

Adsorption behavior in disordered nanoporous solids

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Strain - adsorption behavior in disordered nanoporous solids

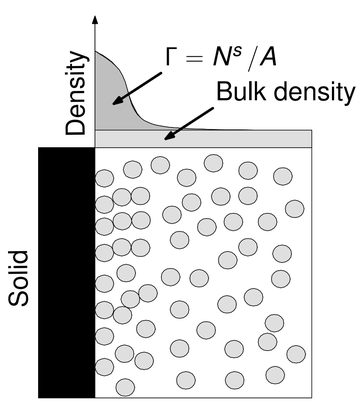
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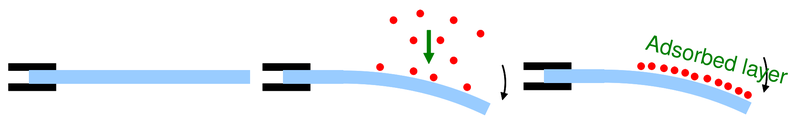
ABSTRACT

The swelling of coal induced by an adsorption of CO_2 impedes a large scale deployment of carbon sequestration projects in coal fields.
In this work we study how adsorption modifies the mechanical behavior of coal. Constitutive equations for generic porous (and nanoporous) solids are derived. These equations require the knowledge of the adsorption behavior in function of the solid strain. In order to better understand the coupling between strain and adsorption, we explore by molecular simulation the adsorption of fluid on 1D nanoporous solids. We first study an ordered nanoporous 1D solid, in which all nanopores are of the same size. The adsorption depends in a complex manner on the strain of the solid, which can be understood in terms of the pore commensurability to the size of the adsorbed fluid molecules. The consequence on the mechanical behavior of the chain is complex (swelling or shrinkage, pressure-dependence of the poroelastic coefficients...). We then study an amorphous nanoporous 1D solid, made of nanopores with various sizes. In such a case, the adsorption depends linearly on the strain of the solid and a simpler form of the constitutive equations can be derived. These simpler constitutive equations enable to capture satisfactorily how coal swells under an adsorption of CO_2.

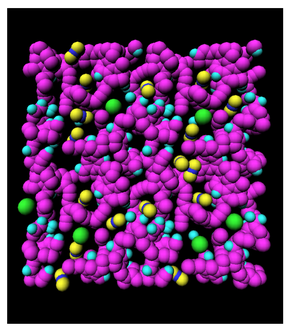
ADSORPTION AND POROMECHANICS



Adsorption is the adhesion of fluid molecules at the surface of a solid due to favorable fluid-solid molecular interaction.
From the mechanical point of view, adsorption is known to induce mechanical stresses.
The mechanical impact of adsorption can be sketched in the case of a thin plate:

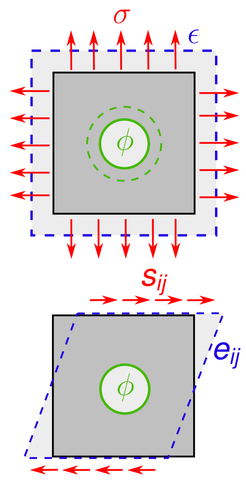


In coal, adsorption occurs in the nanopores of the solid matrix. Poromechanics can be extended to account for adsorption in nanopores. The constitutive equations are:



General poromechanics

$$\begin{cases} \sigma = K\epsilon - \frac{\partial}{\partial \epsilon}\left(\int_0^p n\bar{V}_b dp\right)\Big|_{p,e_{ij}=0} \\ n\bar{V}_b = n(\epsilon=0,p)\,\bar{V}_b(p) - \frac{\partial}{\partial p}\left(\int_0^\epsilon \sigma d\epsilon\right)\Big|_{\epsilon,e_{ij}=0} \\ s_{ij} = 2Ge_{ij} \end{cases} \quad (1)$$

