

Multi-physics Multi-scale Modelling in Geomechanics

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Never Stand Still

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First Question: Why Multi-physics?





Source: US DOE 2008

DIAGENETIC SETTINGS BASED ON MINERALOGY, GEOCHEMISTRY, PETROLEUM, AND HYDROGEOLOGY



Figure 2. Classification of diagenetic settings on the basis of mineralogy, petroleum, hydrogeochemistry, and hydrogeology. For illustrative simplicity, the geologic section is assumed to be isotropic and homogeneous, with idealized groundwater flow lines. The hydrocarbon-contaminated plume is slightly deflected by the local and regional groundwater flow systems. The depth limits separating the burial diagenetic settings are approximate and based on geologic phenomena that are easily recognizable. Near-surface settings may be meteoric, brackish, marine, or hypersaline. Adapted from Machel (1999).



Second Question: Why Multi-scale?



ICME framework, Horstemeyer 2009



Current Paradigm: computational homogenisation/upscalling



How does it work?



Stack of CT-scan images Chemical composition

Chemical system reduction (chemical homogenisation)

$$\frac{d[S]}{dt} = -[S]R_{1}$$

$$\frac{d[X]}{dt} = [S]R_{1}$$

$$\frac{d[X]}{dt} = [S]R_{1}$$

$$\frac{d[X]}{dt} = f[I][L]R_{3}$$

$$\frac{d[X]}{dt} = [F]R_{2} - [K][A][X]^{f}R_{3}$$

$$\frac{d[K]}{dt} = [F]R_{2} - [K][A][X]^{f}R_{3}$$

$$\frac{d[A]}{dt} = [F]R_{2} - [K][A][X]^{f}R_{3} + [L](R_{4}^{-} - R_{4}^{+})$$

$$\frac{d[Q]}{dt} = [L](R_{4}^{+} - R_{4}^{-})$$

$$\frac{d[Y]}{dt} = -[F]R_{2}$$

$$\frac{d[W]}{dt} = n[S]R_{2}$$

Alevizos et al. RMRE 2016 See also the poster by Sotiris Alevizos



d)

How does it work?



Chemical system reduction (chemical homogenisation)

Invariant manifold selection. E.g. steady state approximation for the intermediate species:

$$\frac{d[X]}{dt} = \frac{d[A]}{dt} = \frac{d[L]}{dt} = 0$$
$$B_{\text{(solid)}} \stackrel{r^+}{\rightleftharpoons} A_{\text{(solid)}} + B_{\text{(fluid)}}$$

Stack of CT-scan images Chemical composition

$$r^+ = C_{AB}k^+(T) = [\mathbf{S}][\mathbf{F}]R_1R_2$$

Alevizos et al. RMRE 2016 $r^- = C_A C_B k^-(T) = 2nf[I][S][F]^2 \frac{R_2 R_3}{(R_4^+ - R_4^-)}$ See also the poster by Sotiris Alevizos

How does it work?

Navier-Stokes fluid flow (hydraulic homogenisation)







See also the poster by Martin Lesueur





How do we scale up from lab scale to geodynamics?

- THMC systems obey MaxEP, MinEP or something else? Does the choice of BCs make any difference?
- Current paradigm in computational homogenisation follows the MaxEP path
- Is MaxEP representative for THMC systems? How do we deal with the cascade of length/time scales of localisation?



The multiphysics (THMC) approach

- Fluid-saturated rock
- Coaxial Elasto-visco-plasticity, deviatoric and volumetric components







Towards a unified THMC approach

- Fluid-saturated rock
- Coaxial Elasto-visco-plasticity, deviatoric and volumetric components
- Mechanical (Shear) heating
- Endothermic fluid release reaction producing excess pore pressure

$$AB_{(solid)} \xrightarrow{r_F} A_{(solid)} + B_{(fluid)}$$

 Porosity and permeability linked with Kozeny-Carman law

$$k_{\pi} = k_{\pi 0} \frac{(1 - \phi_0)^2}{\phi_0^3} \frac{\phi^3}{(1 - \phi)^2}$$



$$\phi = \phi_0 + \Delta \phi_{mech} + \Delta \phi_{chem}$$

$$\Delta \phi_{\text{chem}} = A_{\phi} \frac{1 - \phi_{0}}{1 + \frac{\rho_{B}}{\rho_{A}} \frac{M_{A}}{M_{B}} \frac{1}{s}},$$

$$s = \frac{\omega_{\text{rel}}}{1 + \omega_{\text{rel}}}, \text{ and}$$

$$\omega_{\text{rel}} = \frac{\rho_{AB}}{\rho_{A}} \frac{M_{A}}{M_{AB}} K_{c} \exp\left(\frac{\Delta H}{RT}\right)$$



Do we need chemistry? Triaxial experiments (THM) in soft rocks

Distribution of shear strain Compression 0.25 0.20 CD1 CD2 CD3 CD4 CD5 CD6 0.15 0.25MPa 0.5MPa 0.75MPa 1.0MPa 1 5MPa 2.0MPa 0.10 0.05 0.00 Distribution of volumetric strain Oka et al, IJNAMG, 2011

