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## Adsorption behavior in disordered nanoporous solids

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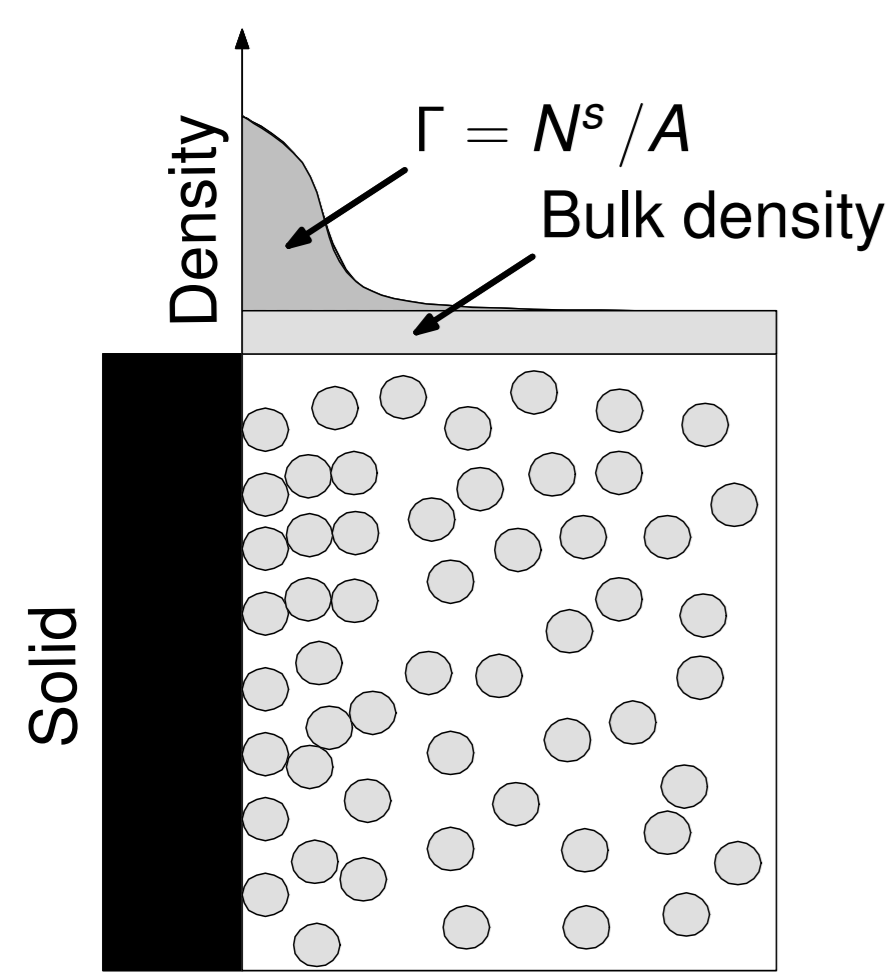
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## ABSTRACT

The swelling of coal induced by an adsorption of CO<sub>2</sub> 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<sub>2</sub>.