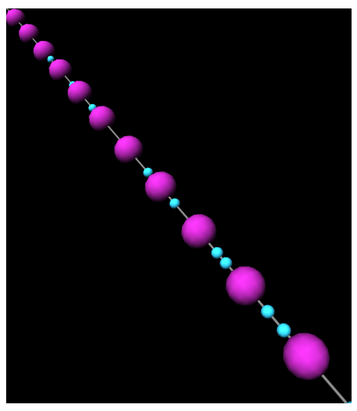


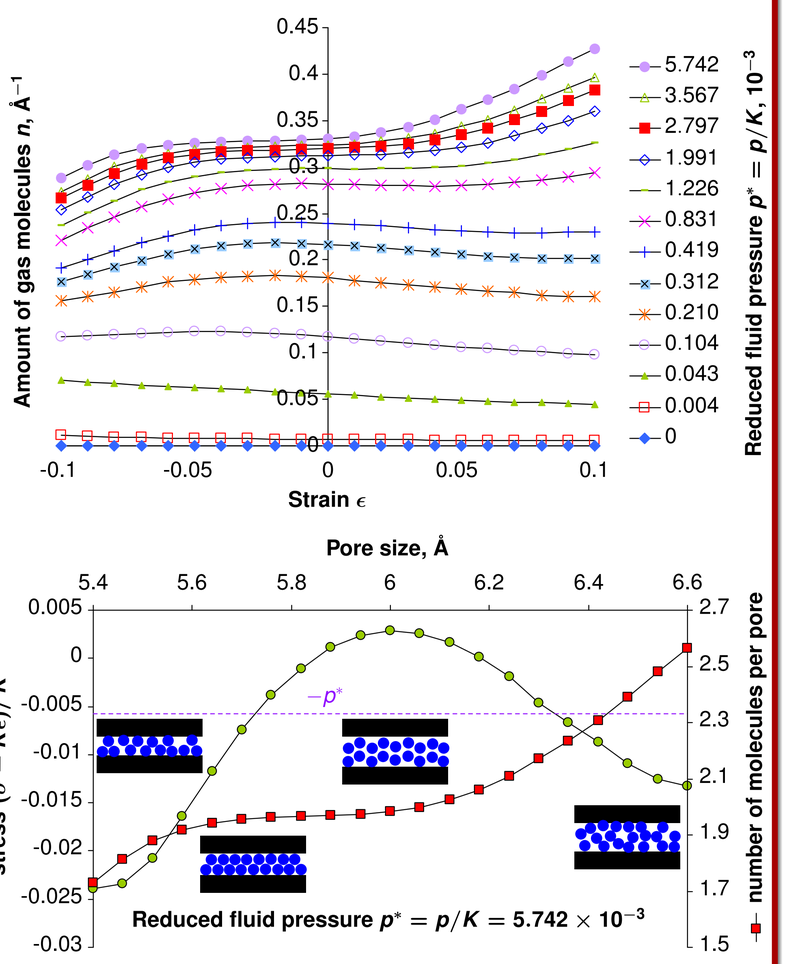
- K and G are the elastic moduli of the dry sample.
- $n(\epsilon, p)$ is the adsorbed amount per unit volume which depends on the strain ϵ and on the bulk pressure p of the fluid
- Adsorption can make the sample swell or shrink, and can make the poroelastic moduli non-linear

Requires to know the adsorbed amount as a function of both the pressure p and the strain ϵ.

CRYSTALLINE ONE DIMENSIONAL CHAIN

Case of a linear elastic chain subjected to the adsorption of a Lennard-Jones fluid

