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# Mechanical effect of absorption Carbon sequestration and swelling of coal

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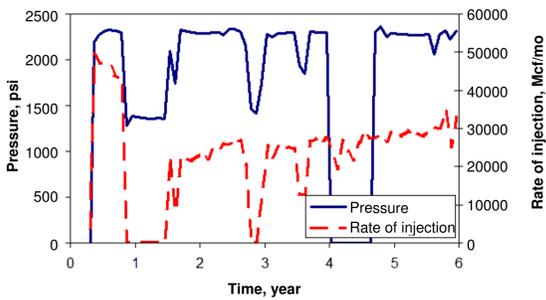
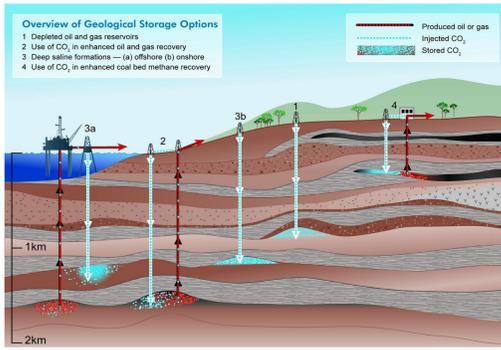
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## CONTEXT - CARBON SEQUESTRATION AND SWELLING OF COAL

In most scenarios for stabilization of atmospheric greenhouse gas concentrations [...] CCS contributes 15 - 55% to the cumulative mitigation effort worldwide

(From: IPCC report on Carbon Capture and Sequestration (2005))

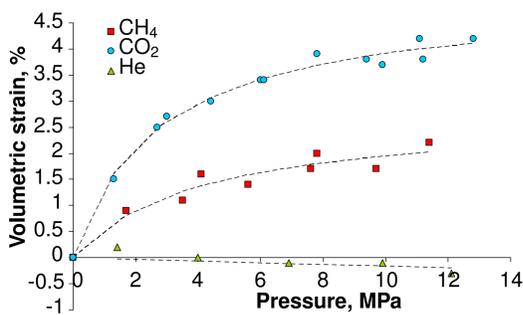
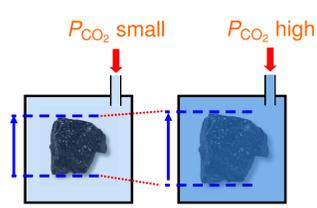


Sequestration in coalbeds is promising (long term storage is safe and natural gas can be recovered, which improves the financial viability), but it is affected by a permeability issue. The injection pilots have encountered an important loss of permeability of the reservoir, after a few months of injection. Left: case of the Allison Unit, San Juan Basin (NM), US DOE.

(adapted from Pekot & Reeves (2002))

**Cause: coal swells more in a CO<sub>2</sub> atmosphere than in a CH<sub>4</sub> atmosphere**

Experiment: inject either CO<sub>2</sub> or CH<sub>4</sub> in a coal sample free of stress



(adapted from Ottiger et al. (2008))

**Conventional poromechanics fails to explain the swelling**

Helmholtz free energy of the solid matrix of a saturated isotropic porous medium:

$$f_{solid} = \frac{1}{2} (K + b^2 N) \epsilon^2 - b N \epsilon \varphi + \frac{N}{2} \varphi^2 + \sum_{ij \in \{1,2,3\}} \frac{G}{2} e_{ij}^2$$

where:

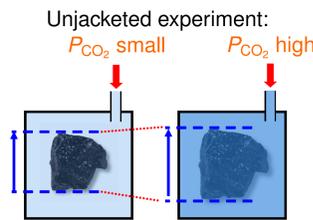
- $\epsilon$  is the volumetric strain,
- $\varphi$  the change of porosity,
- $G$  the shear modulus,
- and  $N$  the Biot modulus.
- $e_{ij}$  the deviatoric strains,
- $K$  the bulk modulus,
- $b$  the Biot coefficient,

