



# **Coupled Thermal-Hydrodynamic-Mechanical -Chemical (THMC) Processes in CO<sub>2</sub> Geological Storage**

## **地质封存的热-流-力-化耦合过程**

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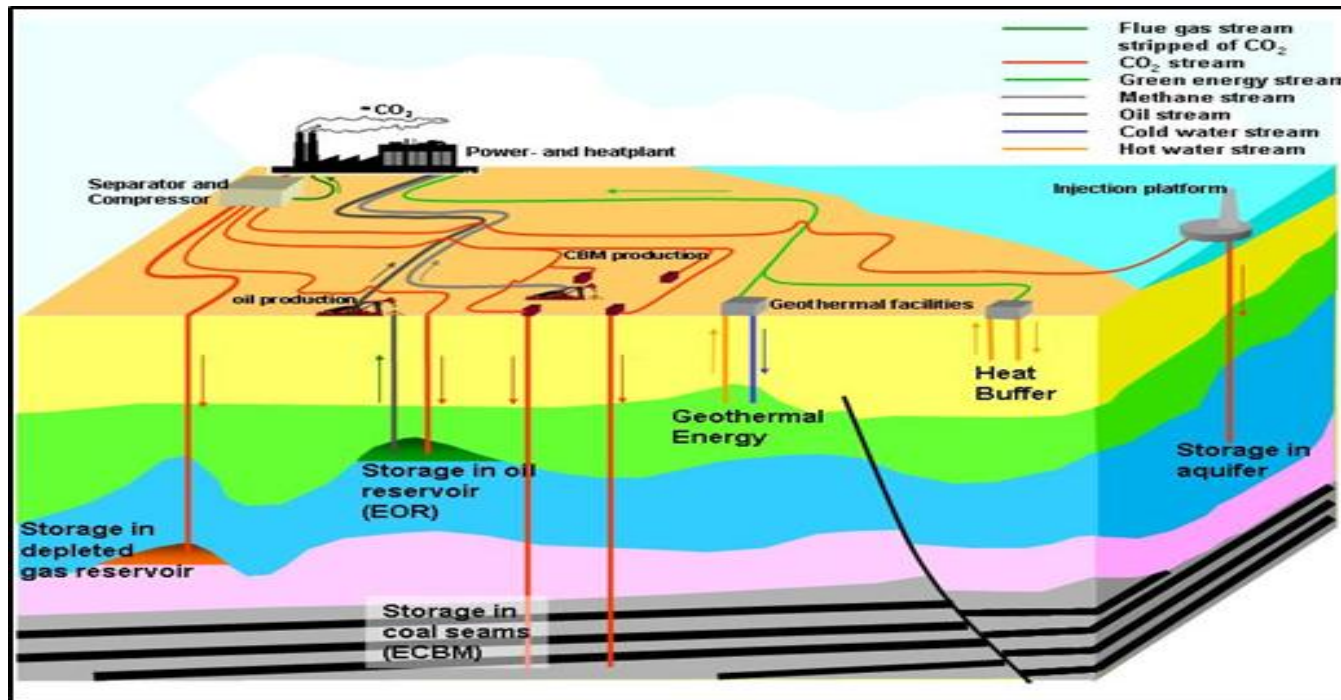
# Outlines

- Background
- Interactions between THMC processes
- Individual processes
- Coupled processes
- Conclusions and recommendations



# Background

## CO<sub>2</sub> Geological utilization and storage (CGUS)

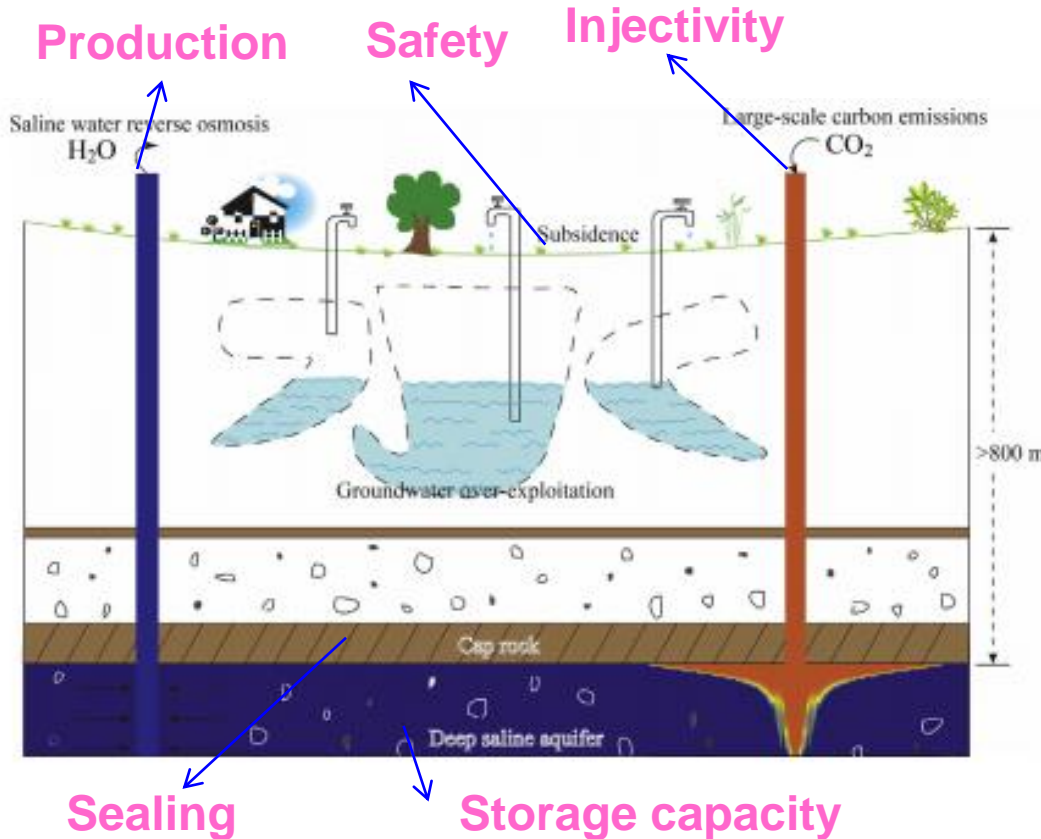


- EOR 驱油
- ECBM 驱煤层气
- EGR 驱天然气
- ESGR 驱页岩气
- EGS 强化采热
- EUL 溶浸采铀
- EWR 驱水

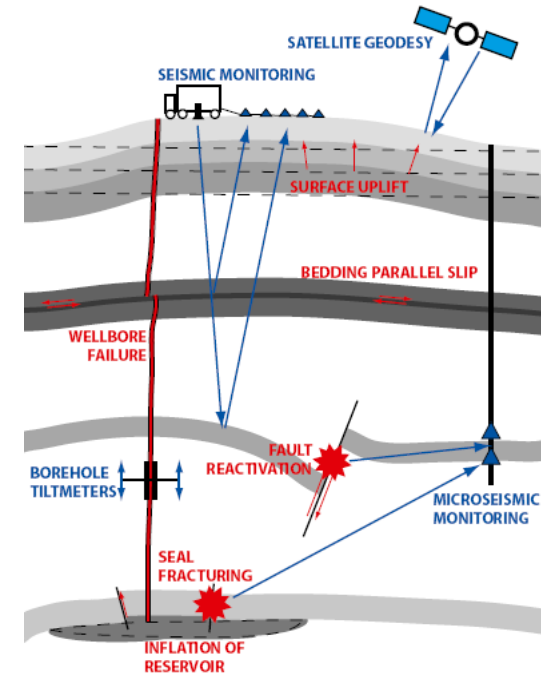
Common scientific issue? 共同的基础科学问题



# Background



## Mechanical Stability



- ◆ **Large scale:** tens of millions ton of CO<sub>2</sub> injected at single site, area of about 1000km<sup>2</sup> involved
- ◆ **Long term:** hundreds of years
- ◆ **Multi-physical coupling:** T-H-M-C coupling

**Aims:** Current understanding, theory framework



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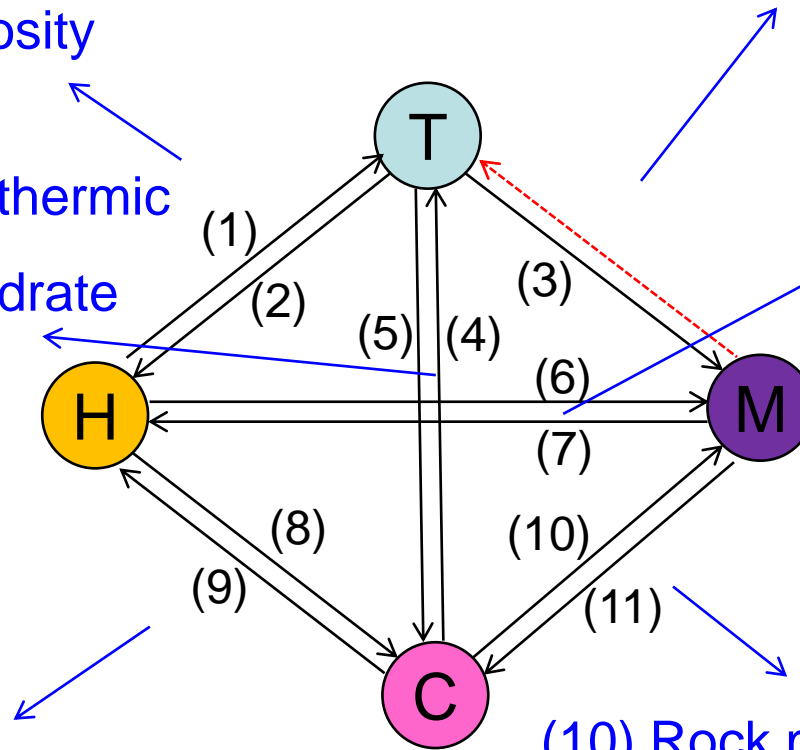
# Interaction among THMC processes

- (1) Heat convection, enthalpy
- (2) Density, viscosity

- (3) Thermal stress, thermal damage

- (4) Exothermic/endothemic
- (5) Reaction rate, hydrate

- (6) Effective stress
- (7) Porosity & permeability



- (8) Species convection transport
- (9) Density, viscosity, porosity & permeability

- (10) Rock mechanical properties, adsorption-induced swelling and softening
- (11) Pressure solution



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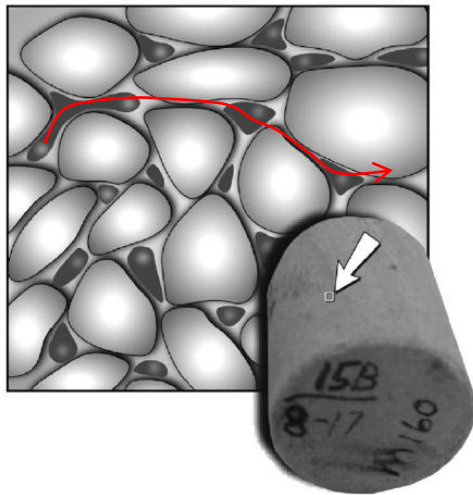




# Individual process-Hydrodynamic process

Multiphase and multicomponent

CO<sub>2</sub>, H<sub>2</sub>O, NaCl  
Aqueous, gaseous



Darcy's law for Multiphase flow

## Mass conservation

$$\frac{d}{dt} \int_{V_n} M^\kappa dV = \int_{\Gamma_n} \mathbf{F}^\kappa \cdot \mathbf{n} d\Gamma + \int_{V_n} q^\kappa dV$$

$$M^\kappa = \sum_{\beta=A,G} \phi S_\beta \rho_\beta X_\beta^\kappa, \quad \kappa = w, i, g$$

$$\mathbf{F}_\beta^\kappa = -k \frac{k_{r\beta} \rho_\beta}{\mu_\beta} X_\beta^\kappa (\nabla P_\beta - \rho_\beta \mathbf{g}) + \mathbf{J}_\beta^\kappa, \quad \kappa = w, i, g$$

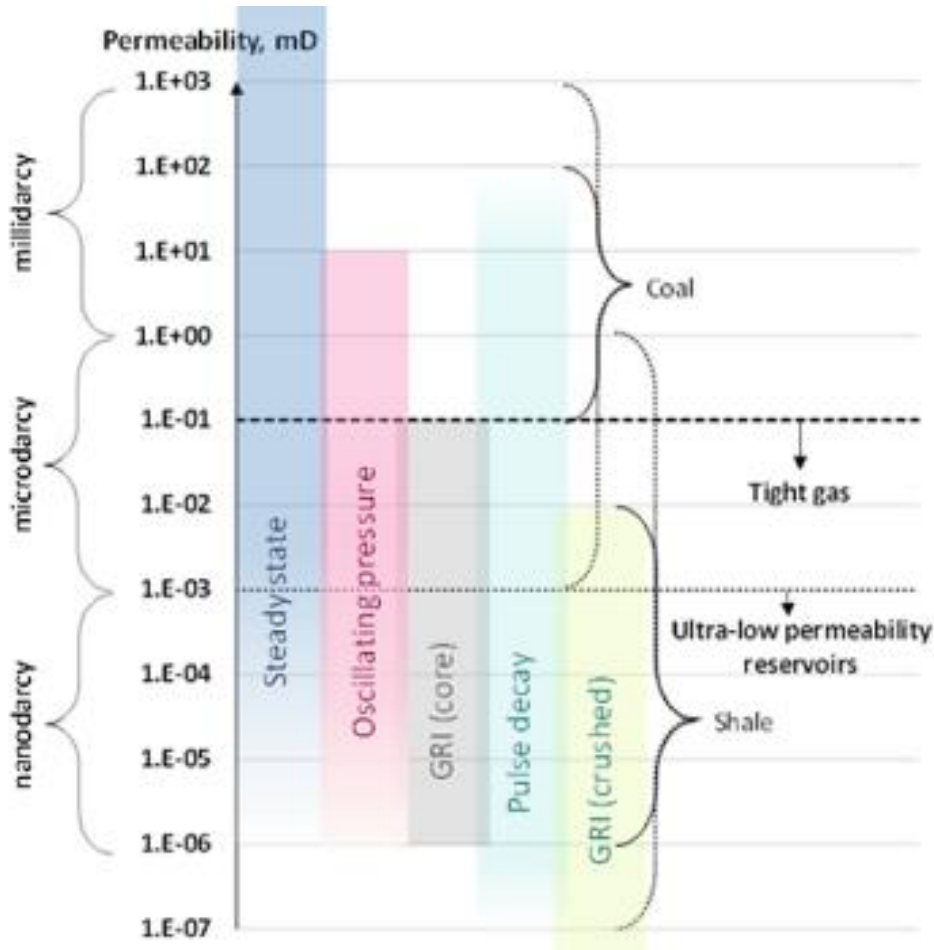
$$\sum_{\beta=A,G} S_\beta = 1 \quad P_g - P_l = P_c$$



