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# Mechanical effect of adsorption Carbon sequestration and swelling of coal

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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))

2500 **5** 1500 **<u>ខ</u>** 1000 20000 500 10000 Pressure - Rate of injection

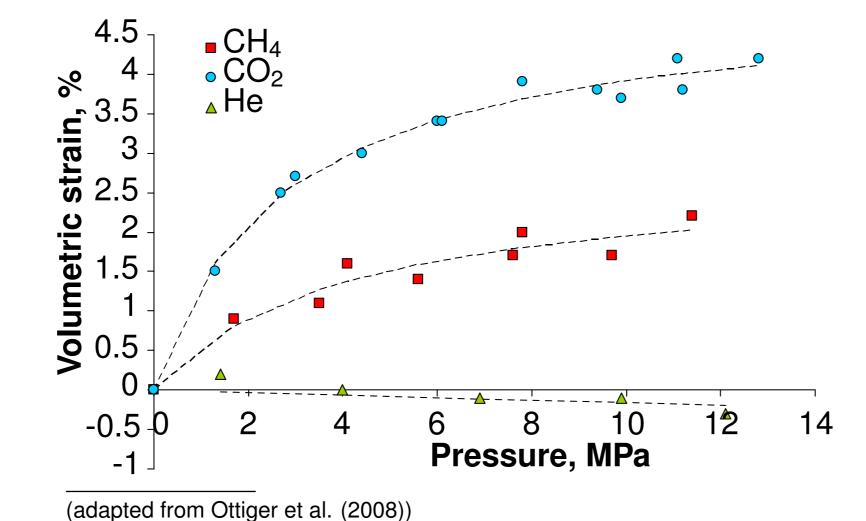
Sequestration in coalbeds is promising (long term storage is safe and natural gas can be recovered, which improves the financial viability), but it is affected by a permeability issue. The injection pilots have encountered an important loss of permeability of the reservoir, after a few months of injection.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

(adapted from Pekot & Reeves (2002))

Experiment:

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

inject either CO<sub>2</sub> or CH<sub>4</sub> in a coal sample free of stress P<sub>CO<sub>2</sub></sub> high  $P_{\text{CO}_2}$  small



### Conventional poromechanics fails to explain the swelling

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

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

(Coussy (2010))

- $\epsilon$  is the volumetric strain,
- G the shear modulus,

and N the Biot modulus.

- $\varphi$  the change of porosity,
- $\bullet$   $e_{ij}$  the deviatoric strains,
- K the bulk modulus,
- b the Biot coefficient,

The volumetric stress is obtained with the state equation:

$$\sigma = \left. rac{\partial f_{solid}}{\partial \epsilon} \right|_{arphi, oldsymbol{e}_{ii}} = oldsymbol{K} \epsilon - oldsymbol{b} oldsymbol{P}$$

P<sub>CO<sub>2</sub></sub> high  $P_{CO_2}$  small

Unjacketed experiment:

Conventional poromechanics predicts a shrinkage, and the same whatever the gas!

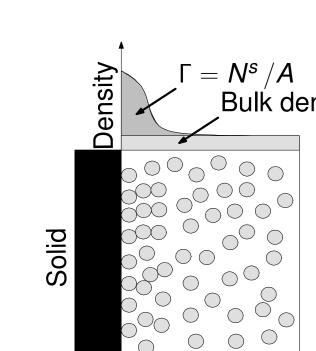
 $\sigma = -P \Rightarrow \epsilon = -\frac{1-b}{\kappa}P < 0$ 

specific to each fluid:

with  $\Delta \gamma = -\int_{\mu}^{\mu} \left( \frac{N^{Ex}}{\Delta} d\mu \right)$  and

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

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 Bulk density 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:

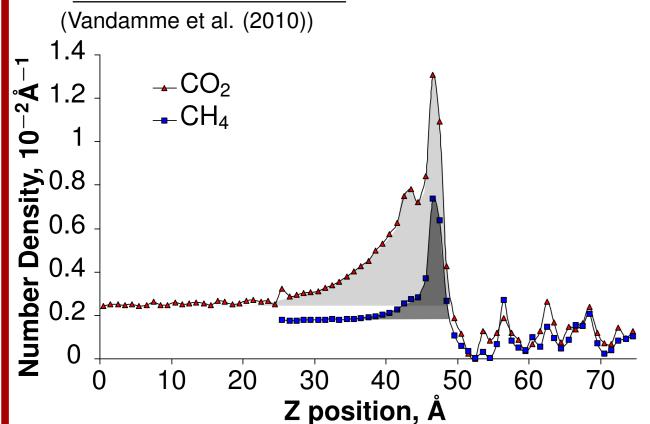
Helmholtz free energy of the (solid matrix + interface): Predicts a possible swelling,