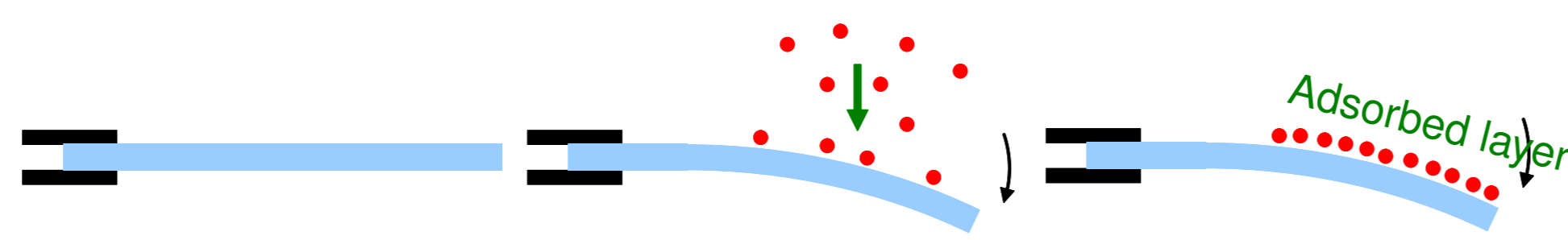
## ADSORPTION AND POROMECHANICS



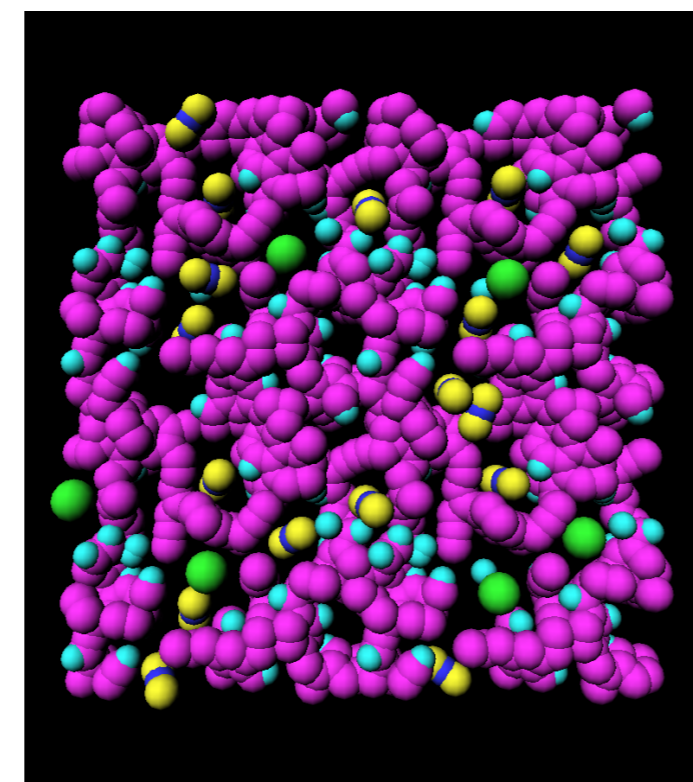
Adsorption is the adhesion of fluid molecules at the surface of a solid due to favorable fluid-solid molecular interaction.

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:

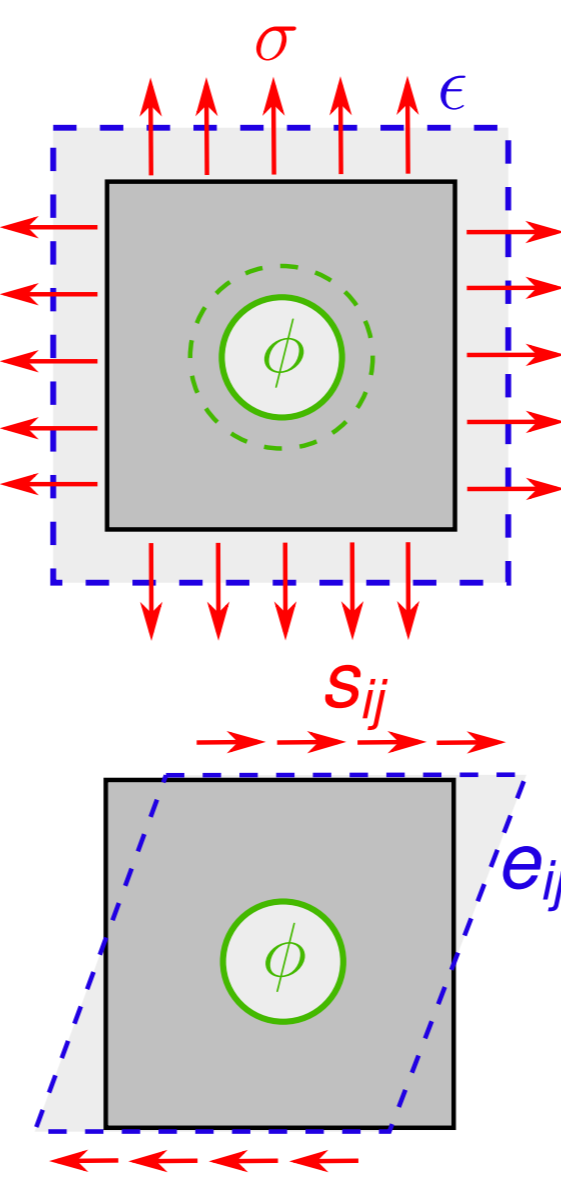


In coal, adsorption occurs in the nanopores of the solid matrix. Poromechanics can be extended to account for adsorption in nanopores. The constitutive equations are:



### General poromechanics

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

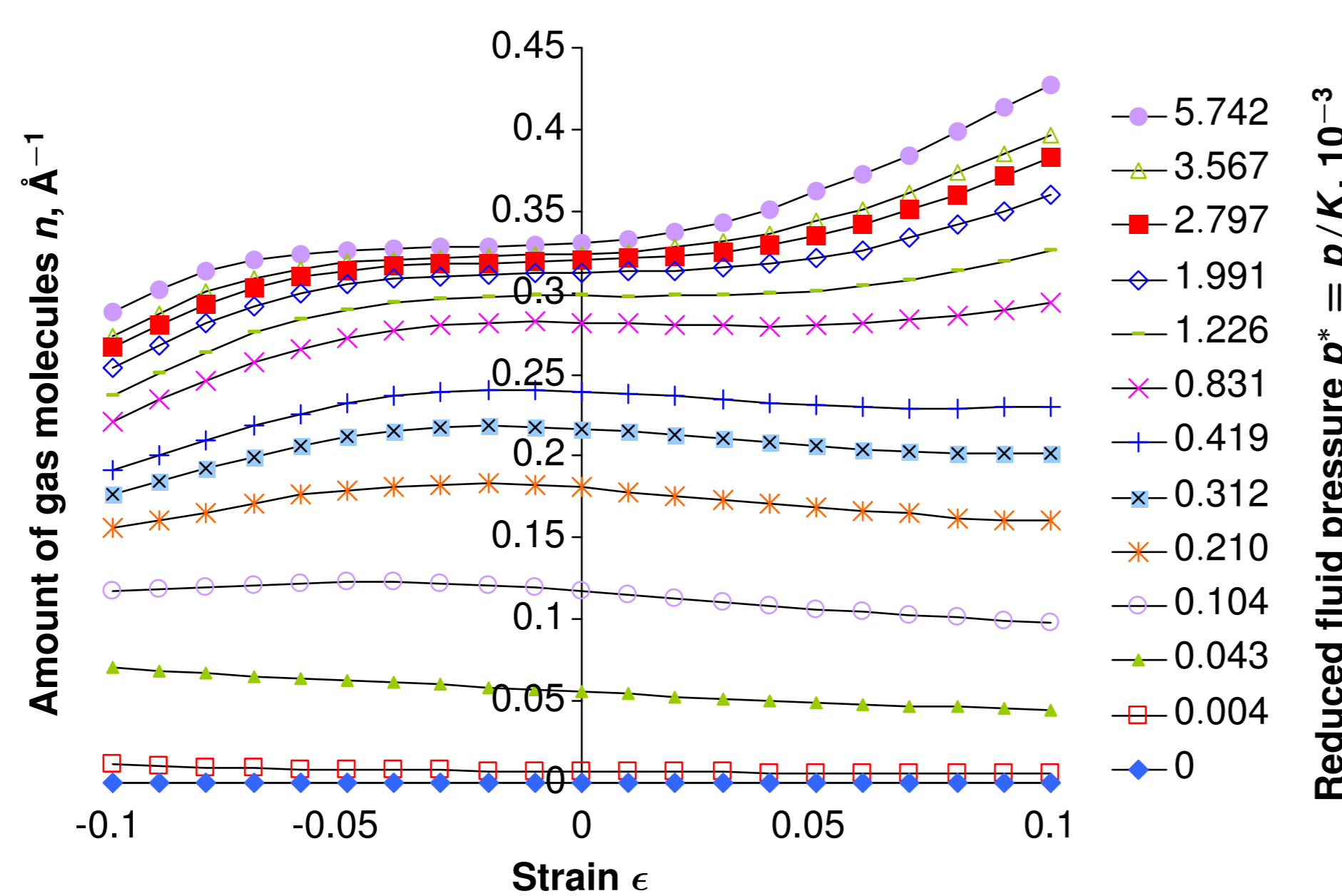
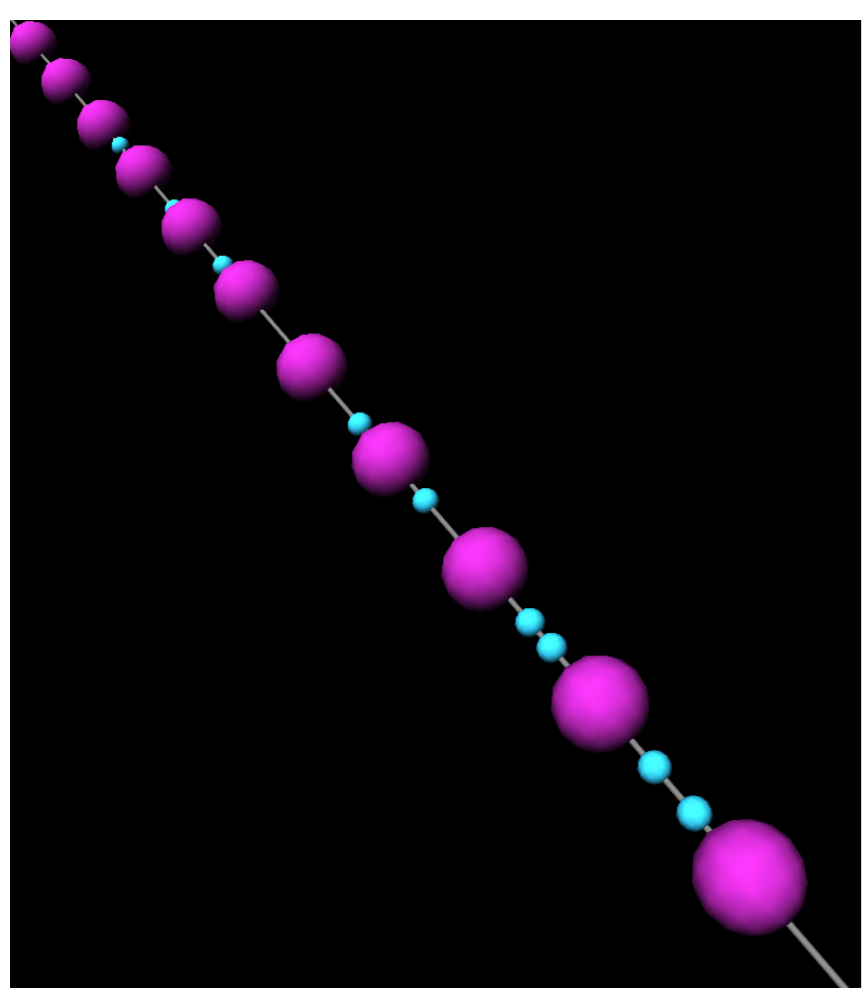