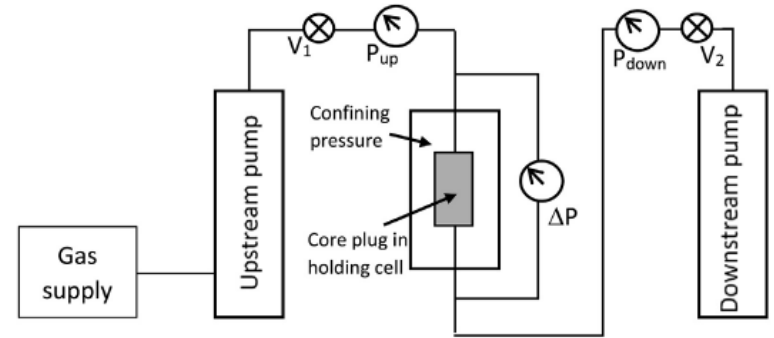


# Single process-Hydrodynamic process

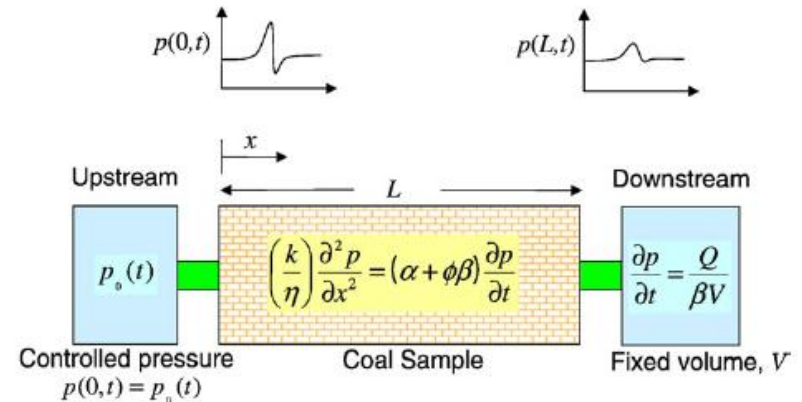
## Key Parameter-permeability



### Steady state method

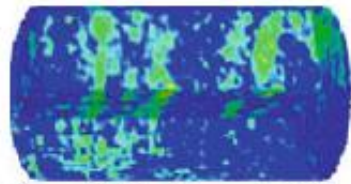
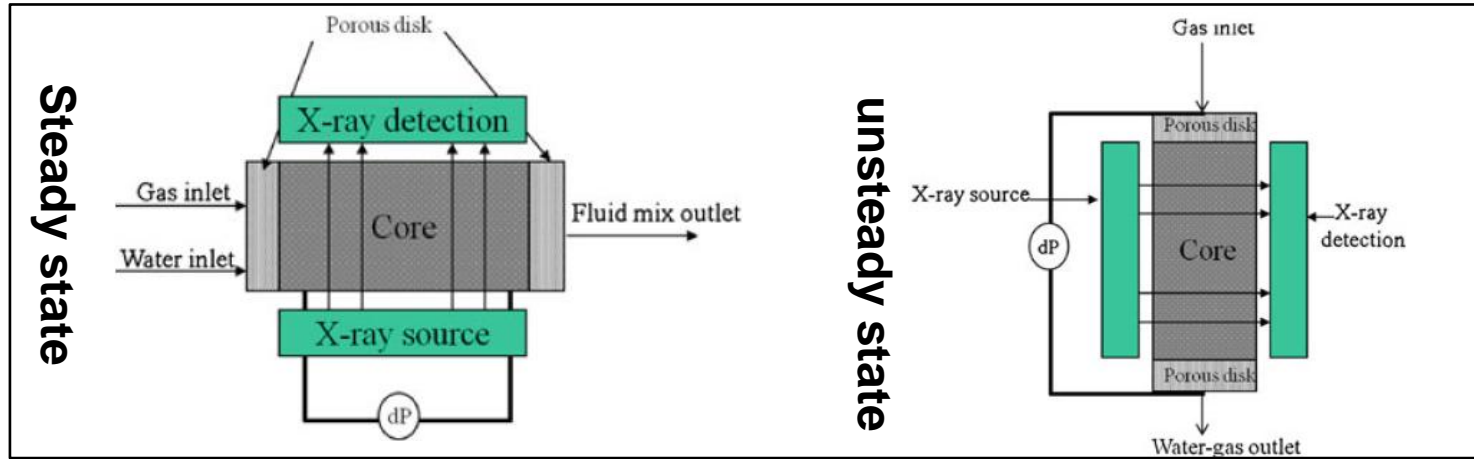


### Pressure transient method

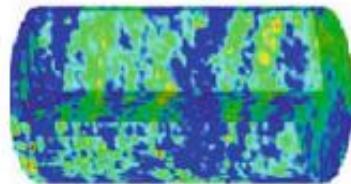


# Single process-Hydrodynamic process

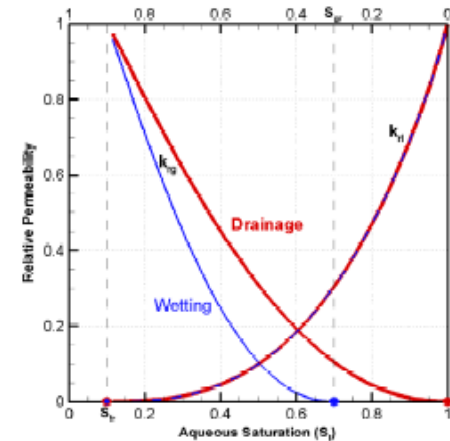
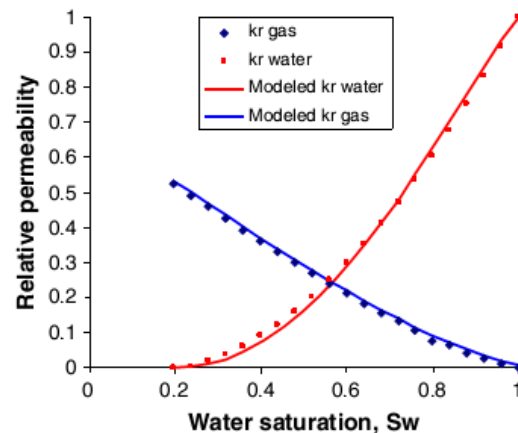
## Key Parameter-relative permeability



$$f_{CO_2} = 0.05, S_{CO_2} = 0.132$$



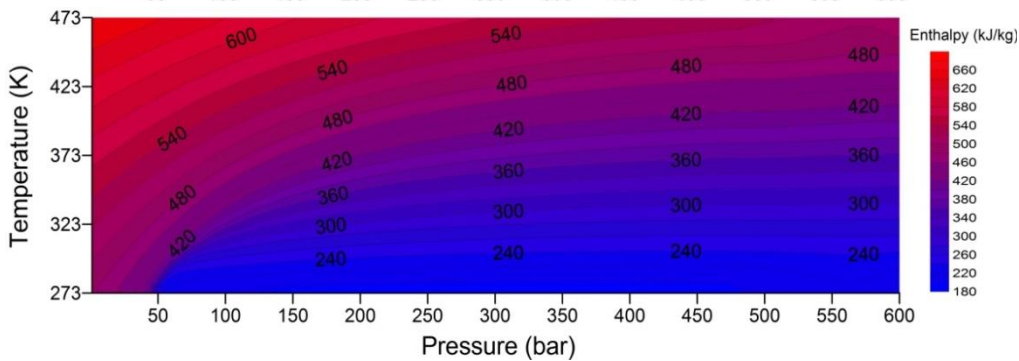
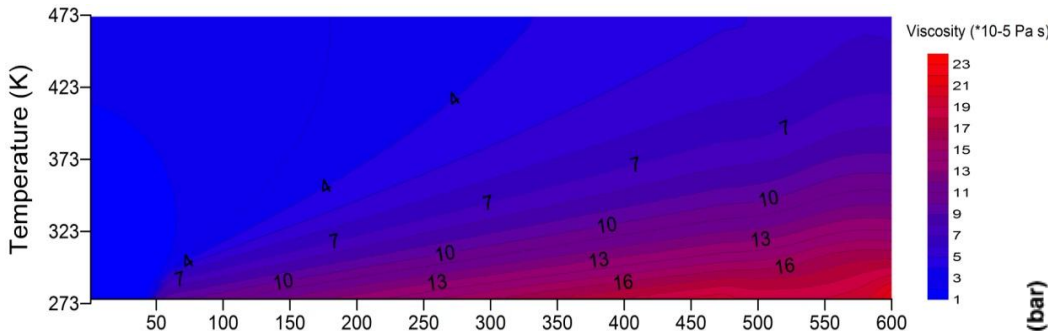
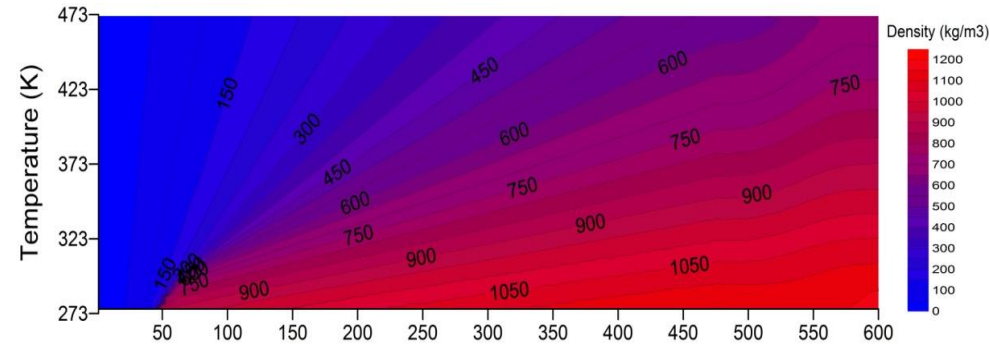
$$f_{CO_2} = 0.70, S_{CO_2} = 0.278$$



# Single process-Hydrodynamic process

## Fluid property

Pure CO<sub>2</sub>

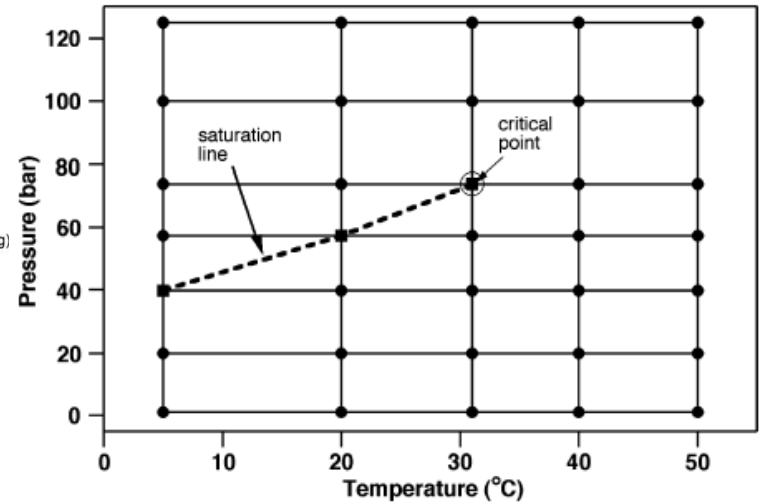


Pure H<sub>2</sub>O

International Formulation Committee (1967)

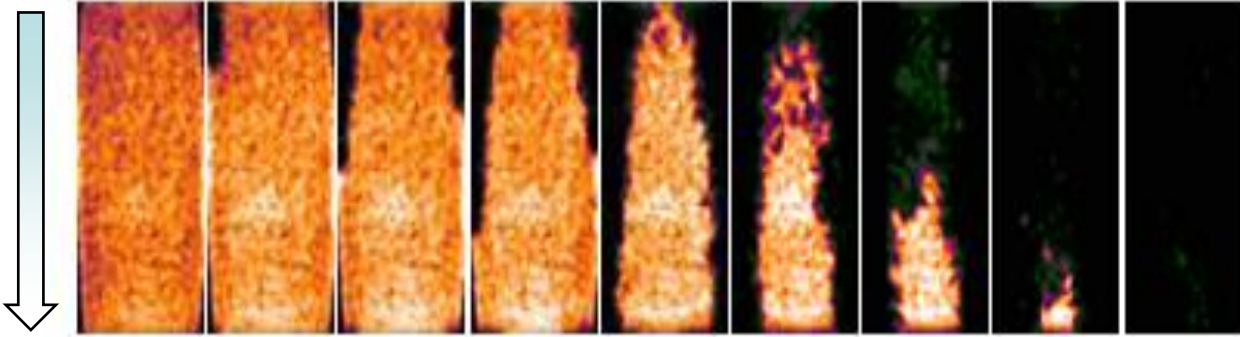
Mixtures

Density, viscosity, enthalpy

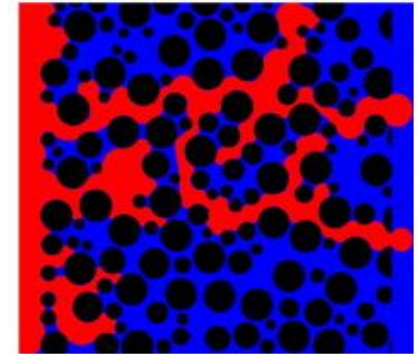


# Coupled processes-Hydrodynamic process

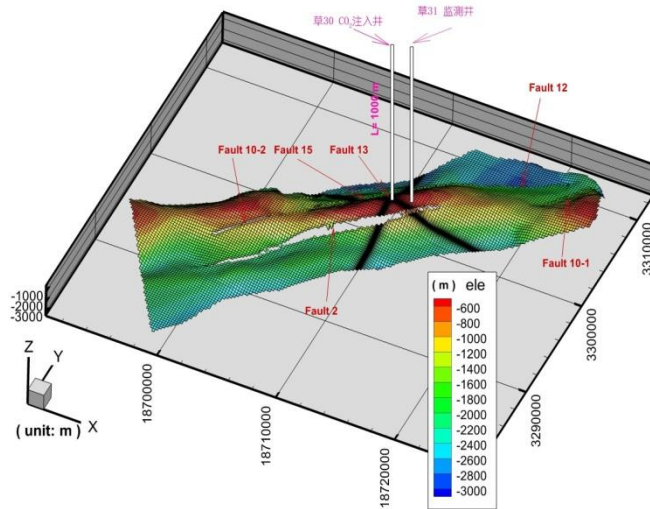
MRI images of CO<sub>2</sub> displacement (Jiang LL, 2016)



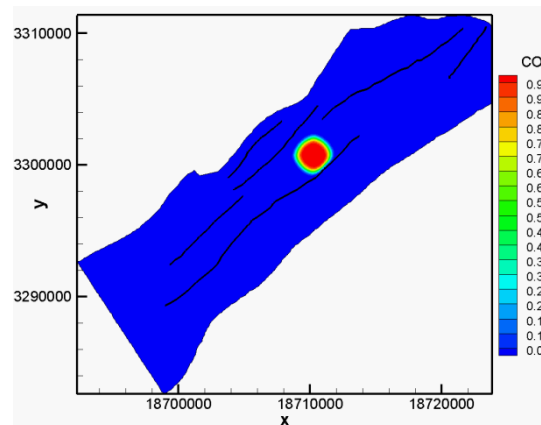
Pore-scale



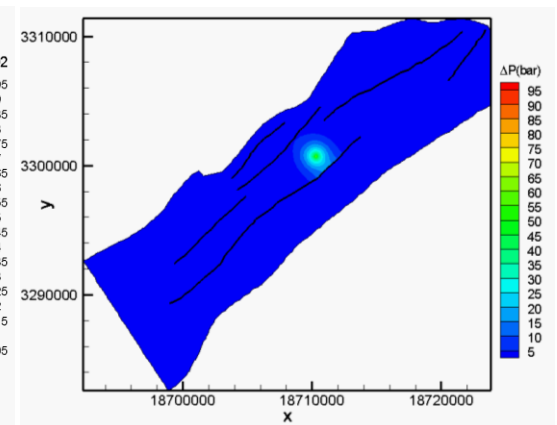
Numerical simulation of CO<sub>2</sub> injection (site-scale)