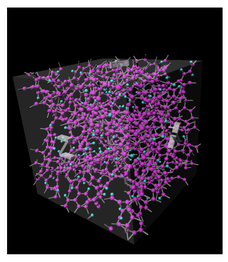


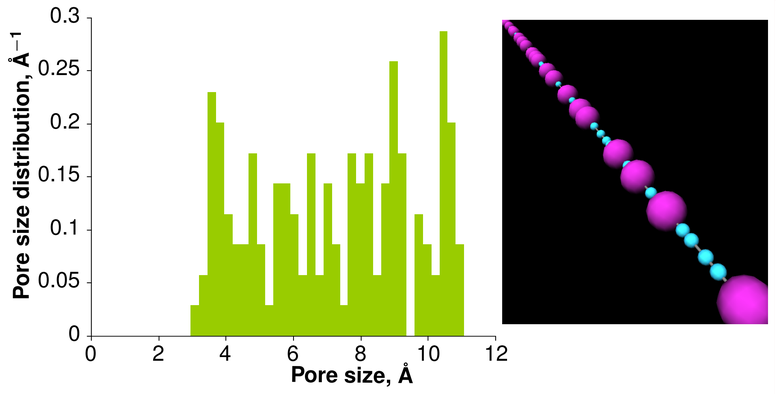


The uneven adsorption behavior can be explained by the commensurability of the size of the pores to the size of the adsorbed fluid molecules.

AMORPHOUS ONE DIMENSIONAL CHAIN

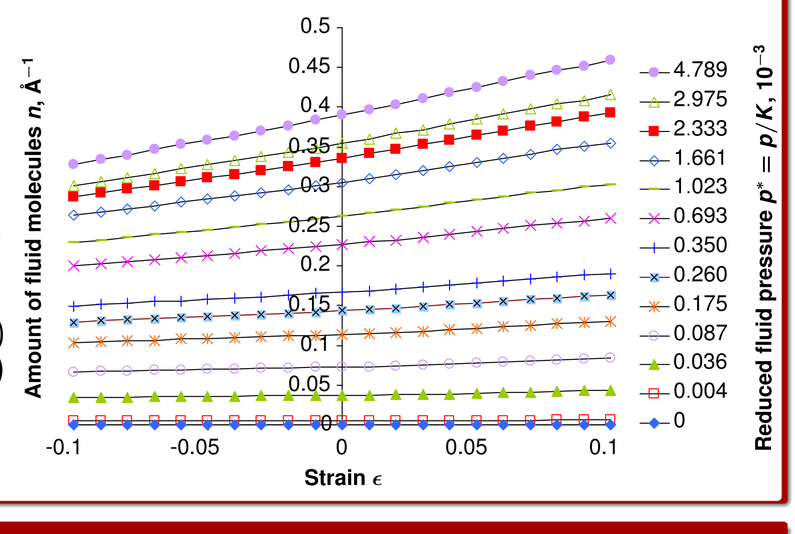
Coal is an amorphous medium and is expected to exhibit the same type of dependence of the adsorbed amount of fluid on the strain of the medium
What about an amorphous chain?





The adsorption behavior in the amorphous chain is linear:

$$n(\epsilon, p) = n(\epsilon = 0, p)\cdot(1 + C * \epsilon) \quad (2)$$

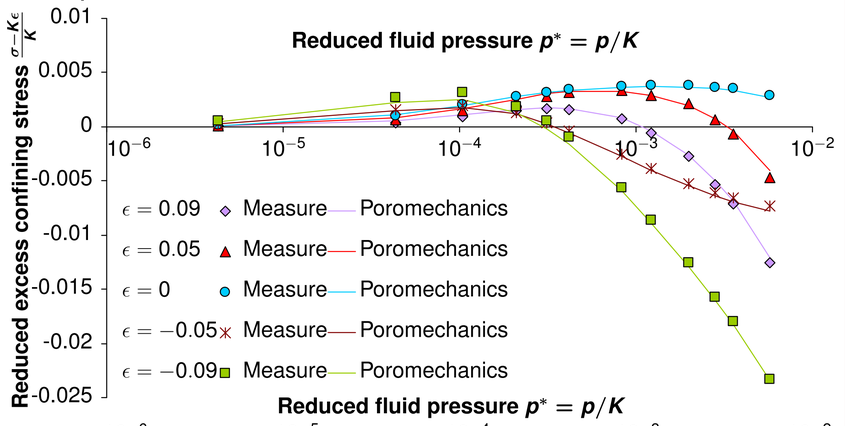


CONSEQUENCE ON THE MECHANICAL BEHAVIOR

The first constitutive equation of the general poromechanics (Eq. 1) relates the mechanical effect to the adsorption isotherms