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

s the specific surface.,

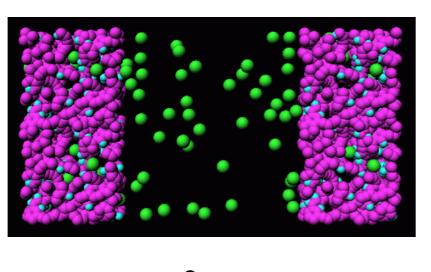
• and  $\gamma_{FS}$  the fluid-solid interface energy.

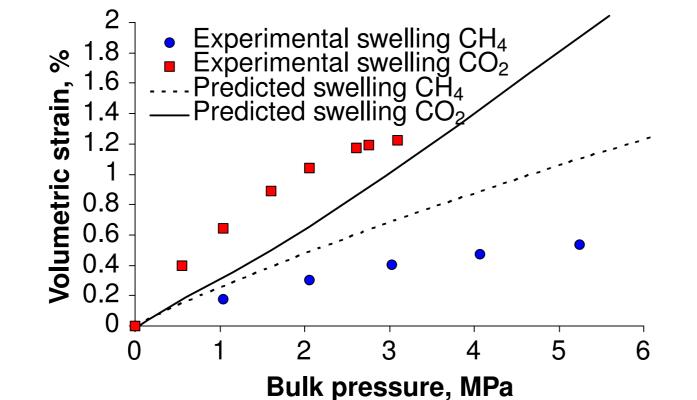
where  $\widetilde{\sigma}_s = \gamma + s \frac{\partial \gamma}{\partial s}$  is the interface stress.



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

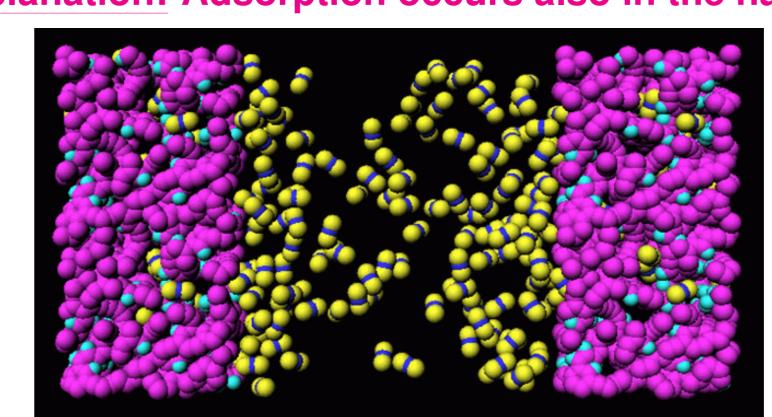


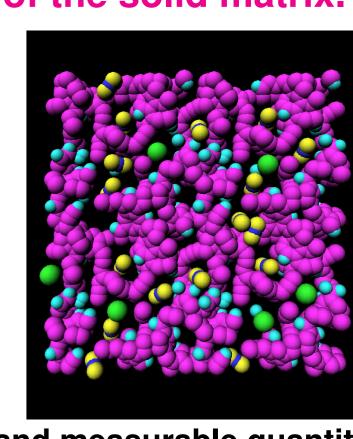


(Experimental data from Levine (1996))