The volumetric stress is obtained with the state equation:

$$\sigma = \frac{\partial f_{solid}}{\partial \epsilon} \Big|_{\varphi, e_{ij}} = K \epsilon - b P$$

(Coussy (2010))

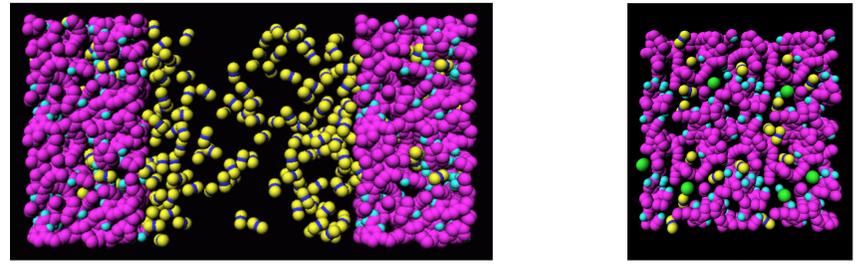
**Objective: Understand the physics of swelling and predict the permeability loss**



Conventional poromechanics predicts a shrinkage, and the same whatever the gas!  
 $\sigma = -P \Rightarrow \epsilon = -\frac{1-b}{K} P < 0$

## POROMECHANICS OF NANOPORE ADSORPTION

**Explanation: Adsorption occurs also in the nanopores of the solid matrix.**



Guideline for the poromechanics of nanopore adsorption: Use **known and measurable quantities only**. Questionable quantities (porosity, specific surface) should not intervene.

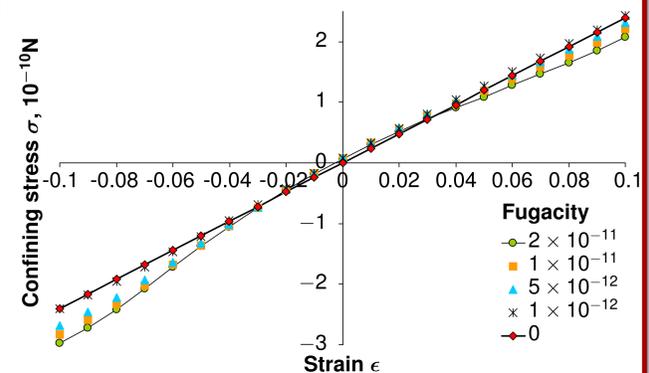
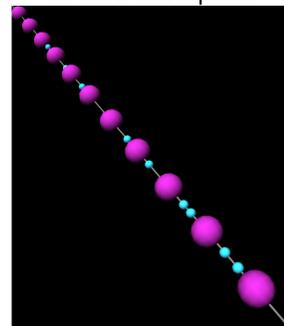
**Behavior law of a porous solid subjected to a fluid under any form (bulk, surface adsorption, nanopore adsorption...)**

$$\sigma = \frac{df_s}{d\epsilon} - \frac{\partial}{\partial \epsilon} \left( \int_{-\infty}^{\mu} \frac{N}{V_0} d\mu \right) \Big|_{\mu} \quad (2)$$

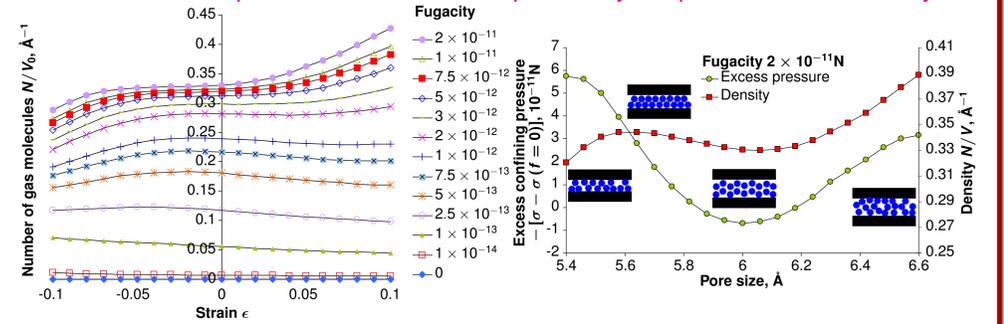
**Requires to know the adsorbed amount as a function of both  $\mu$  and  $\epsilon$ .**