Incremental pressure

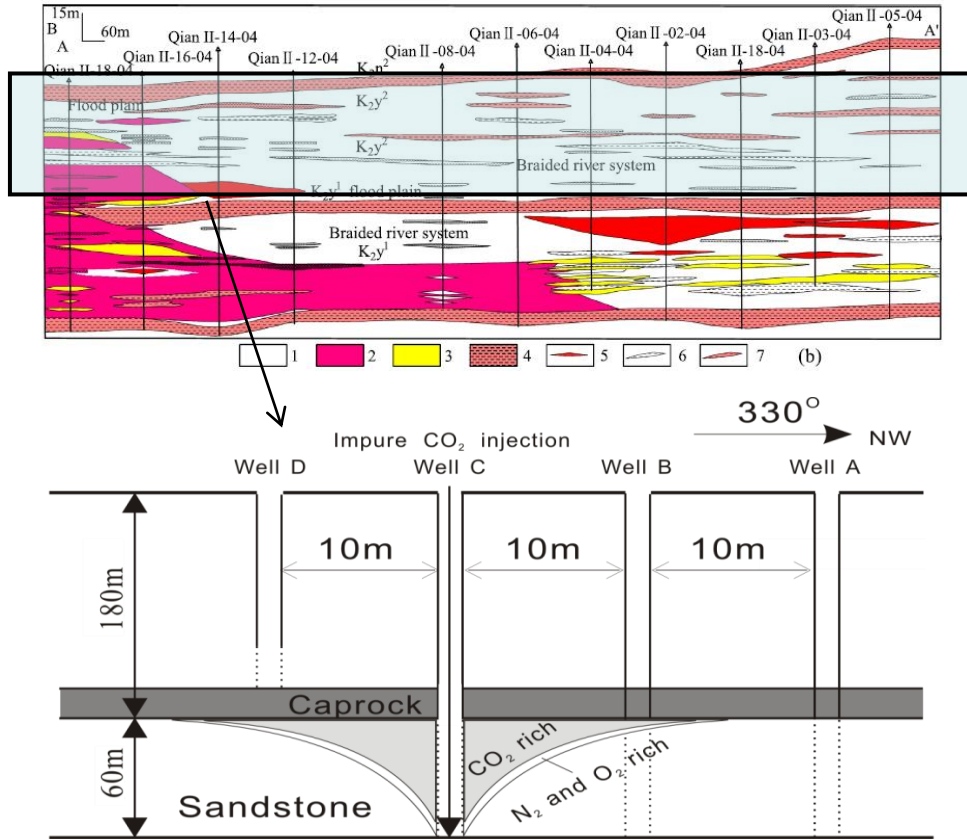


CO<sub>2</sub> mass fraction

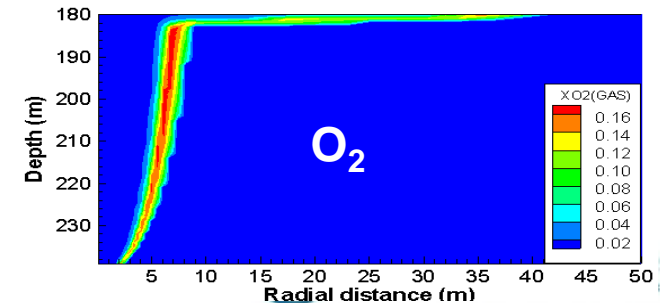
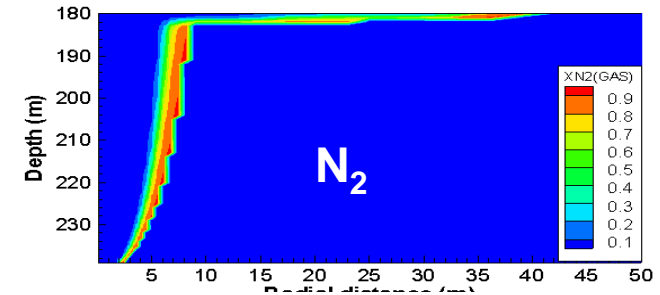
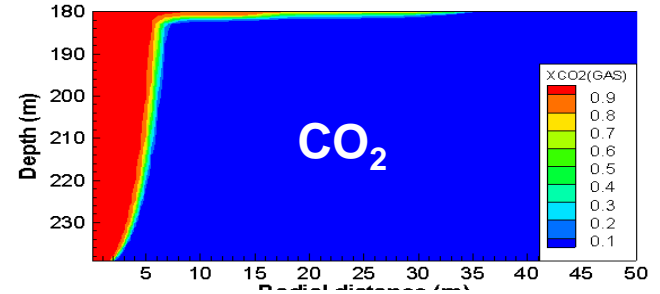
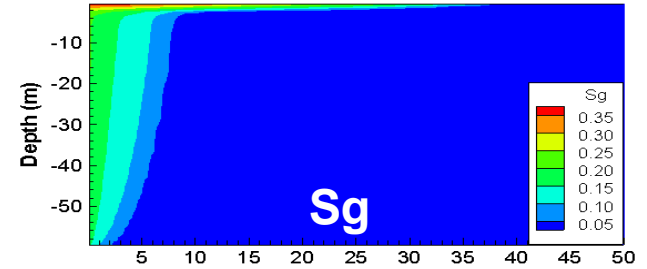


# Coupled processes-Hydrodynamic process

## Impure CO<sub>2</sub> injection at Tongliao



Lei, et al. 2016

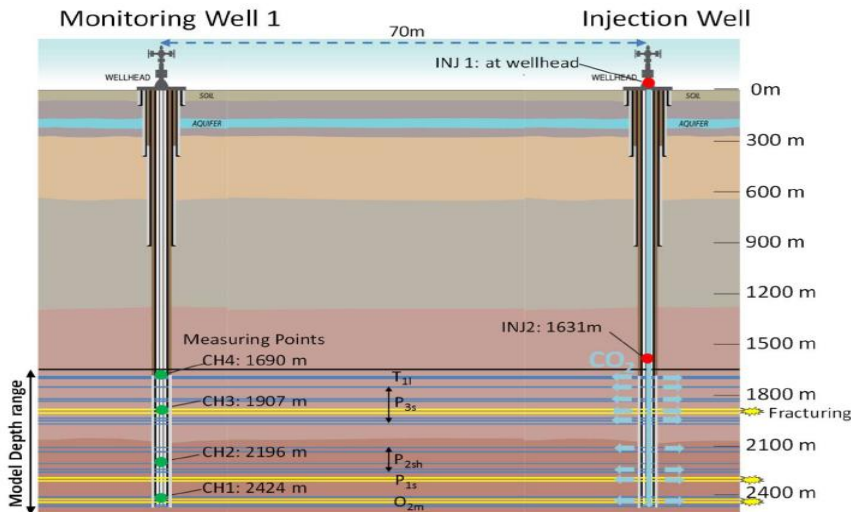
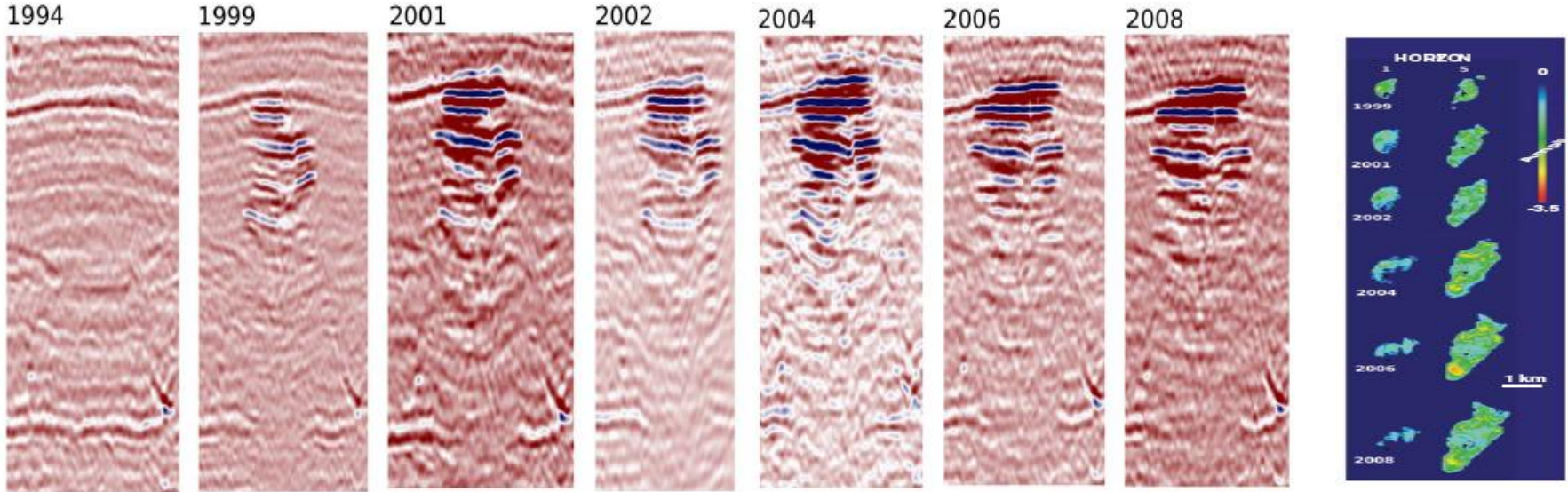


# Coupled processes-Hydrodynamic process

## Monitoring of CO<sub>2</sub> migration

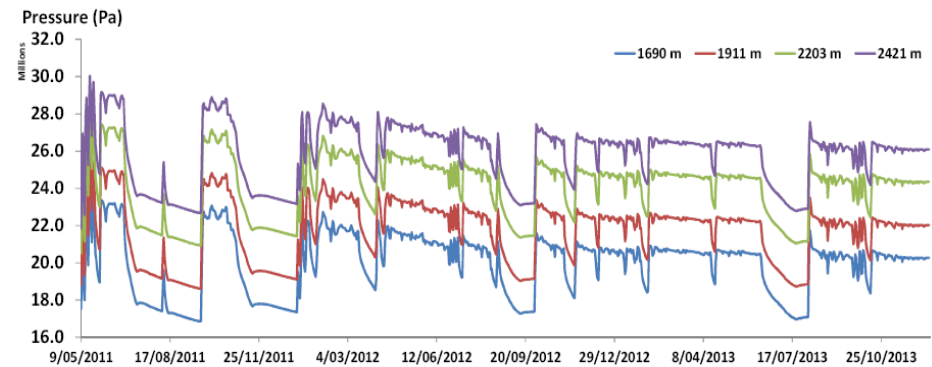
Sleipner Field

Boait, et al. 2012



Shenghua CCS site

Li, et al. 2016



# Single process-Thermal process

Energy conservation

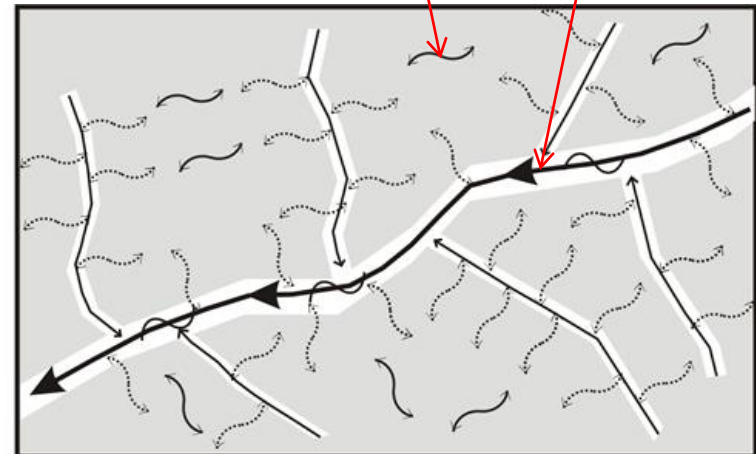
Must be coupled with H !

$$\frac{d}{dt} \int_{V_n} M^\kappa dV = \int_{\Gamma_n} \mathbf{F}^\kappa \cdot \mathbf{n} d\Gamma + \int_{V_n} q^\kappa dV$$

$$M^{\kappa+1} = (1 - \phi) \rho_R C_R T + \sum_{\beta=A,G} \phi S_\beta \rho_\beta u_\beta$$

$$\mathbf{F}_\beta^{\kappa+1} = -\lambda \nabla T + \sum_{\beta} h_\beta F_\beta$$

conduction      convection





# Single process-Mechanical process

## Motion equation

$$\left. \begin{aligned} -G\nabla^2 w_x - \frac{G}{1-2\nu} \frac{\partial}{\partial x} \left( \frac{\partial w_x}{\partial x} + \frac{\partial w_y}{\partial y} + \frac{\partial w_z}{\partial z} \right) + \frac{\partial P}{\partial x} + 3\beta_T K \frac{\partial T}{\partial x} &= 0 \\ -G\nabla^2 w_y - \frac{G}{1-2\nu} \frac{\partial}{\partial y} \left( \frac{\partial w_x}{\partial x} + \frac{\partial w_y}{\partial y} + \frac{\partial w_z}{\partial z} \right) + \frac{\partial P}{\partial y} + 3\beta_T K \frac{\partial T}{\partial y} &= 0 \\ -G\nabla^2 w_z - \frac{G}{1-2\nu} \frac{\partial}{\partial z} \left( \frac{\partial w_x}{\partial x} + \frac{\partial w_y}{\partial y} + \frac{\partial w_z}{\partial z} \right) + \frac{\partial P}{\partial z} + 3\beta_T K \frac{\partial T}{\partial z} &= \gamma_{sat} \end{aligned} \right\}$$

Must be coupled  
with H and T !