#### 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.

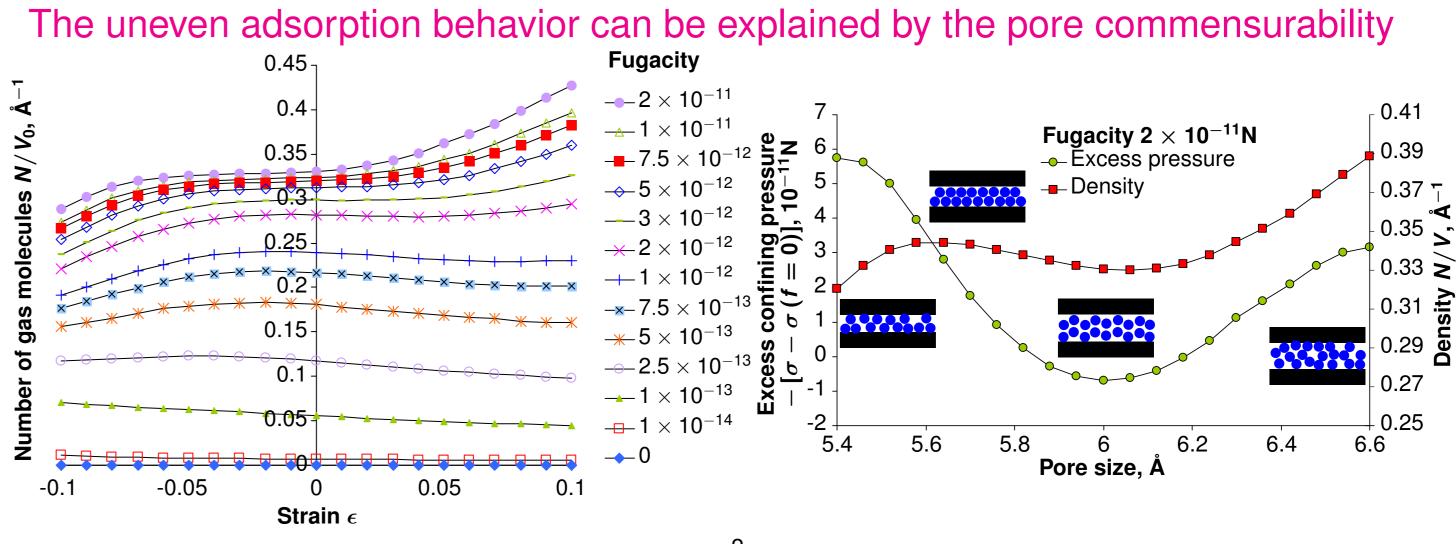
Behavior law of a porous solid subjected to a fluid under any form (bulk, surface adsorption, nanopore adsorption...)

 $\left. rac{ extbf{d}f_{ extsf{S}}}{ extbf{d}\epsilon} - rac{\partial}{\partial\epsilon} \left( \int_{-\infty}^{\mu} rac{ extbf{N}}{ extbf{V}_{ extbf{0}}} extbf{d}\mu 
ight) 
ight|_{\mu}$ 

- $\circ$   $V_0$  is the volume of the porous solid under unstressed
- 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.

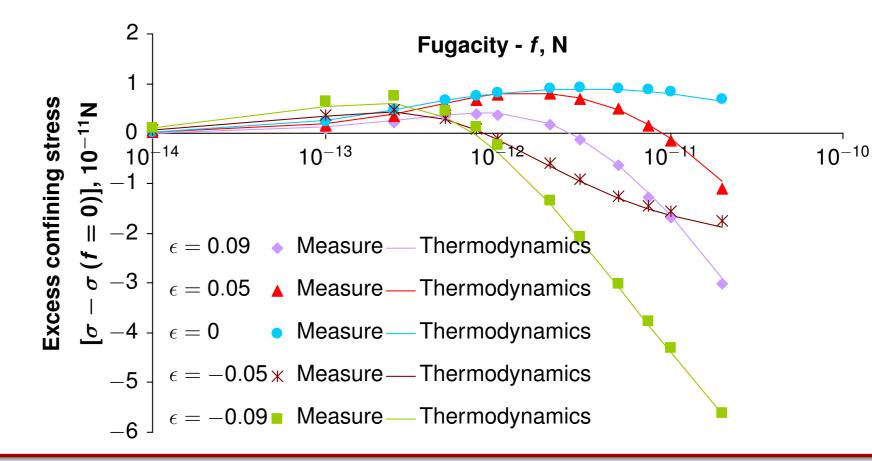
Requires to know the adsorbed amount as a function of both  $\mu$  and  $\epsilon$ .