- $V_0$  is the volume of the porous solid under unstressed conditions,
- $N$  is the number of fluid molecules whatever their state (adsorbed in nanopores, on surfaces, bulk...),
- $f_s = F_s / V_0$  and  $F_s$  is the free energy of the sole solid, that is when there is no fluid molecule in the pores.  $f_s = \frac{1}{2} K \epsilon^2$  for an elastic solid.

Case of a 1D chain subjected to fluid adsorption

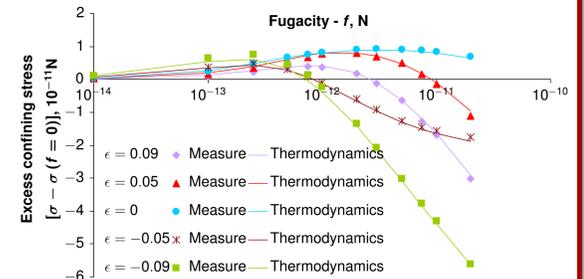


**The uneven adsorption behavior can be explained by the pore commensurability**

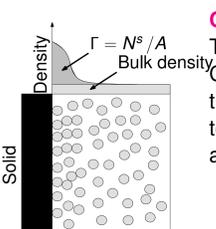


The excess stress directly computed (virial estimate) and the excess stress predicted by the proposed thermodynamics (Equation 2) are consistent.

$$\sigma - \sigma(f=0) = - \frac{\partial}{\partial \epsilon} \left( \int_{-\infty}^{\mu} \frac{N}{V_0} d\mu \right) \Big|_{\mu}$$



## CONVENTIONAL POROMECHANICS EXTENDED TO SURFACE EFFECTS



**Contrary to CO<sub>2</sub> and CH<sub>4</sub>, helium behaves as predicted by poromechanics.**

The difference stems from the adsorption (low for Helium, high for CO<sub>2</sub> and CH<sub>4</sub>) which may have an impact on the mechanics of a solid, since it modifies the fluid-solid interface energy  $\gamma_{FS}$  (Gibbs adsorption equation, at fixed temperature and interface area):  $d\gamma_{FS} = -\Gamma d\mu$ . The mechanical impact of adsorption can be sketched in the case of a thin plate:

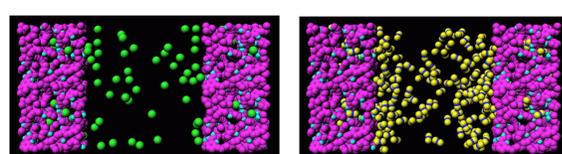
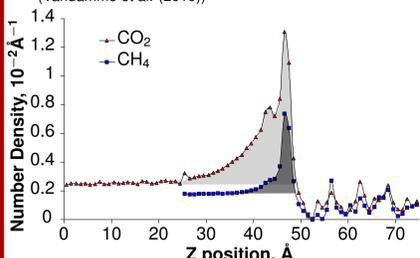
Helmholtz free energy of the (solid matrix + interface):

$$f_{solid} = \frac{1}{2} (K + b^2 N) \epsilon^2 - b N \epsilon \varphi + \frac{N}{2} \varphi^2 + \sum_{ij \in \{1,2,3\}} \frac{G}{2} e_{ij}^2 + \gamma s$$

- $s$  the specific surface, and  $\gamma_{FS}$  the fluid-solid interface energy.