## Stress-strain

$$\left. \begin{aligned} \sigma'_x &= 2G \left( \frac{\nu}{1-2\nu} \varepsilon_v + \varepsilon_x \right) + 3\beta_T K \Delta T \\ \sigma'_y &= 2G \left( \frac{\nu}{1-2\nu} \varepsilon_v + \varepsilon_y \right) + 3\beta_T K \Delta T \\ \sigma'_z &= 2G \left( \frac{\nu}{1-2\nu} \varepsilon_v + \varepsilon_z \right) + 3\beta_T K \Delta T \\ \tau'_{yz} &= G\gamma_{yz}, \tau'_{zx} = G\gamma_{zx}, \tau'_{xy} = G\gamma_{xy} \end{aligned} \right\}$$

## Strain-displacement

$$\left. \begin{aligned} \varepsilon_x &= -\frac{\partial w_x}{\partial x}, \gamma_{yz} = -\left( \frac{\partial w_y}{\partial z} + \frac{\partial w_z}{\partial y} \right) \\ \varepsilon_y &= -\frac{\partial w_y}{\partial y}, \gamma_{zx} = -\left( \frac{\partial w_z}{\partial x} + \frac{\partial w_x}{\partial z} \right) \\ \varepsilon_z &= -\frac{\partial w_z}{\partial z}, \gamma_{xy} = -\left( \frac{\partial w_x}{\partial y} + \frac{\partial w_y}{\partial x} \right) \end{aligned} \right\}$$







# Single process-Chemical process

**Mass conservation**

**Solute transport**

Mechanical dispersion  
Molecular diffusion

$$\frac{d}{dt} \int_{V_n} M^K dV = \int_{\Gamma_n} \mathbf{F}^K \cdot \mathbf{n} d\Gamma + \int_{V_n} q^K dV$$

**convection**

**dispersion**

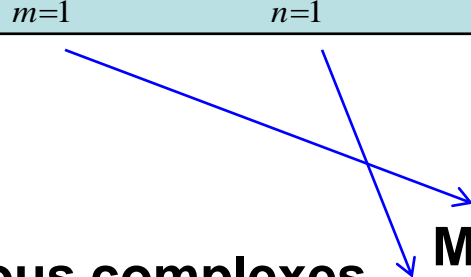
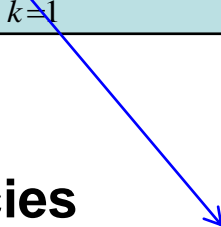
$$M_l^K = \phi S_l C_l^K$$

$$F_l^K = F_l C_l^K - (\tau \phi S_l D_l^K) \nabla C_l^K$$

**Chemical reaction**

- Gas solution
- Aqueous complexation
- Redox
- Ion exchange
- Adsorption
- Mineral dissolution /precipitation

$$T_j = c_j + \sum_{k=1}^{N_x} v_{kj} c_k + \sum_{m=1}^{N_p} v_{mj} c_m + \sum_{n=1}^{N_q} v_{nj} (c_n^0 - r_n \Delta t_r) = T_j^0$$



**Basis species**

**Aqueous complexes**

**Mineral at equilibrium and kinetic constraint**



# Single process-Chemical process

## Chemical reaction-gas solution

Cubic model for fugacity

$$\mu_i^{NA} = \mu_i^{AQ}$$

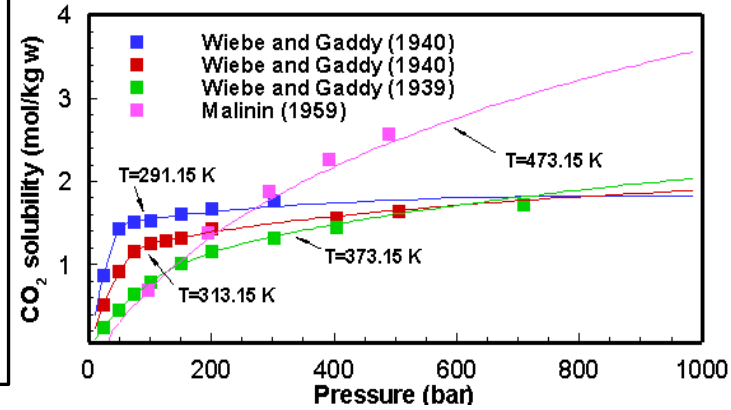
Pitzer model for water activity

$$\begin{aligned} \mu_i^{NA}(T, P, y_i) &= \mu_i^{NA(0)}(T) + RT \ln f_i(T, P, y_i) \\ &= \mu_i^{NA(0)}(T) + RT \ln y_i P + RT \ln \phi_i(T, P, y_i) \end{aligned}$$

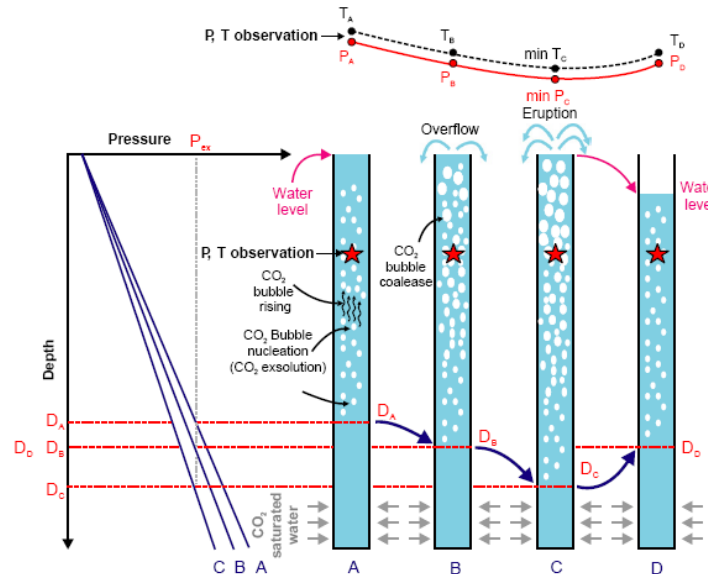
$$\begin{aligned} \mu_i^{AQ}(T, P, m_{sol}) &= \mu_i^{AQ(0)}(T, P) + RT \ln a_i(T, P, m_{sol}) \\ &= \mu_i^{AQ(0)}(T, P) + RT \ln(Nw \times x_i) + RT \ln \gamma_i(T, P, m_{sol}) \end{aligned}$$

$$P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b) + b(V-b)}$$

$$\ln \gamma_i = \sum_c 2m_c \lambda_{i-c} + \sum_a 2m_a \lambda_{i-a} + \sum_c \sum_a m_a m_c \zeta_{i-a-c}$$



CO2 eruption from Crystal Geyser, UT

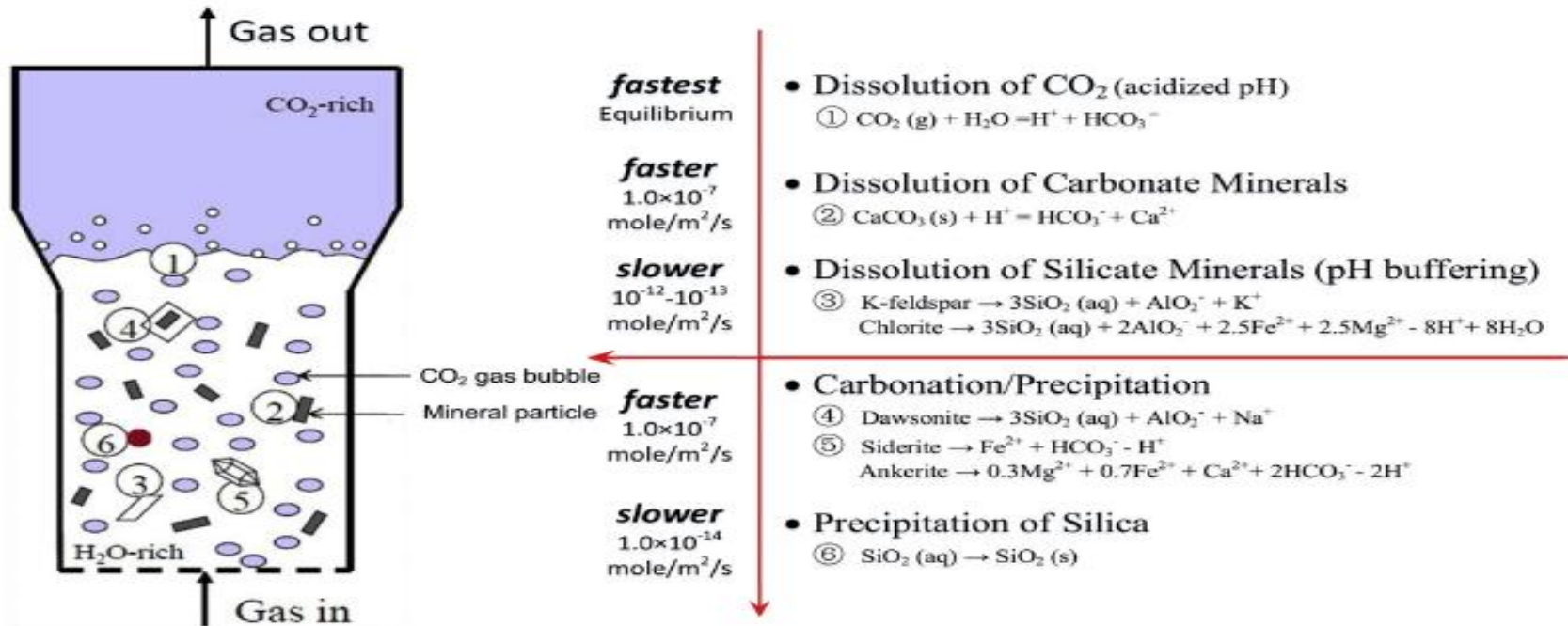


Han WS et al., 2013



# Single process-Chemical process

## Chemical reaction-water/rock reaction



### Reaction rate for kinetic minerals

$$r_m = \pm k(T)_m \left| 1 - \left( \frac{Q_m}{K_m} \right)^\theta \right|^\eta$$

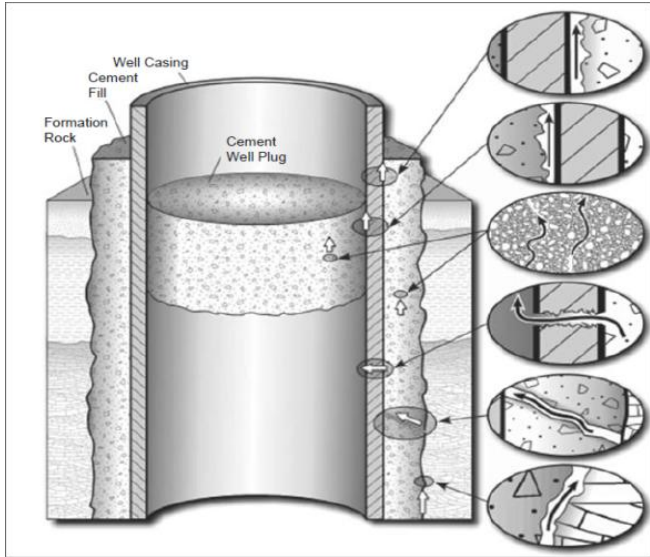
$$k(T) = k_{25}^{nu} \exp \left[ \frac{-E_a^{nu}}{R} \left( \frac{1}{T} - \frac{1}{298.15} \right) \right]$$

$$+ k_{25}^H \exp \left[ \frac{-E_a^H}{R} \left( \frac{1}{T} - \frac{1}{298.15} \right) \right] a_H^{n_H}$$

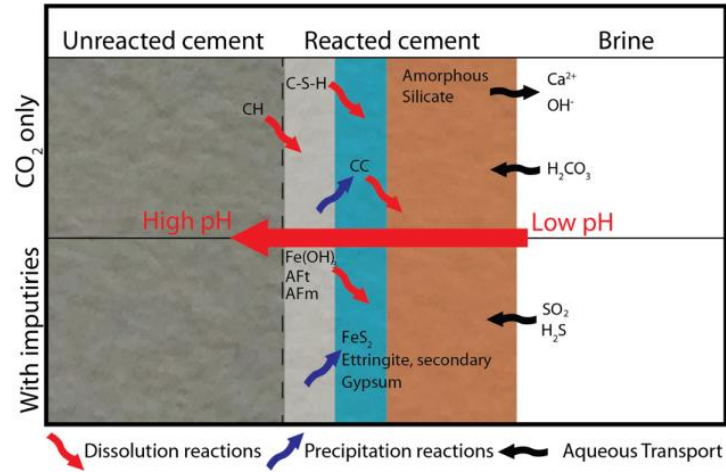
$$+ k_{25}^{OH} \exp \left[ \frac{-E_a^{OH}}{R} \left( \frac{1}{T} - \frac{1}{298.15} \right) \right] a_{OH}^{n_{OH}}$$

# Coupled processes-**Chemical process**

## CO<sub>2</sub>-water-rock reaction-batch experiment



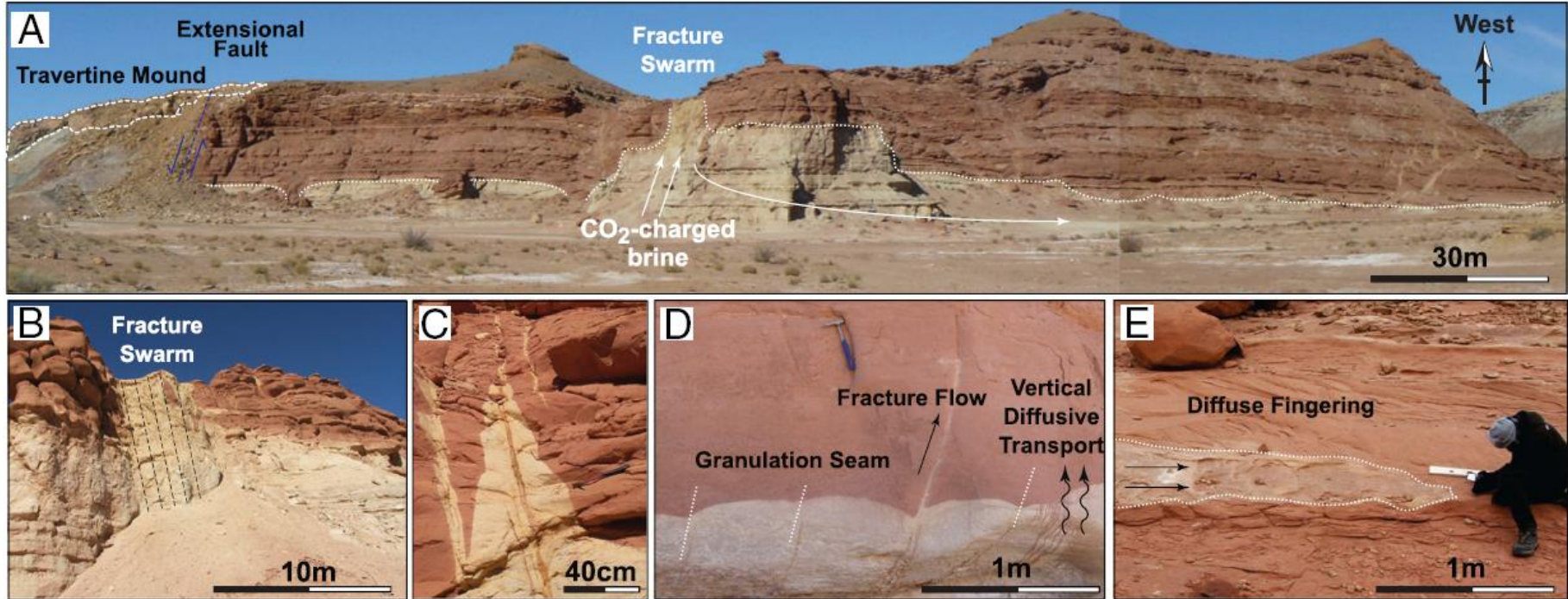
### CO<sub>2</sub>-water-rock reaction near the wellbore