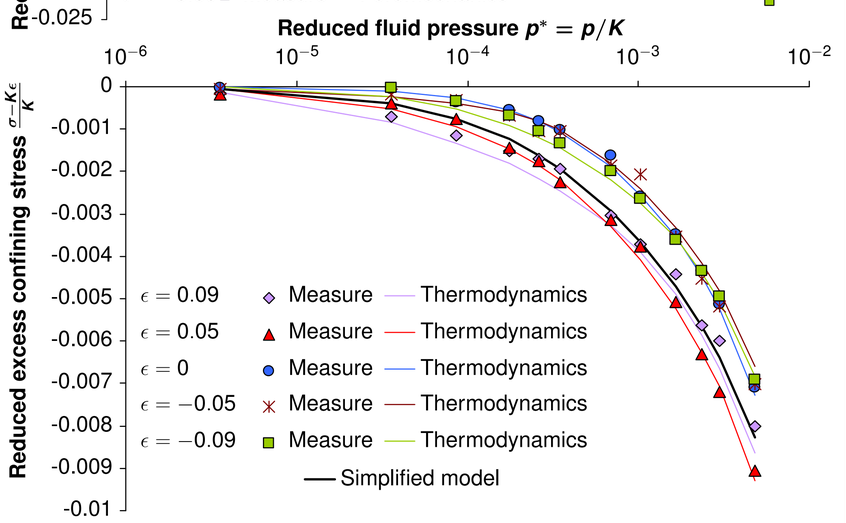
Crystalline chain:

Complex adsorption
⇒ Complex mechanical effect
The fluid can make the solid swell or shrink



Amorphous chain:

Linear adsorption
⇒ Uniform disjoining effect
The fluid always makes the solid swell



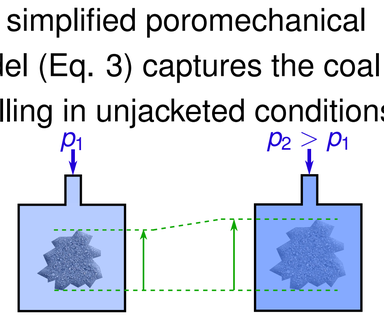
Given the simple dependence (Eq. 2) of the adsorption on the strain, the constitutive equation (1) can be simplified.

Simplified model

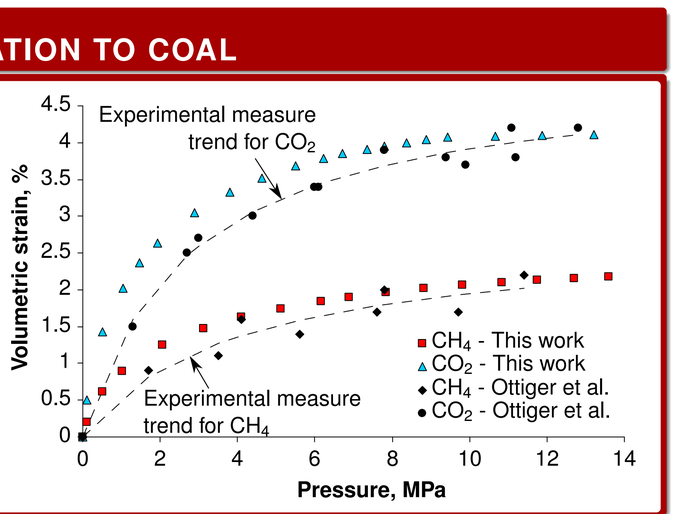
$$\sigma = K\epsilon - C\int_0^p n(\epsilon = 0, p)\,\bar{V}_b dp \quad (3)$$

APPLICATION TO COAL

The simplified poromechanical model (Eq. 3) captures the coal swelling in unjacketed conditions



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



CONCLUSIONS

- In order to understand the mechanical effect of adsorption, the strain-adsorption behavior is needed.
- For amorphous solids the adsorption is linear with strain, which means that the impact on poromechanics can be captured by a simple model
- How adsorption in nanopores depends on the strain can be understood in terms of pore commensurability
- Application to coal is satisfying