- $K$  and  $G$  are the elastic moduli of the dry sample.
- $n(\epsilon, p)$  is the adsorbed amount per unit volume which depends on the strain  $\epsilon$  and on the bulk pressure  $p$  of the fluid
- Adsorption can make the sample swell or shrink, and can make the poroelastic moduli non-linear

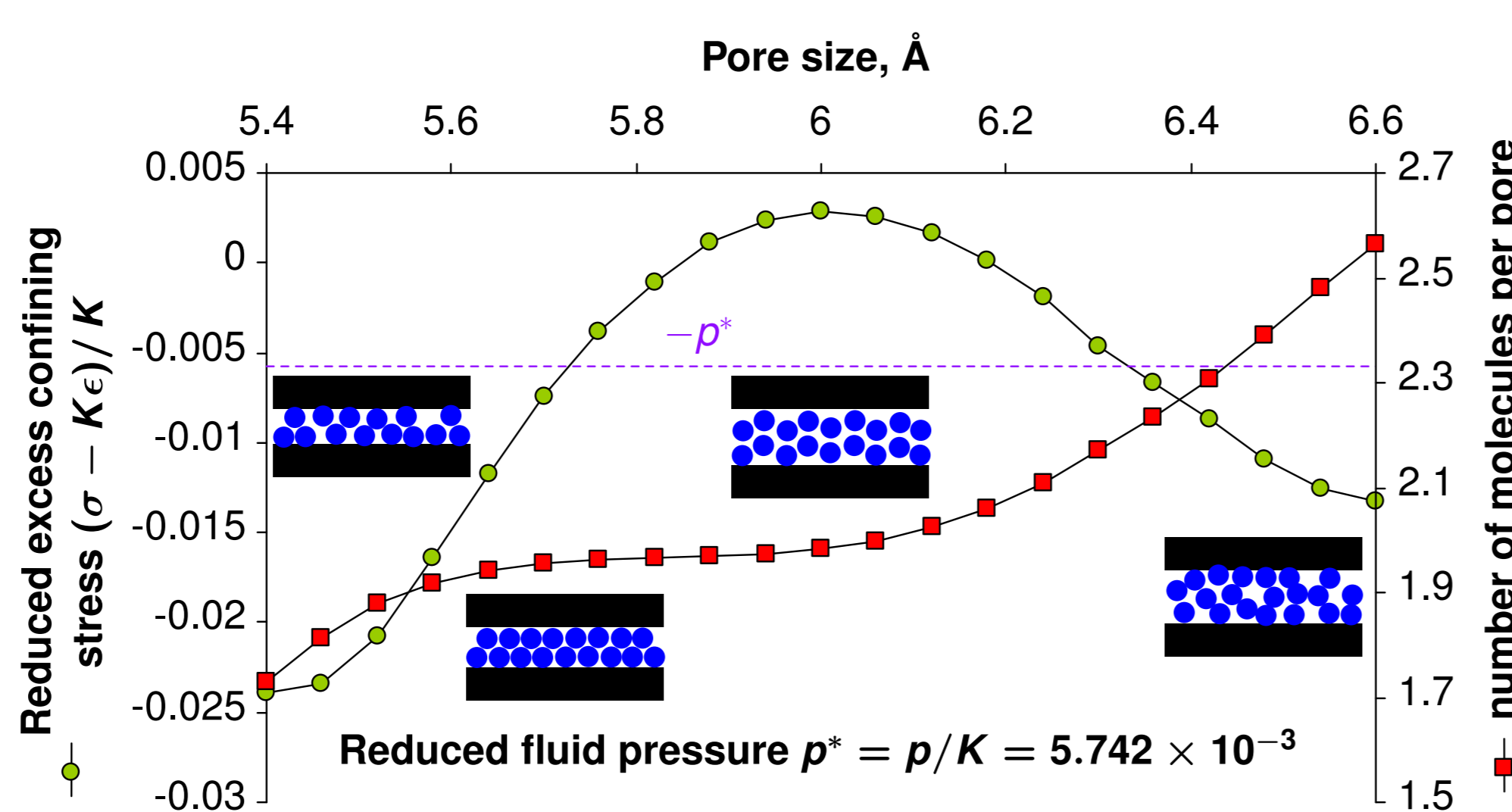
Requires to know the adsorbed amount as a function of both the pressure  $p$  and the strain  $\epsilon$ .