The goal is to constrain the hardening law:

 $Q_{mech} = E + p_f V_{act}$

 $E = E_0 + \Delta E$



a (T)HM system for pore collapse

$$\mathbf{0} = \partial_j \sigma'_{ij} - \partial_i \Delta p_f + b_i,$$

$$\mathbf{0} = \partial_t \Delta p_f - \partial_i \left[\frac{1}{Le} \partial_i \Delta p_f \right] - \Lambda \partial_t T + \frac{\dot{\epsilon_V}}{\bar{\beta}},$$

$$\mathbf{0} = \partial_t T - \partial_{ii}^2 T - Gr \,\sigma_{ij} \dot{\epsilon}_{ij}^{pl}.$$

The energy and entropy balance laws are solved explicitly to determine the global attractor of the system



Diagenesis (pore collapse) in sandstone

Isotropic consolidation of saturated Bleurwiller sandstone



Drained consolidation of diatomaceous mudstone



Matching the experiments



Deviatoric plastic strain

0.110

0.339

4.940e-01

Poulet and Veveakis COGE 2016



MaxEP or MinEP Where do THM systems self-organise?



Paesold et al JoMMS 2016

Temperature θ 0 4 8 12 16 22





T(H)M systems self-organise at MaxEP





T(H)M systems self-organise at MaxEP



Paesold et al JoMMS 2016





Where do THMC systems self-organise?





Alevizos et al, Mathematics 2016

What changes when chemistry is included?



System of equations

$$AB_{(solid)} \underbrace{\stackrel{r_{F}}{\longleftarrow} A_{(solid)}}_{r_{R}} + B_{(fluid)} \qquad r_{F,R} = k_{F,R}\rho_{i} e^{-\frac{Ar}{1+\theta}}$$
$$\frac{\partial P}{\partial t} + Pe_{mass} v \cdot \nabla P - Pe_{temp} v \cdot \nabla \theta - \nabla \left[\frac{1}{Le}\nabla P\right] - \overline{\Lambda} \frac{\partial \theta}{\partial t} + \frac{\dot{\varepsilon}_{v}^{pl}}{\beta^{*}} - \mu \cdot r_{F} = 0$$

$$\frac{\partial \theta}{\partial t} + Pe_{thermal} v \cdot \nabla \theta - \nabla^2 \theta - X \cdot \tau \cdot \dot{\varepsilon}_d^p - X \cdot \sigma \cdot \dot{\varepsilon}_v^p + |\Delta H| \cdot r_F - |\Delta H| \cdot r_R = 0$$



System's stability regimes



char. time scale energy transfer



Phase diagrams

Natural localised instability



Temperature



Temperature

THMC systems self-organise around MinEP





Alevizos et al, Mathematics 2016

How do we upscale from here? Constant force vs flux BCs







Exrtapolation to large scales? Large scale modelling





Modelling Subduction zones: Serpentinite dehydration oscillator





Modelling subduction zones



Rogers & Dragert, Science (2003)

Alevizos et al, JGR (2014)



Chaotic signals – Gisborne (New Zealand)



Poulet et al, JGR (2014)



Matching length scales

- Intern. Ocean Discovery Program
- Japan Trench Fast Drilling Project

Nature news, Dec 2013:



Table 3. Material Parameters Inverted From the ETS

"The localization of deformation onto a limited thickness (~5 meters) of pelagic clay is the defining characteristic of the shallow earthquake fault" (Chester et al / Science 2013). "That's just weird" says Emily Brodsky (UC Santa Cruz)

		Sequences, After Fitting the GPS Data ^a				
		Parameter	Units	ALBH	GISB 1	GISB 2
	_	Ý0	s ⁻¹	200	230	230
AGU PUBLICATIONS		d	m	6.4	6.4	6.4
Journal of Geophysical Research: Solid Earth		$\bar{\sigma}'_n$	MPa	49	49	74
RESEARCH ARTICLE	Thermo-poro-mechanics of chemically active creeping faults: 3. The role of serpentinite in episodic tremor and slip sequences, and transition to chaos T. Poulet ¹ , E. Veveakis ^{1,2} , K. Regenauer-Lieb ^{1,3} , and D. A. Yuen ^{4,5}	$\beta_T \bar{\tau}_n$	MPa	0.3	0.26	0.20
		k _F	s ⁻¹	10 ⁸	10 ⁸	10 ⁸
This is a companion paper to Alevizos et al. (2014), doi:10.1002/2013JB010070, and Veuronkir et al. (2014)		Q_F	kJ/mol	114	114	114
		k _R	s ⁻¹	10 ⁻²	10 ⁻²	10 ⁻²
		ΔH	kJ/mol	80	80	80
		Q_R	kJ/mol	34	34	34

In Conclusion



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http://ugg.unsw.edu.au





July 5-7, 2017 Paris, France

The 6th International Conference on Coupled Thermo-Hydro-Mechanical-Chemical (THMC) Processes in Geosystems: Multiphysical instabilities across the scales



Important dates

Abstract submission: 15 November 2016 Abstract acceptance: 15 December 2016 Early-bird registration: 31 January 2017

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