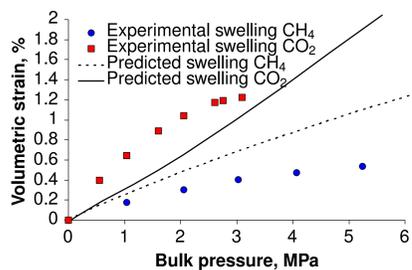
$$\sigma = K \epsilon - b P + \tilde{\sigma}_s \frac{\partial s}{\partial \epsilon} \Big|_P \text{ where } \tilde{\sigma}_s = \gamma + s \frac{\partial \gamma}{\partial s} \text{ is the interface stress.}$$

(Vandamme et al. (2010))



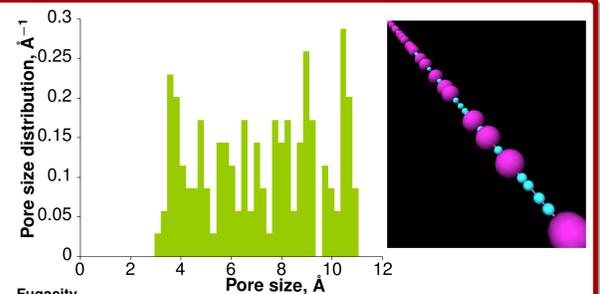
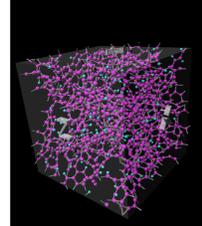
CO<sub>2</sub> and CH<sub>4</sub> density profiles on the surface of coal matrix were obtained by molecular simulation. The swelling predicted by the model (Equation 1) is compared to the experimental swelling.

**The model does not capture the experimental swelling**

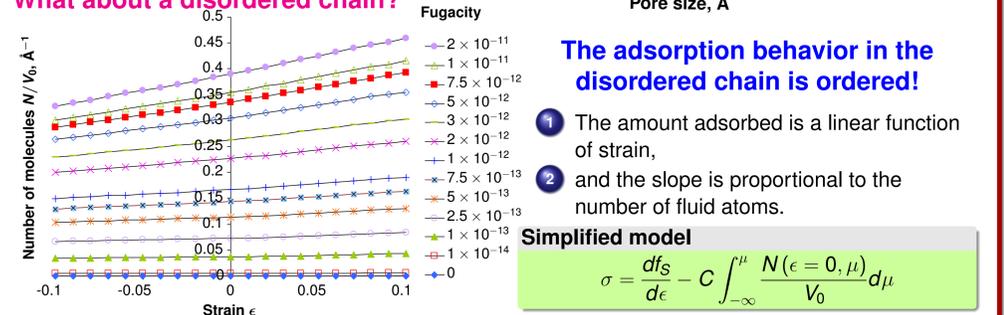


(Experimental data from Levine (1996))

Coal is a disordered nanoporous matrix.



**What about a disordered chain?**



**The adsorption behavior in the disordered chain is ordered!**

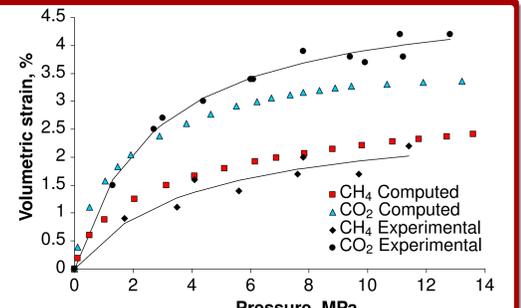
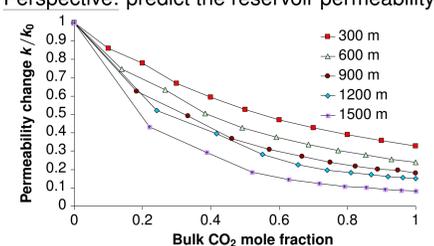
- The amount adsorbed is a linear function of strain,
- and the slope is proportional to the number of fluid atoms.

**Simplified model**

$$\sigma = \frac{df_s}{d\epsilon} - C \int_{-\infty}^{\mu} \frac{N(\epsilon=0, \mu)}{V_0} d\mu$$

**Swellings predicted with the simplified model are satisfying.**

Perspective: predict the reservoir permeability



(Experimental results from Ottiger et al. (2008))