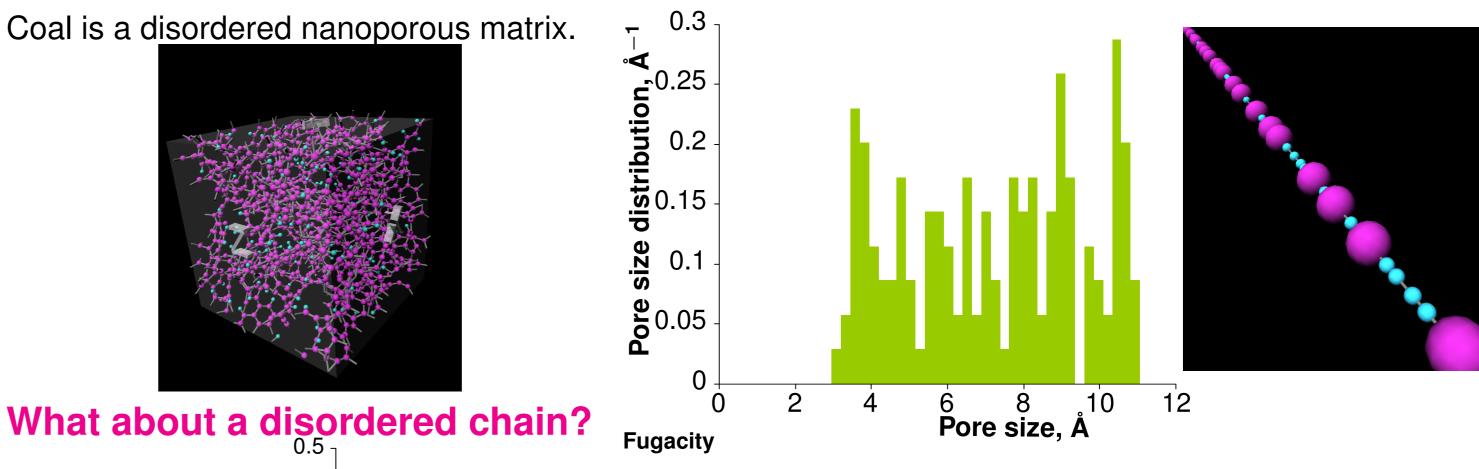
## Case of a 1D chain subjected to fluid adsorption 0.1 -0.08 -0.06 -0.04 -0.02 0.02 0.04 0.06 0.08 0.1 **Fugacity** $-2 \times 10^{-11}$ $1 \times 10^{-11}$ $^{4}$ 5 × 10<sup>-12</sup> $* 1 \times 10^{-12}$ Strain $\epsilon$

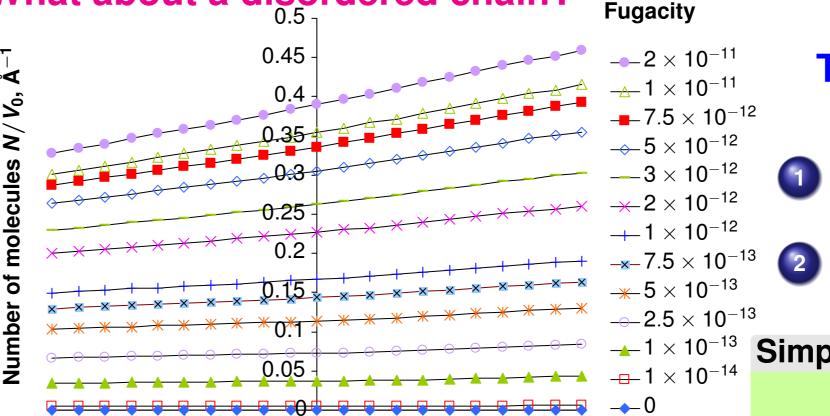


The excess stress directly computed (virial estimate) and the excess stress predicted by the proposed thermodynamics (Equation 2) are consistent.

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







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

## Swellings predicted with the simplified model are satisfying.

Strain  $\epsilon$ 

-0.05

Perspective: predict the reservoir permeability **--** 300 m ---- 600 m **→** 900 m 0.6 → 1200 m **★** 1500 m 0.3 0.2 0.1 0.2 0.6 8.0

Bulk CO<sub>2</sub> mole fraction

CH<sub>4</sub> Computed △ CO<sub>2</sub> Computed ◆ CH<sub>4</sub> Experimental CO<sub>2</sub> Experimental 12 Pressure, MPa

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

January 27<sup>th</sup>, 2011 L. BROCHARD (Laboratoire Navier) Adsorption induced swelling of coal