## 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.

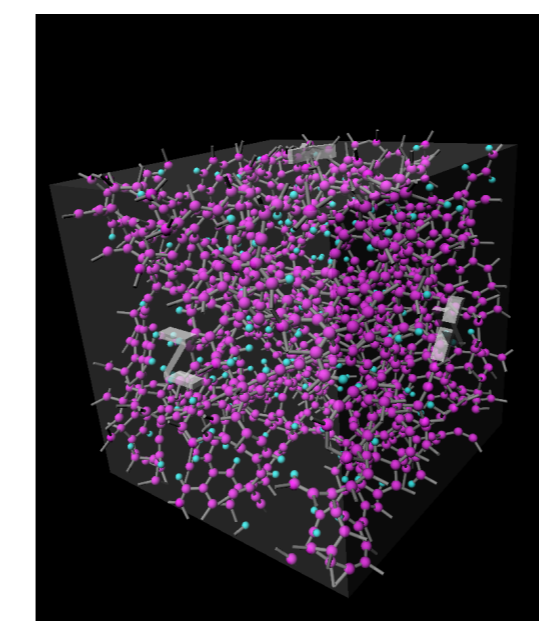


## CONCLUSIONS

- 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

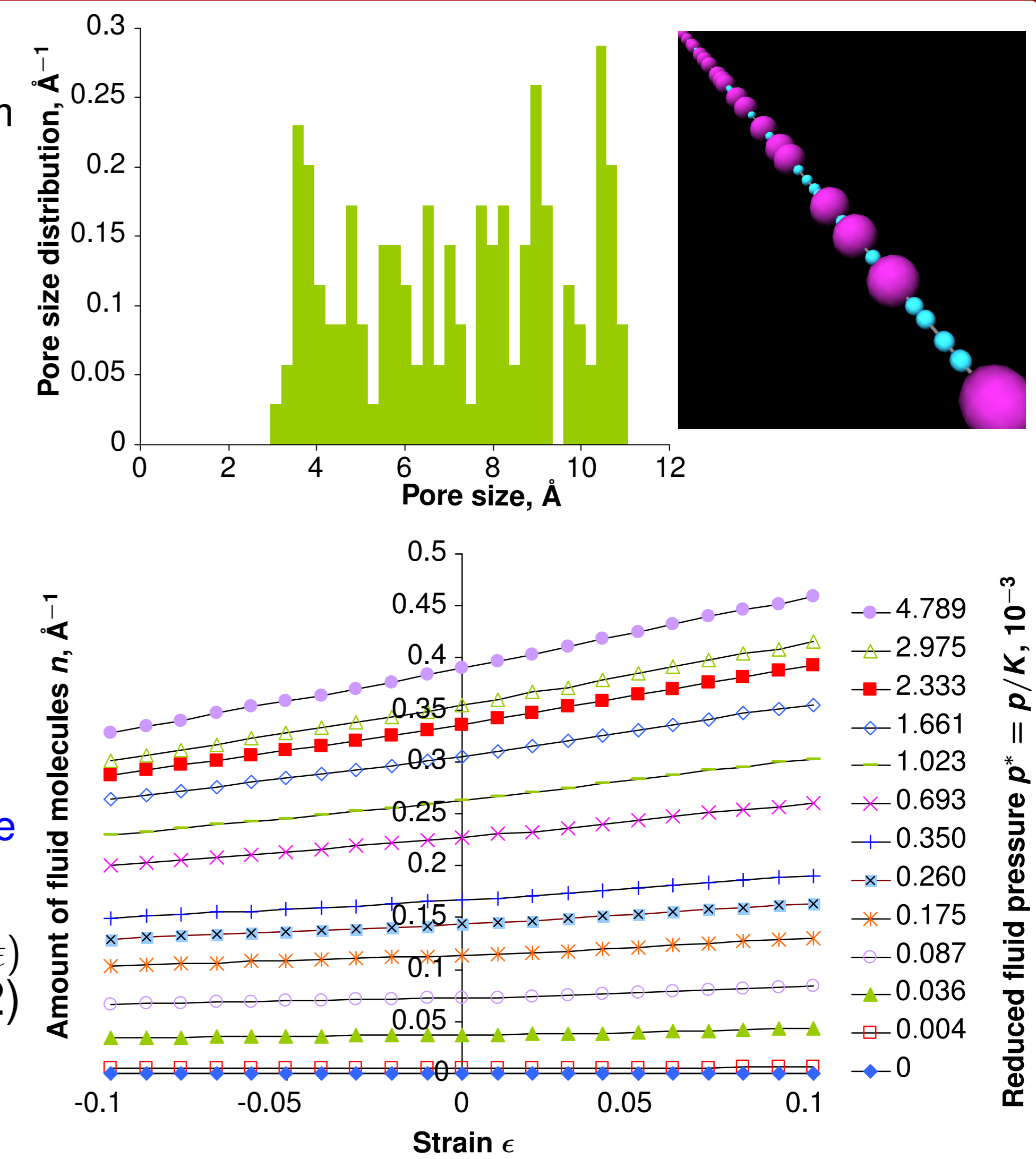
## AMORPHOUS ONE DIMENSIONAL CHAIN

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:

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



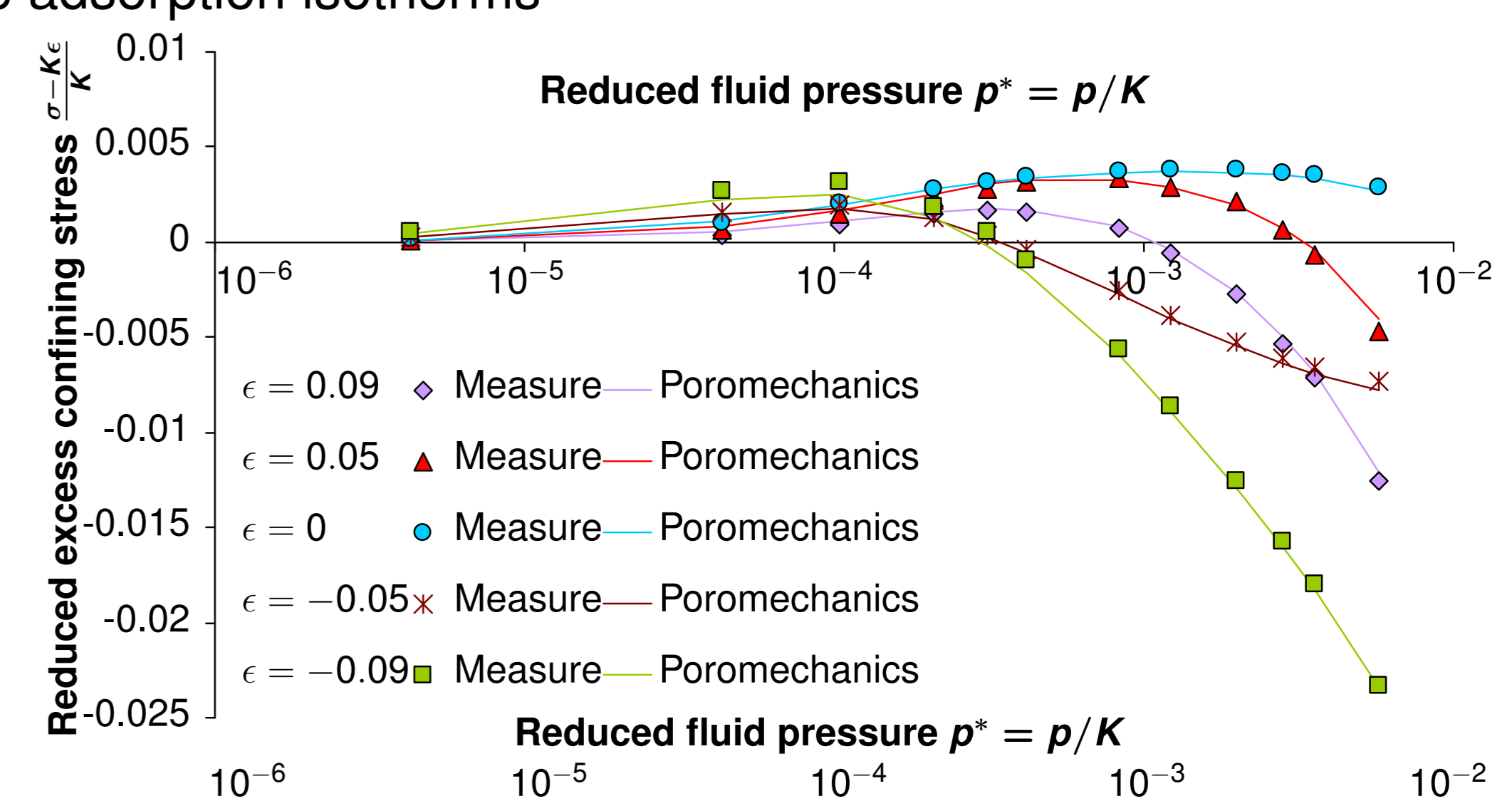
## CONSEQUENCE ON THE MECHANICAL BEHAVIOR

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

Crystalline chain:

Complex adsorption  
 $\Rightarrow$  Complex mechanical effect

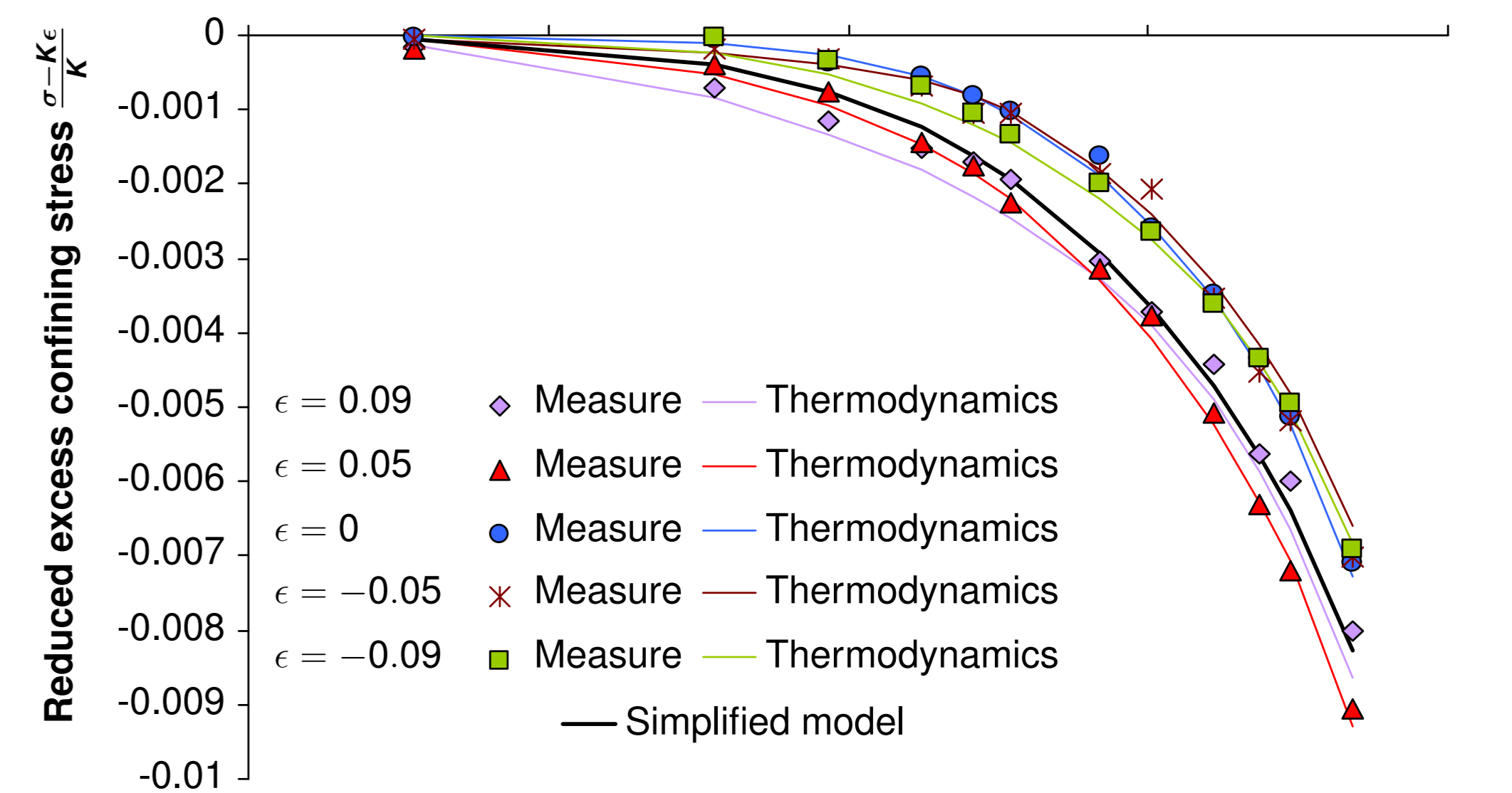
The fluid can make the solid swell or shrink



Amorphous chain:

Linear adsorption  
 $\Rightarrow$  Uniform disjoining effect

The fluid always makes the solid swell



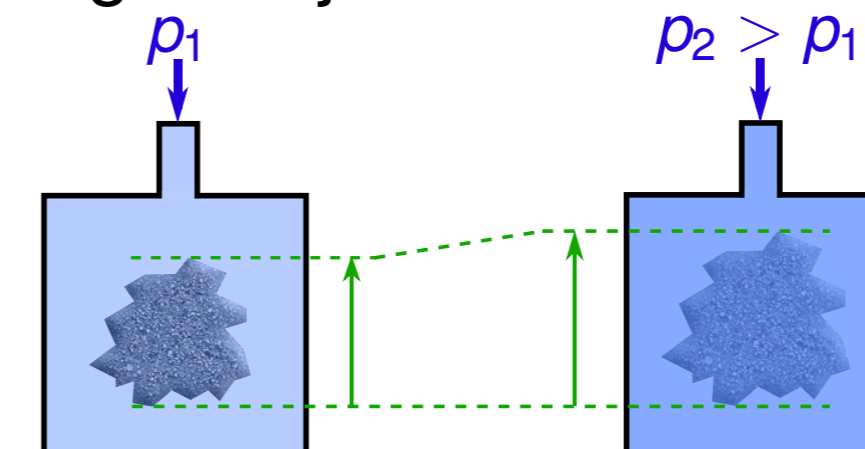
Given the simple dependence (Eq. 2) of the adsorption on the strain, the constitutive equation (1) can be simplified.

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))