Zhang, et al.  
2013

# Coupled processes-**Chemical process**

## Long term CO<sub>2</sub>-water-rock reaction



Kampman, et al. 2014



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# Coupled processes-Focus

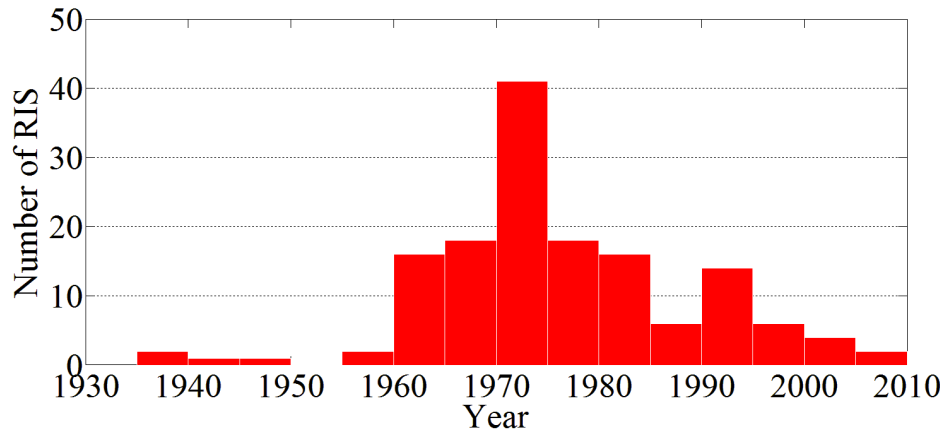
Number of process	Coupling
1	T、H、C、M
2	TH、HM、HC、MC、TM、TC
3	THC、THM、HMC、TCM
4	THMC



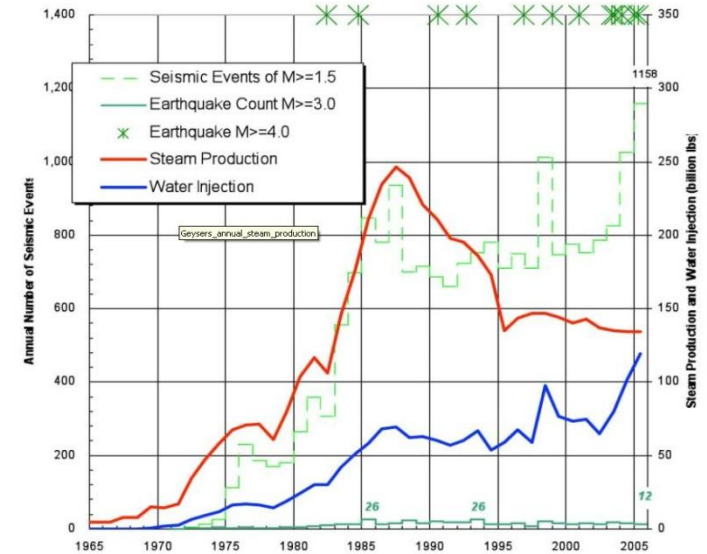
# Coupled processes-HM processes

Induced-seismicities can be mitigated by regulations, site selection, evaluation, monitoring and control

## Seismicity Magnitude $\geq 2.0$



Reservoir-induced seismicities in the world



The Geysers Geothermal Field, California, USA

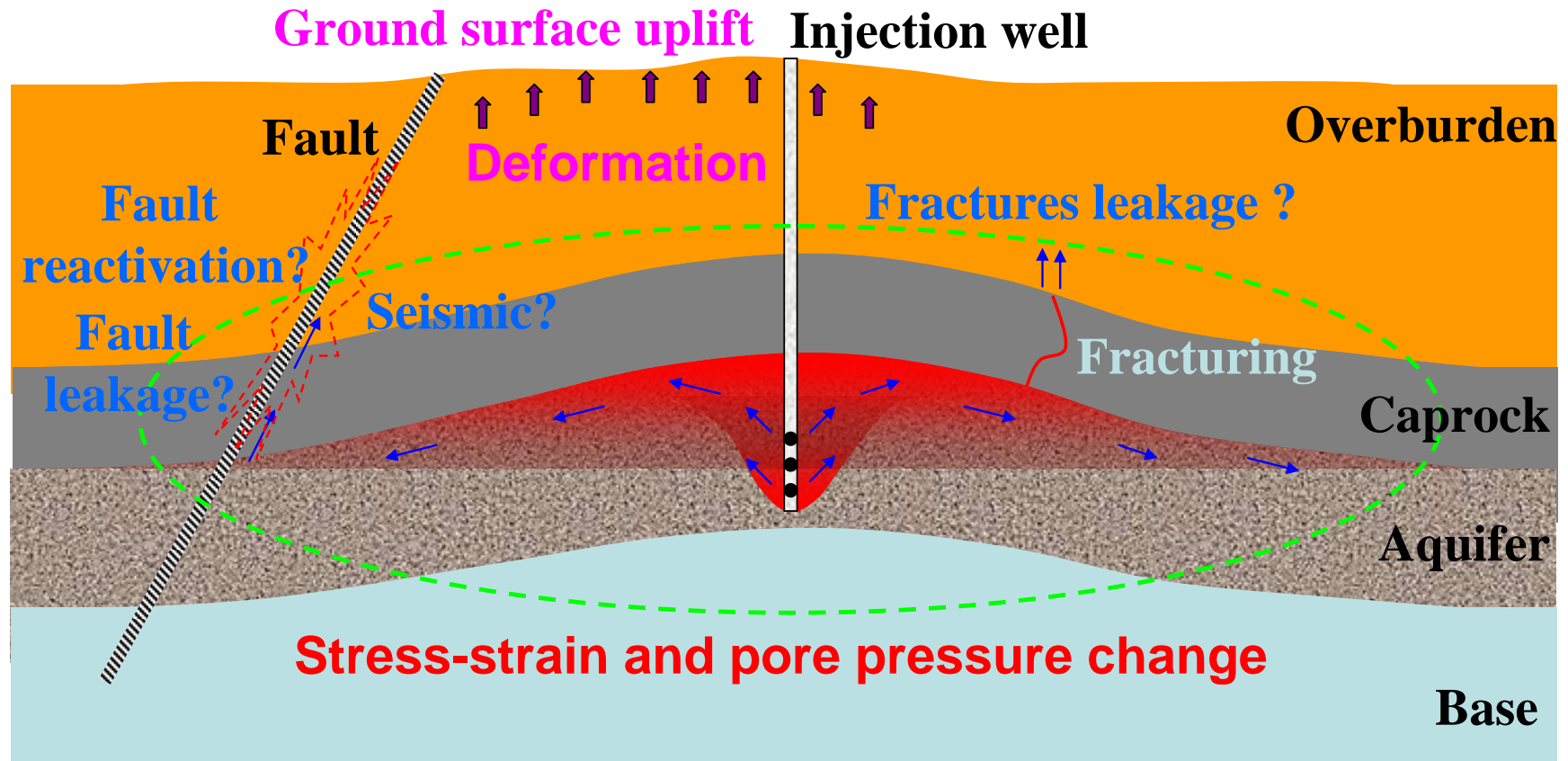
M $\geq 1.5$  events recorded since 1965 (maximum M4.6)





# Coupled processes-HM processes

- ◆ stress-strain and pore pressure change
- ◆ fault stability
- ◆ mechanical integrity of the cap-rock
- ◆ ground surface uplift



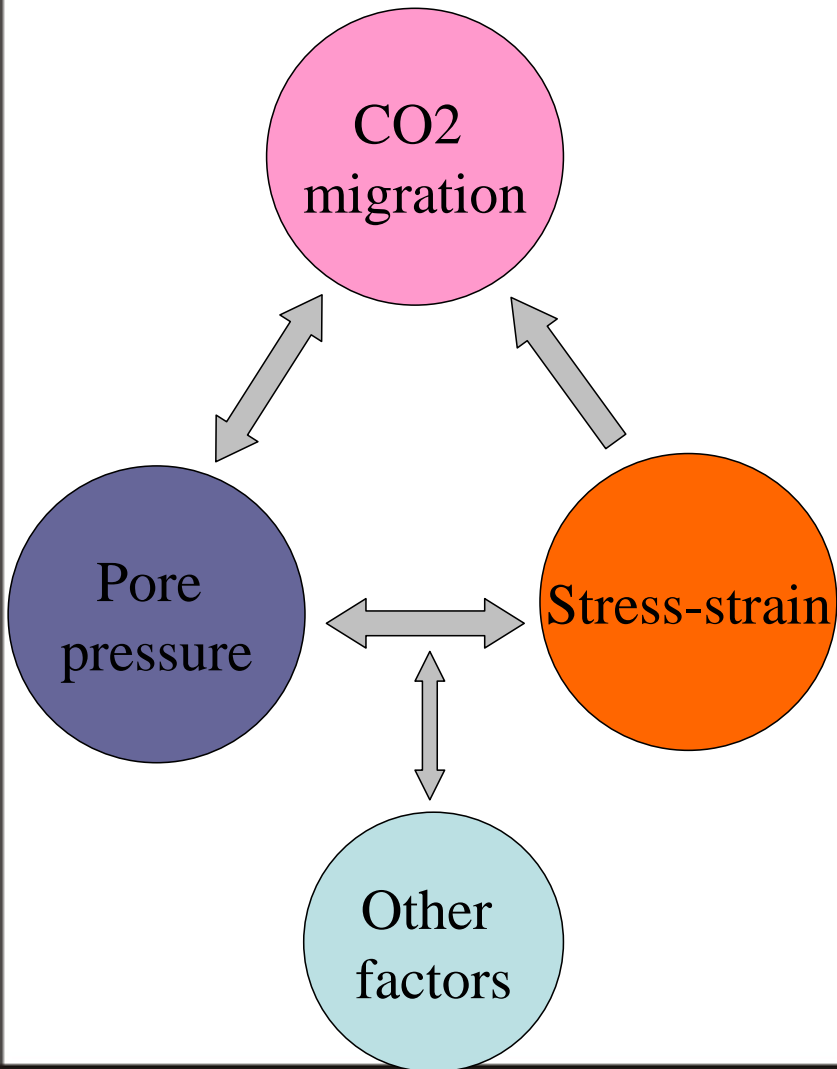
Pressure buildup induced by CO2 injection is the driving force !





# Coupled processes-HM processes

The changes of the stress-strain and pore pressure



CO<sub>2</sub> injection

→ Pore pressure increase

→ Effective stress decrease

→ Pore volume expansion

→ Facilitating the evolution of the pore pressure

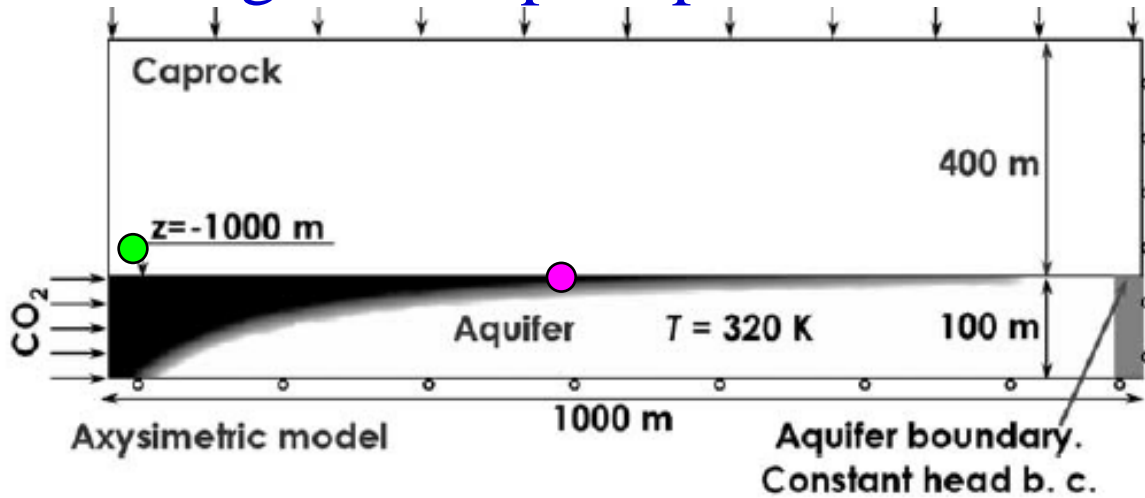
→ Promoting CO<sub>2</sub> migration

**Importance:**

- Preconditions for analyzing other issues
- Basic understandings for the changes of cap-rock and reservoir

# Coupled processes-HM processes

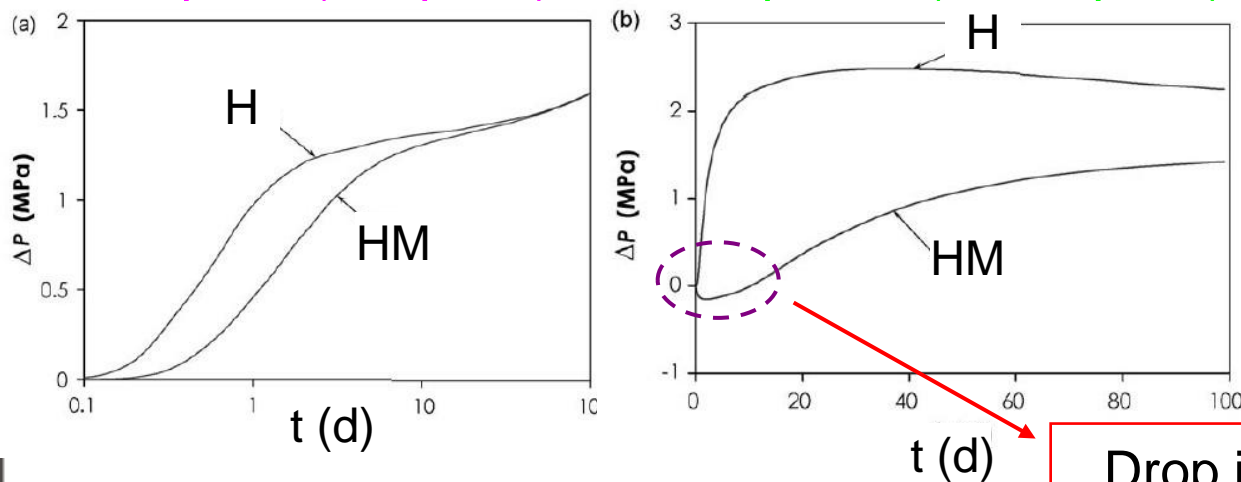
## The change of the pore pressure



- Prominent effect of mechanics to pore pressure.
- Notable difference between the aquifer and cap-rock.

