reactive transport models: from geochemistry to geophysics to exploration targets. pmd*CRC Final Report: Project Y4 PART III.

Cleverley, J. (2008). Deliverable 15: Report on reactive transport models tested against specific sites where paragenesis and structure understood. FINAL REPORT pmd*CRC Y4 Project Part IV.