Aquifer (red point)

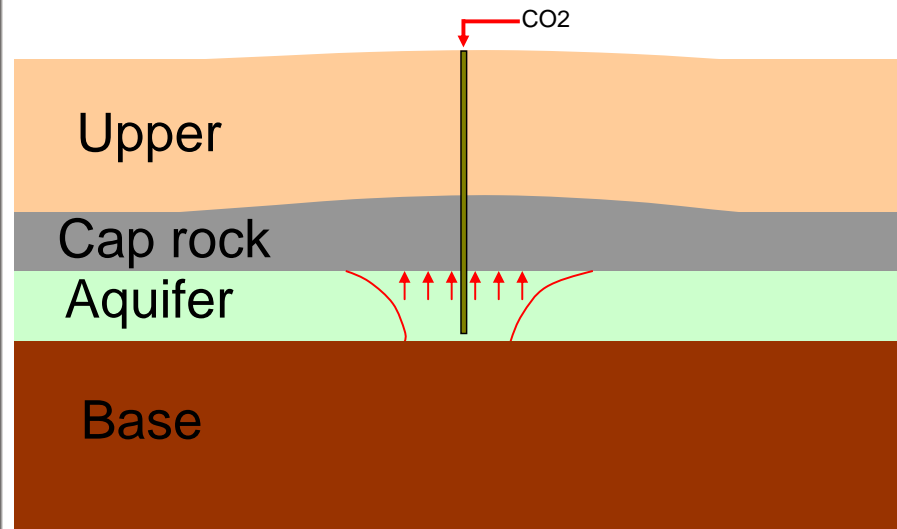
Cap-rock (green point)





# Coupled processes-HM processes

## Ground surface deformation



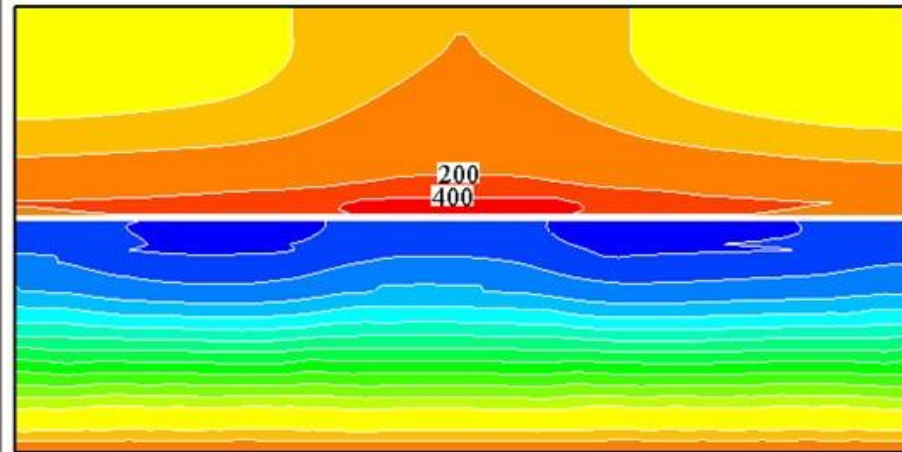
Pore pressure increase

Volumetric expansion in the injection zones

extrusion force from the bended cap-rock

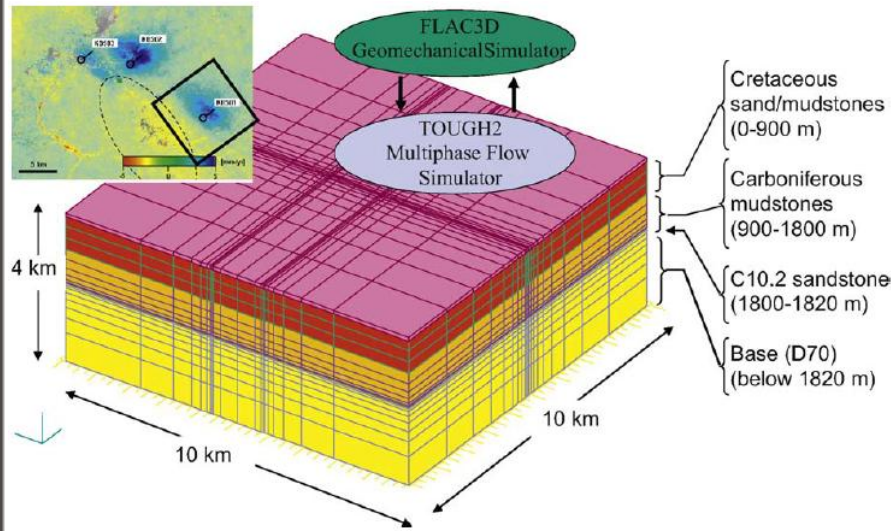
squeezing the overlying rock mass

ground surface deformation

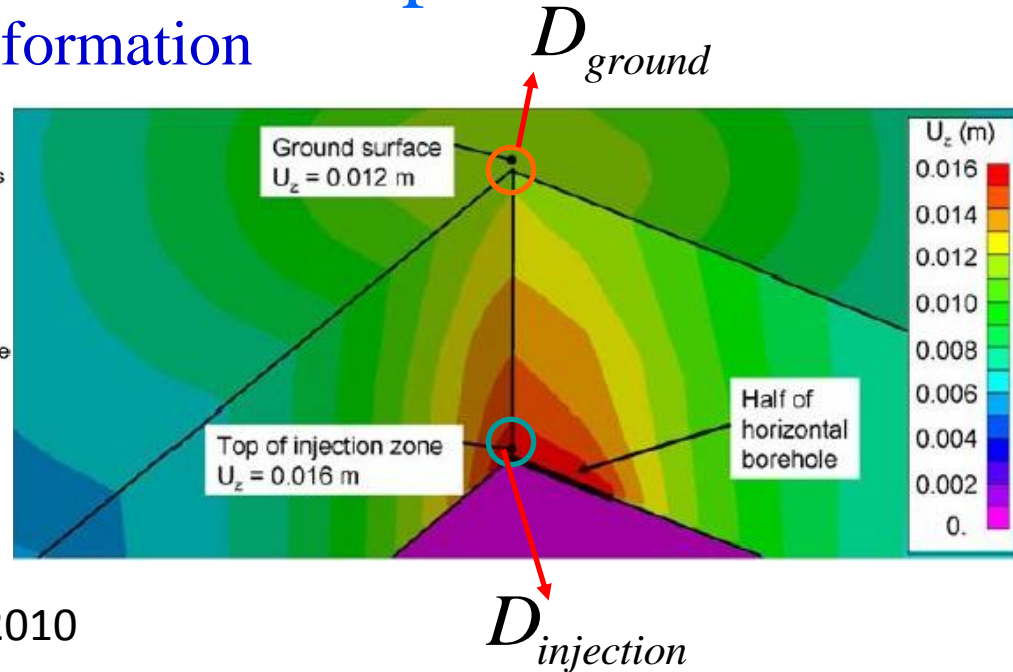


# Coupled processes-HM processes

## Ground surface deformation



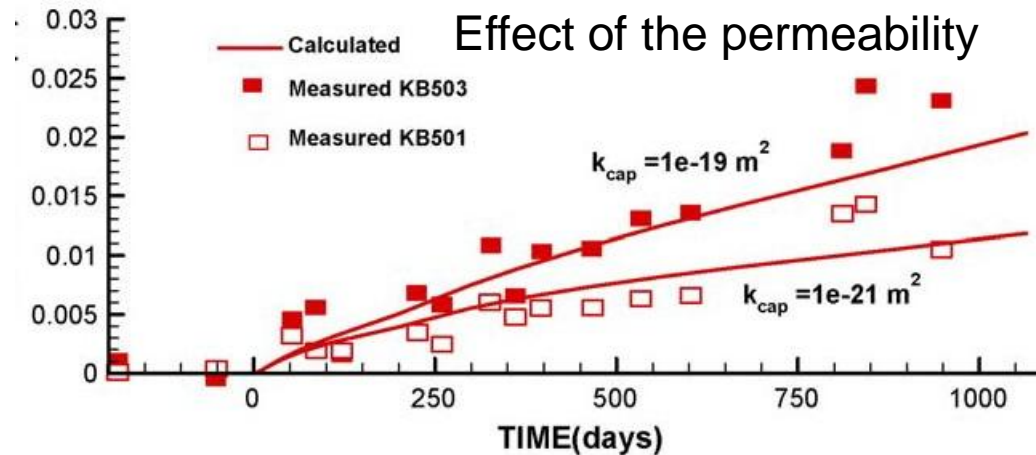
Rutqvist et. al. 2010



●  $D_{ground} < D_{injection}$

● The permeability of the cap-rock has an effect to the surface uplift.

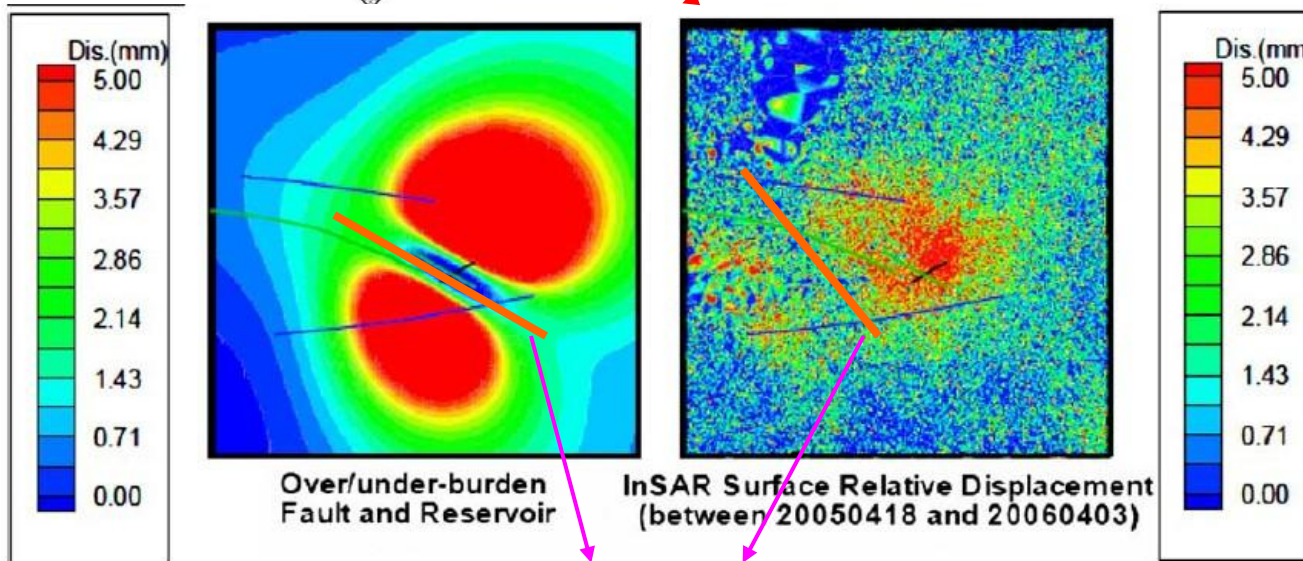
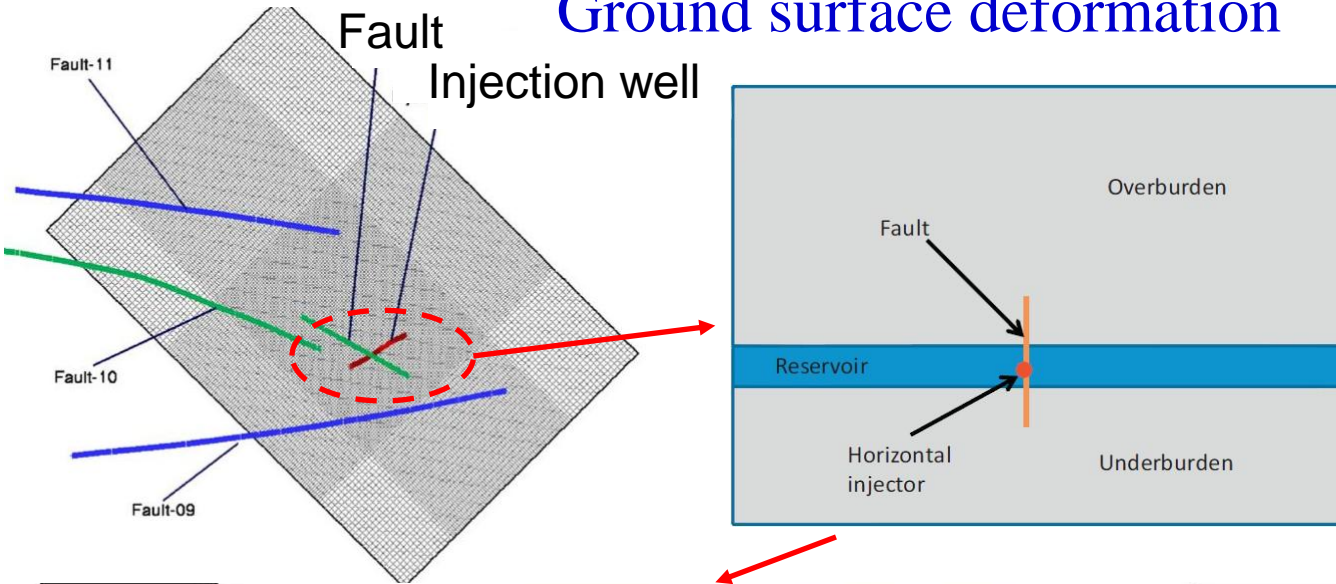
● Temperature and stiffness have a slight effect.



# Coupled processes-HM processes

## Ground surface deformation

- Direct response of the subsurface mechanical issues
- Coinciding with the monitoring results



Over/under-burden  
Fault and Reservoir

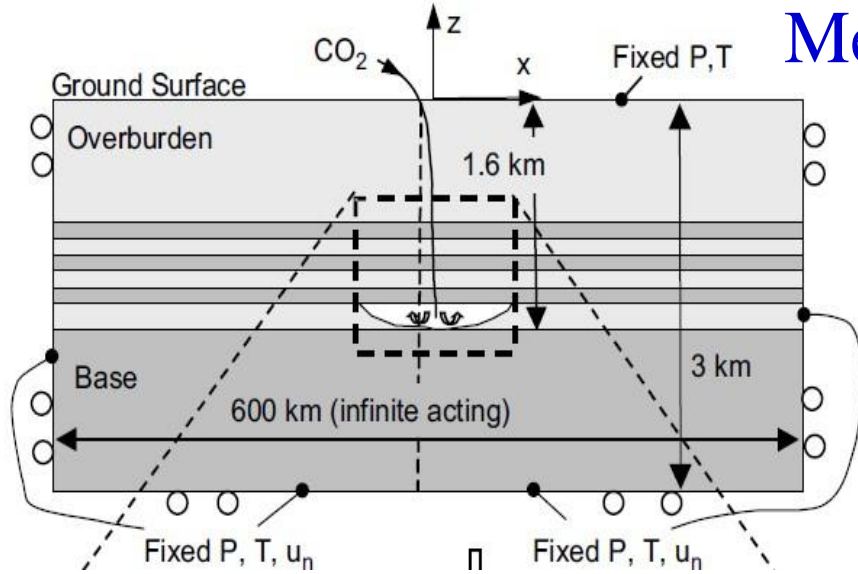
InSAR Surface Relative Displacement  
(between 20050418 and 20060403)

Vertical fault

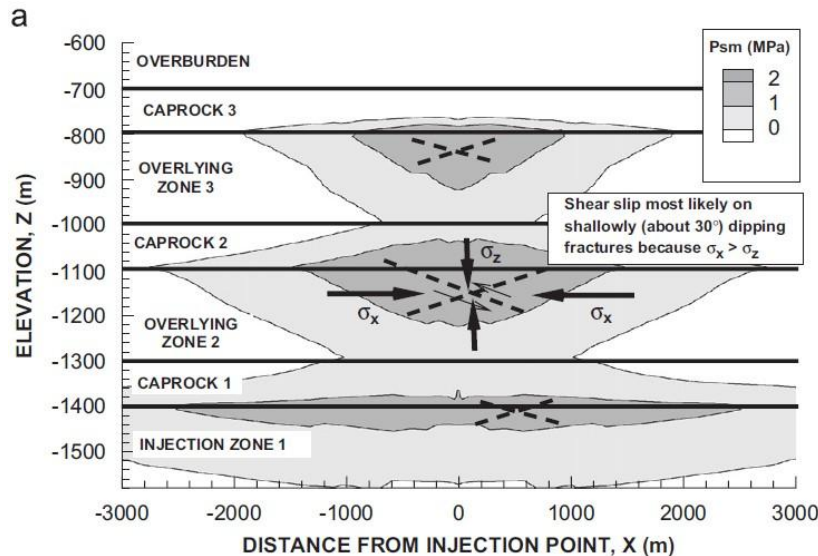
In Salah project  
Left:  
numerical simulation  
Right:  
field monitoring

# Coupled processes-HM processes

Mechanical integrity *Elastic model*



- Two-dimensional plane-strain model
- Partial coupling method
- H-M



Compressive stress regime  $\sigma_x = 1.5\sigma_z$

- Shear failure is likely to be initiated in shallowly dipping at the interface between the reservoir and cap-rock.
- Low possibility for tensile failure.

# Coupled processes-HM processes

## Mechanical integrity

## Elastic model

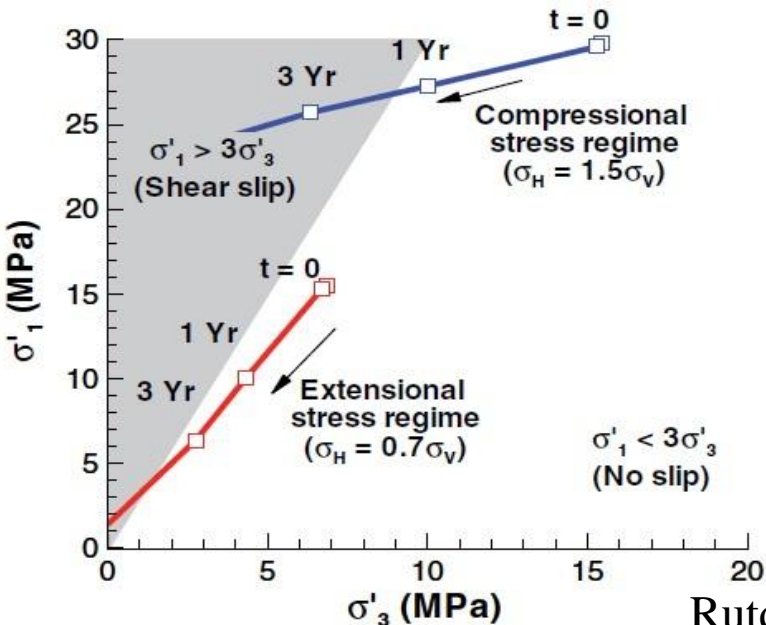
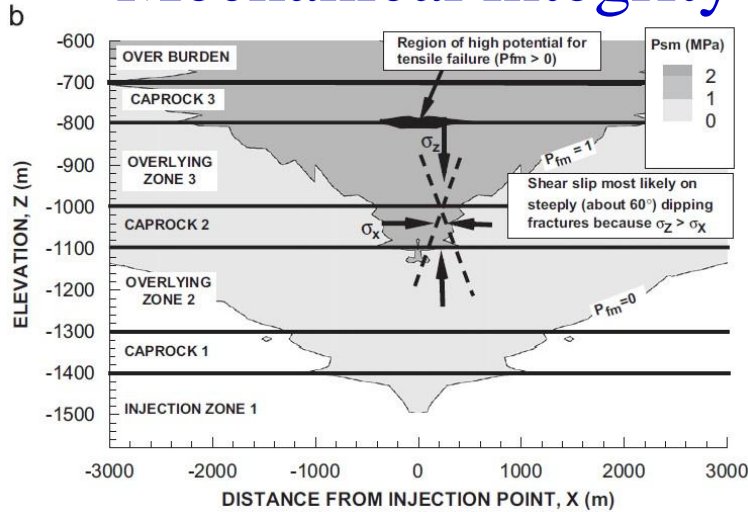
Extensional stress regime  $\sigma_x = 0.7\sigma_z$

- High potential for shear failure occurs throughout the CO<sub>2</sub>-storage system and in preferentially steeply dipping fractures.

- High potential for tensile failure occurs in the bottom of the cap-rock

- In compressional stress regime, shear failure is much more likely to occur.

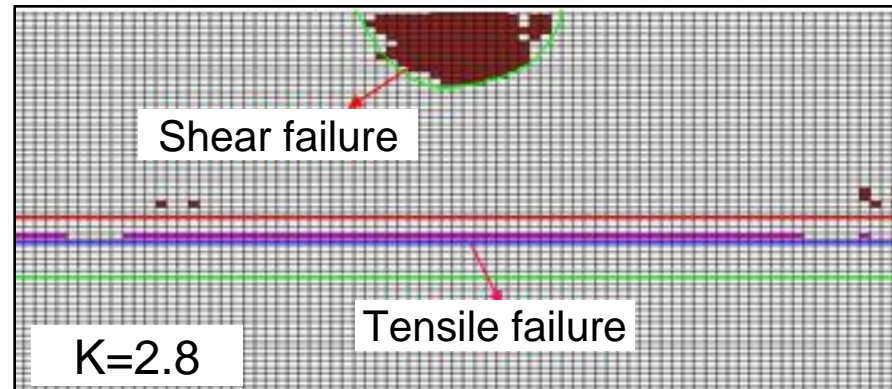
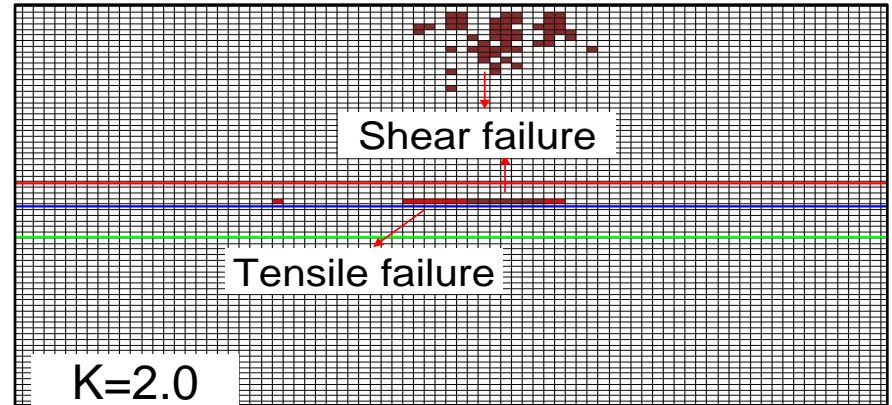
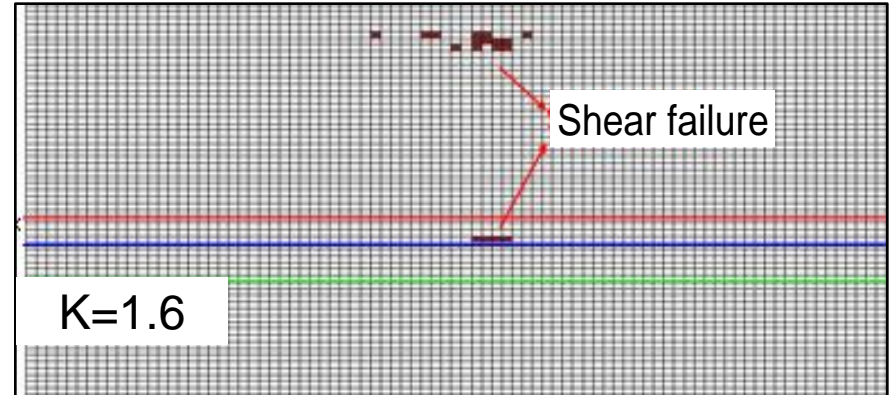
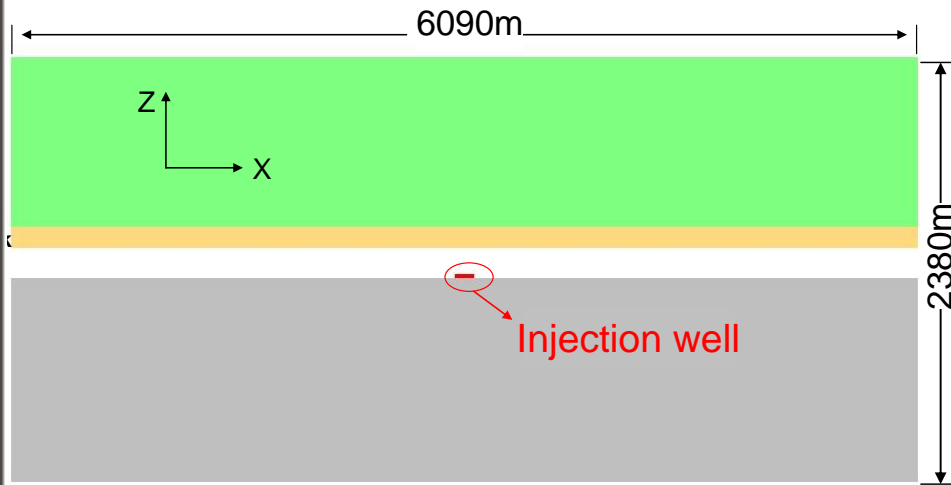
- Compressional stress regime is not favorable for mechanical integrity.





# Coupled processes-HM processes

## Mechanical integrity



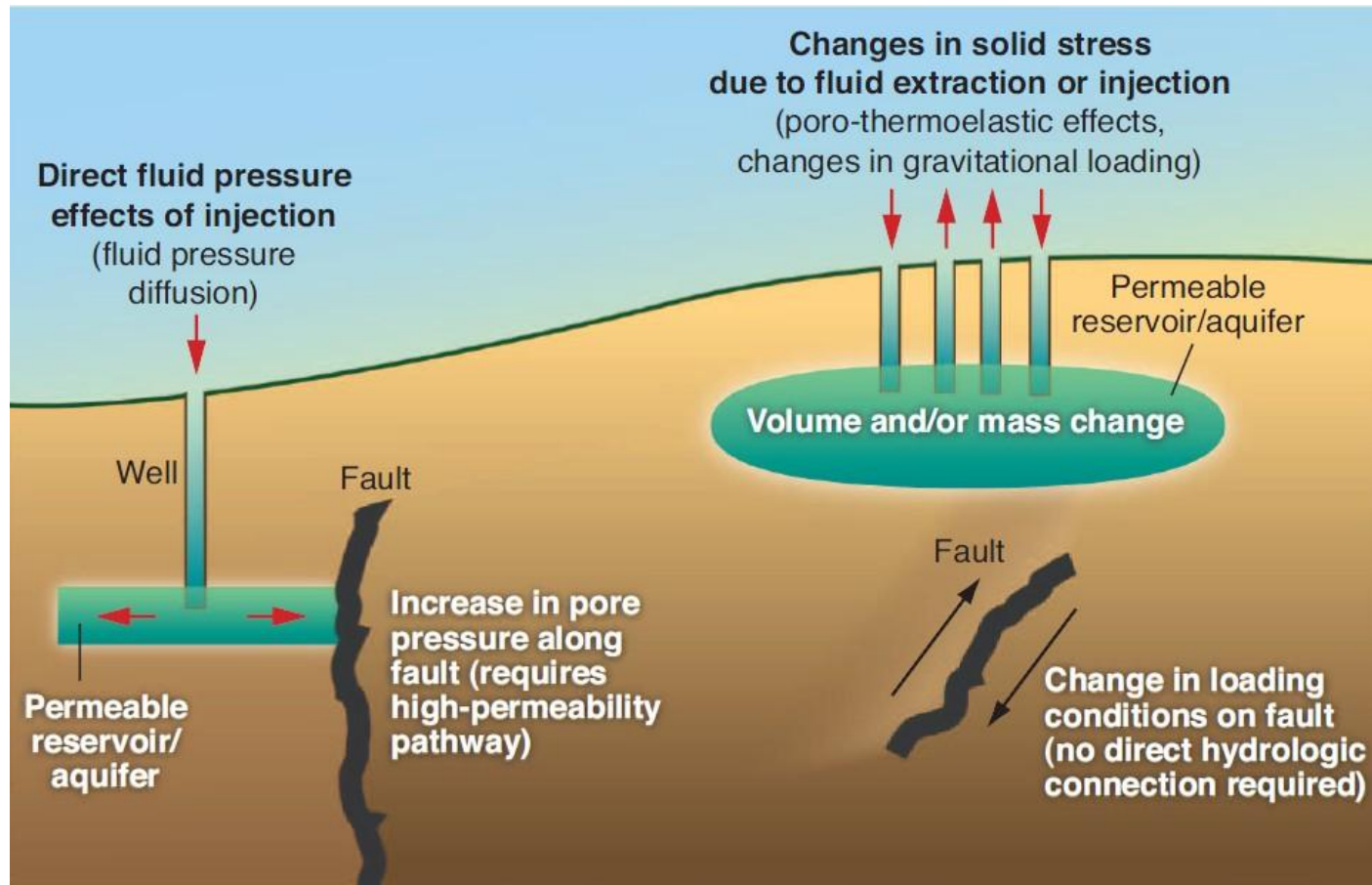
Wei Yuan et. al. 2015

- Elastic-plastic constitutive model
- Criterion: the elements of the cap rock tensile yield
- Method: strength reduction method
- As the reduction factor increase, the failure area enlarge.



# Coupled processes-HM processes

## Mechanisms for inducing earthquakes



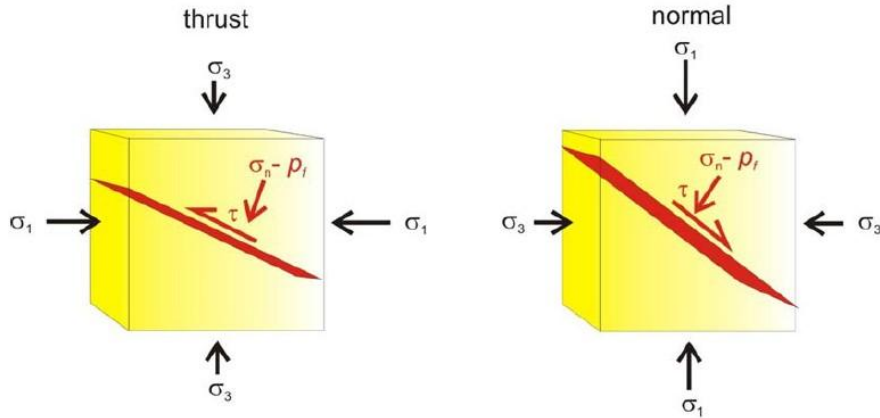
William  
L. Ellsworth  
2013

- The effective stress acting on fault decrease by increasing pore pressure.
- The loading condition on fault has changed.

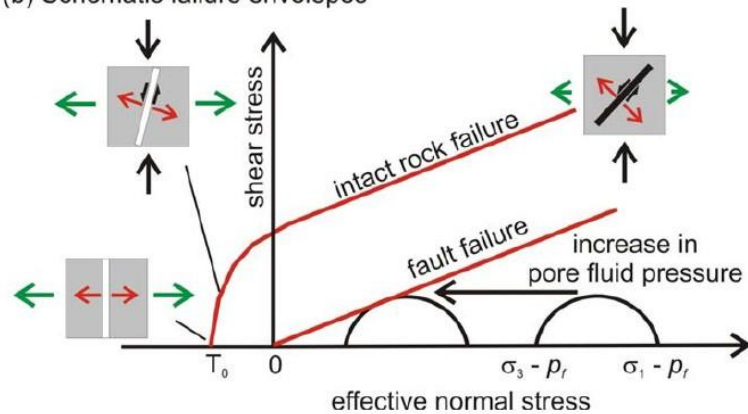
# Coupled processes-HM processes

## Fault stability- Constitutive model and failure criterion

(a) Stress regimes



(b) Schematic failure envelopes

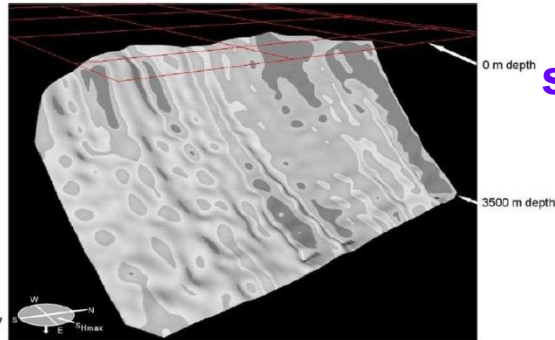


Elastic-perfectly plastic theory

- Mohr-Coulomb criterion
- Zero cohesive strength.
- The coefficients of the static friction:  $0.6 \leq \mu \leq 0.85$

# Coupled processes-HM processes

## Stability evaluation of the fault



Slip tendency on fault surface

The slip tendency is defined as the ratio of the shear stress to the normal effective stress

$$T_s = \frac{\tau}{\sigma_n - p_f}$$

Streit et al.2004

$\sigma_n$  — Normal effective stress

$\tau$  — Shear effective stress

$p_f$  — Pore pressure

## Evaluating the seismic magnitude

Quantification of the overall size of an earthquake is generally based on the seismic moment  $M_0$  defined for a ruptured patch on a fault by the following:

$$M_0 = \mu A d$$

$$M = (\log_{10} M_0 / 1.5) - 6.1$$

$M$  — Seismic magnitude

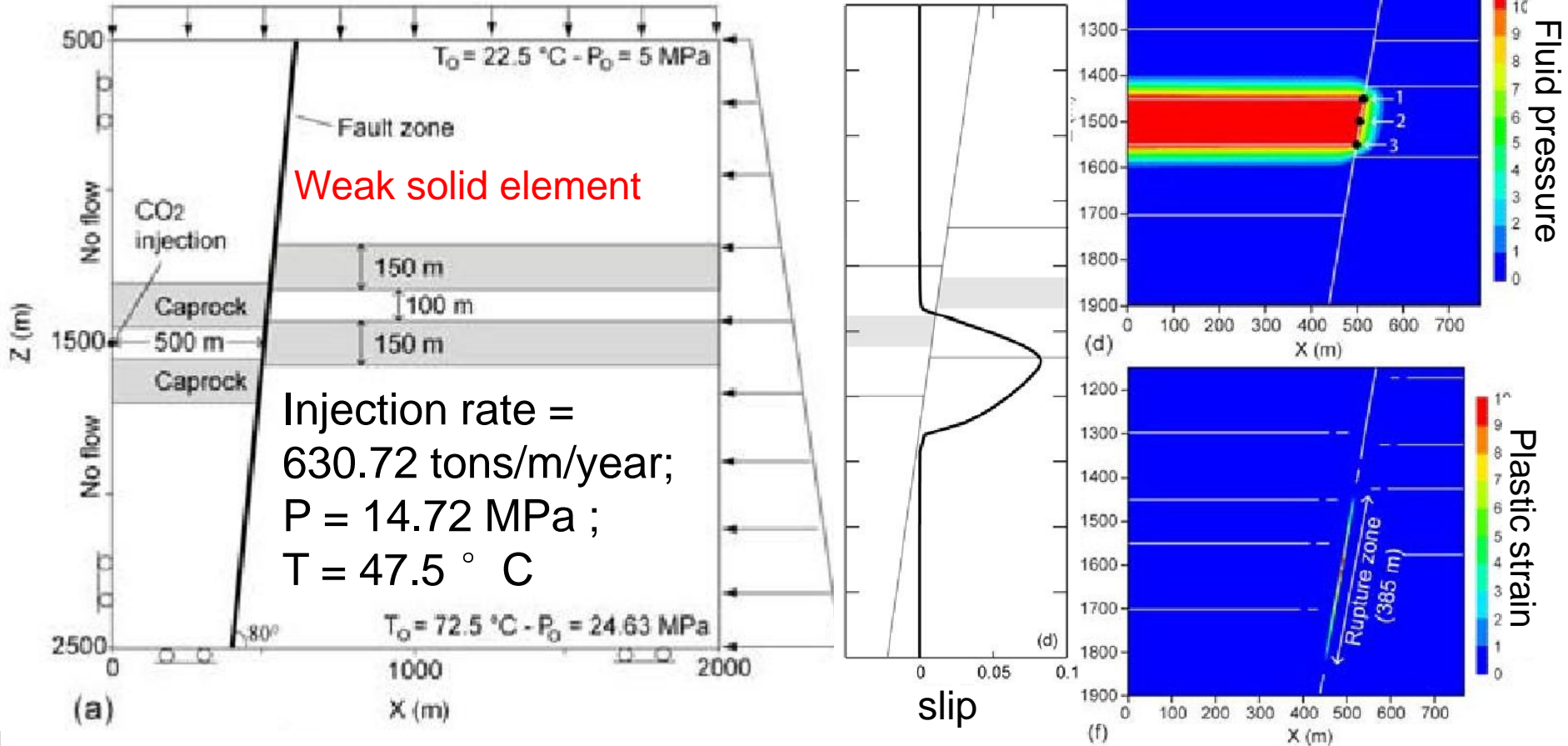
$\mu$  — Shear module

$A$  — Reactive area

$d$  — Slip distance

# Coupled processes-HM processes

## Fault stability Case study



Intention: earthquake magnitude resulting from CO2 injection

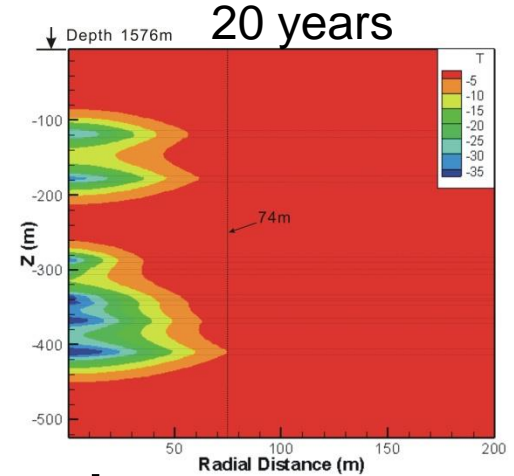
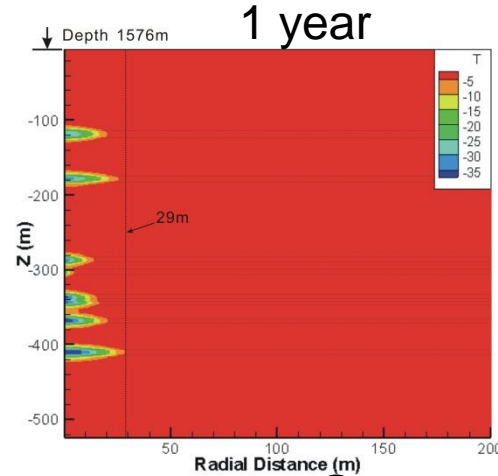
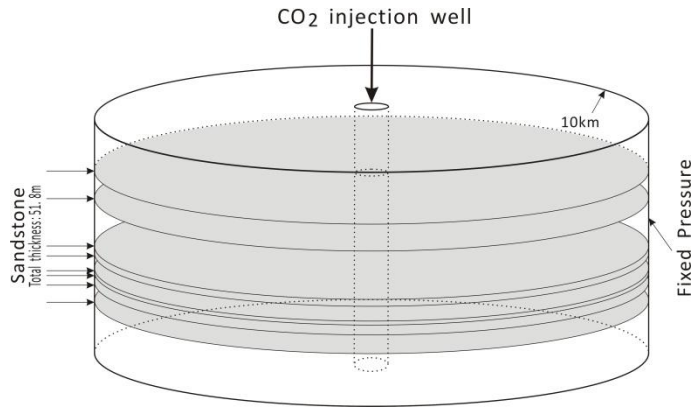
$$M_0 = 4 \times 10^9 \times 1000 \times 385 \times 0.08 = 1.23 \times 10^{14} \text{ Nm}$$

$$M = (\log_{10} M_0 / 1.5) - 6.1 = 3.29$$

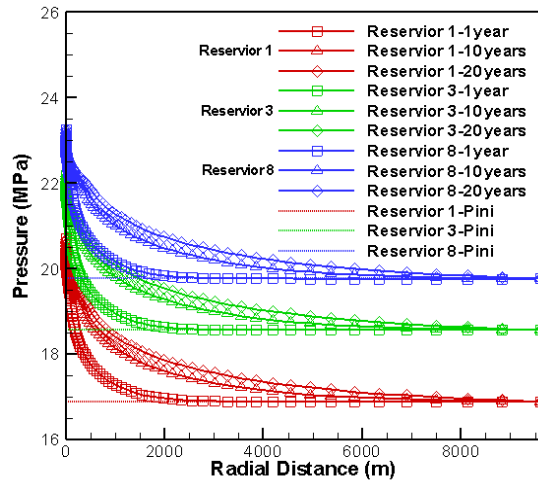
# Coupled processes-TH processes

Shenhua CCS site

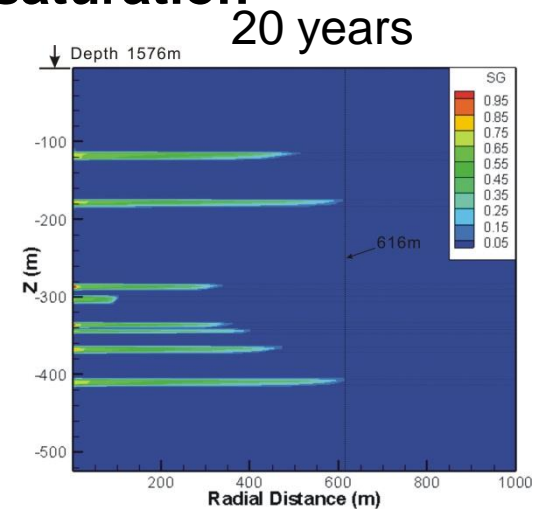
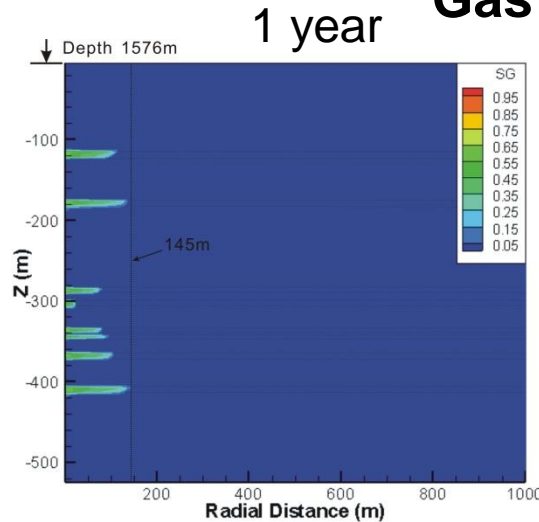
temperature



Pressure



Gas saturation





# Summary

质量守恒：单元含有的=进来的-出去的+内生的

能量守恒：单元含有的=进来的-出去的+内生的

运动规律：运动量=驱动力×常数

T: 热流=温度梯度×热传导系数

H: 流速=压力梯度×导流系数

M: 应力=应变×弹性系数

C: 反应速度=f (平衡浓度差)

耦合途径：

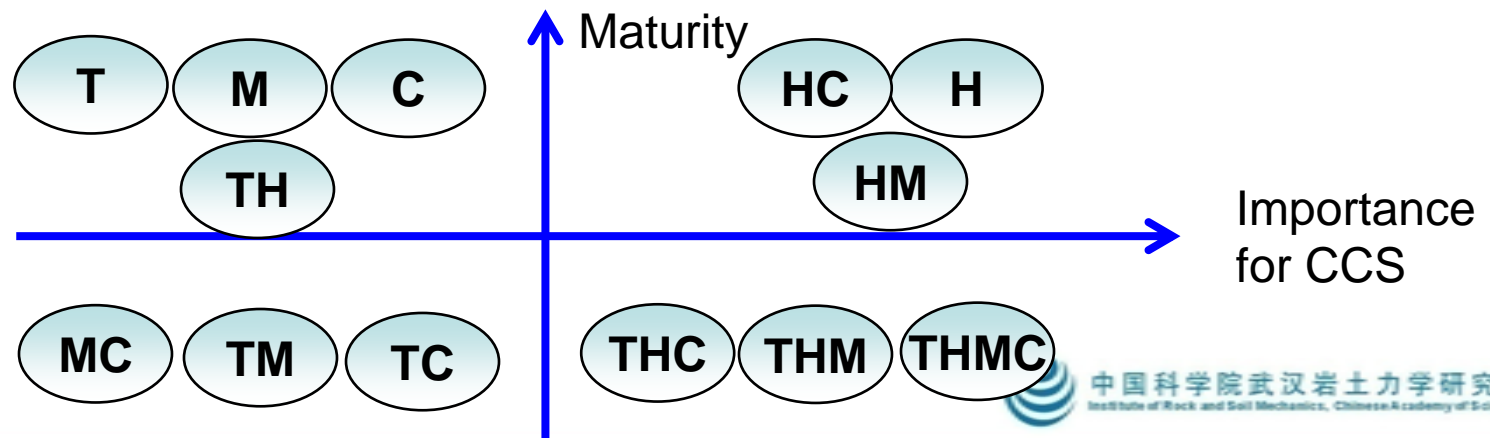
- 通过物质、能量的交换
- 通过对材料特性、结构、相态的改变





# Summary

1. The key indicators of CGUS project performance are capacity, injectivity, sealing, stability and productivity
2. Prediction is based on detailed geological model and on knowledge and analysis of THMC processes
3. Short-term processes in EOR and DSF/EWR have been well understood and reasonably simulated
4. Their long-term processes and the other CGUS options need to be studied
5. Fully coupled analyses are not always necessary. Identifying the dominated processes is critical







# Thank you !

