

# Investigation of the carbon dioxide sorption capacity and structural deformation of coal

## Abstract:

- Due to increasing atmospheric CO<sub>2</sub> concentrations causing the global energy and environmental crises, geological sequestration of carbon dioxide is now being actively considered as an attractive option to mitigate greenhouse gas emissions. One of the important strategies is to use deep unminable coal seams, for those generally contain significant quantities of coal bed methane that can be recovered by CO<sub>2</sub> injection through enhanced coal bed natural gas production, as a method to safely store CO<sub>2</sub>. It has been well known that the adsorbing CO<sub>2</sub> molecules introduce structural deformation, such as distortion, shrinkage, or swelling, of the adsorbent of coal organic matrix. The accurate investigations of CO<sub>2</sub> sorption capacity as well as of adsorption behavior need to be performed under the conditions that coals deform. The U.S. Department of Energy-National Energy Technology Laboratory and Regional University Alliance are conducting carbon dioxide sorption isotherm experiments by using manometric analysis method for estimation of CO<sub>2</sub> sorption capacity of various coal samples and are constructing a gravimetric apparatus which has a visual window cell. The gravimetric apparatus improves the accuracy of carbon dioxide sorption capacity and provides feasibility for the observation of structural deformation of coal sample while carbon dioxide molecules interact with coal organic matrix. The CO<sub>2</sub> sorption isotherm measurements have been conducted for moist and dried samples of the Central Appalachian Basin (Russell County, VA) coal seam, received from the SECARB partnership, at the temperature of 55 °C.

## Sample preparation

- Virginia Tech samples from SECARB partnership: Pocahontas #3 and Pocahontas #9.

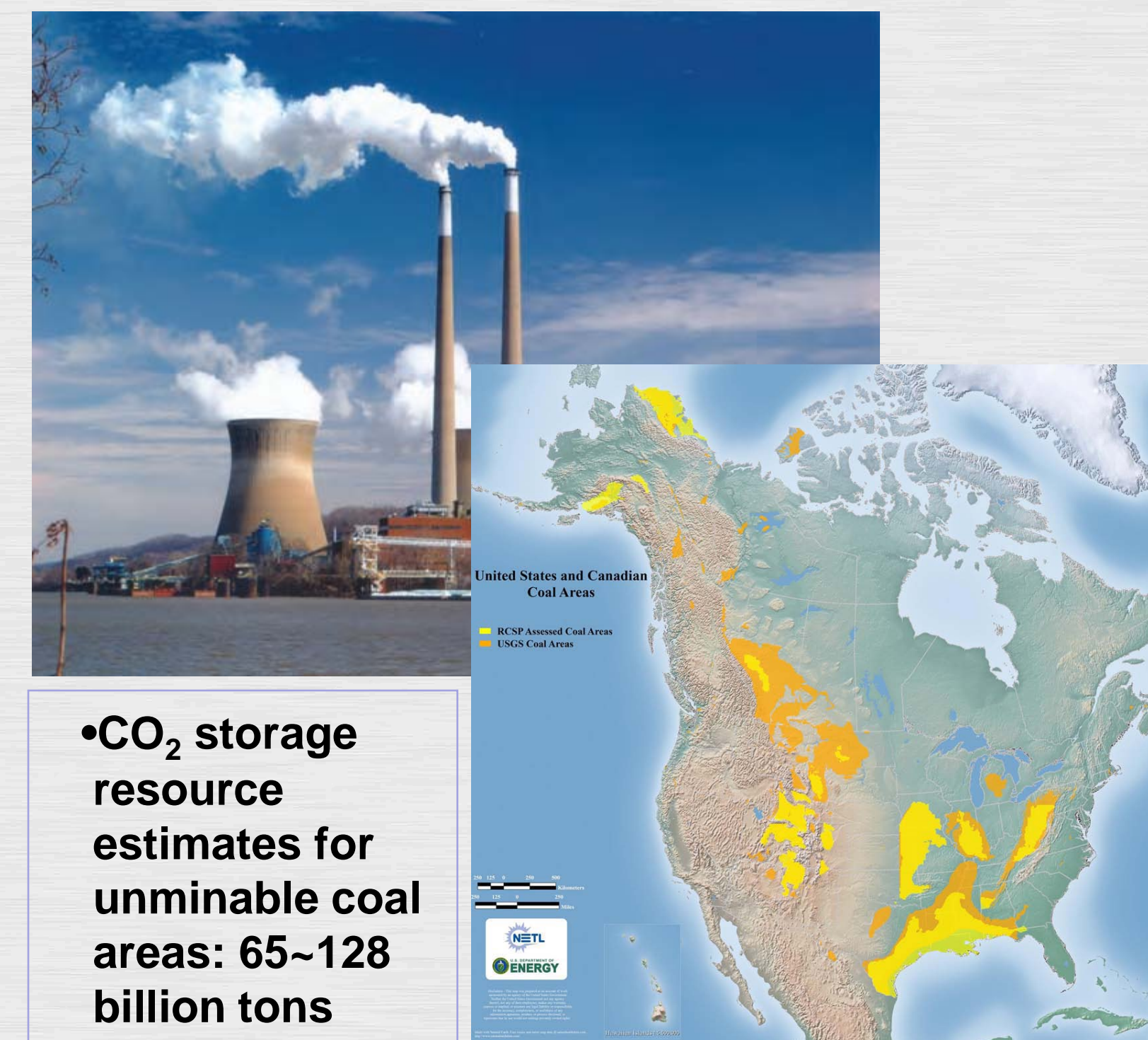


Fig.1. The map displays unminable coal areas that were estimated by the RCSPs [R1]. The carbon dioxide injected into coalbed can recover methane and be physically trapped on the coal.



G- Gas Cylinder  
I- ISCO Series D Syringe Pump  
D- Data Acquisition  
R- Reference Cell  
S- Sample Cell  
P- Pressure Transducer  
V- Vacuum Pump  
T- Thermocouples  
B- Constant Temperature Water Bath

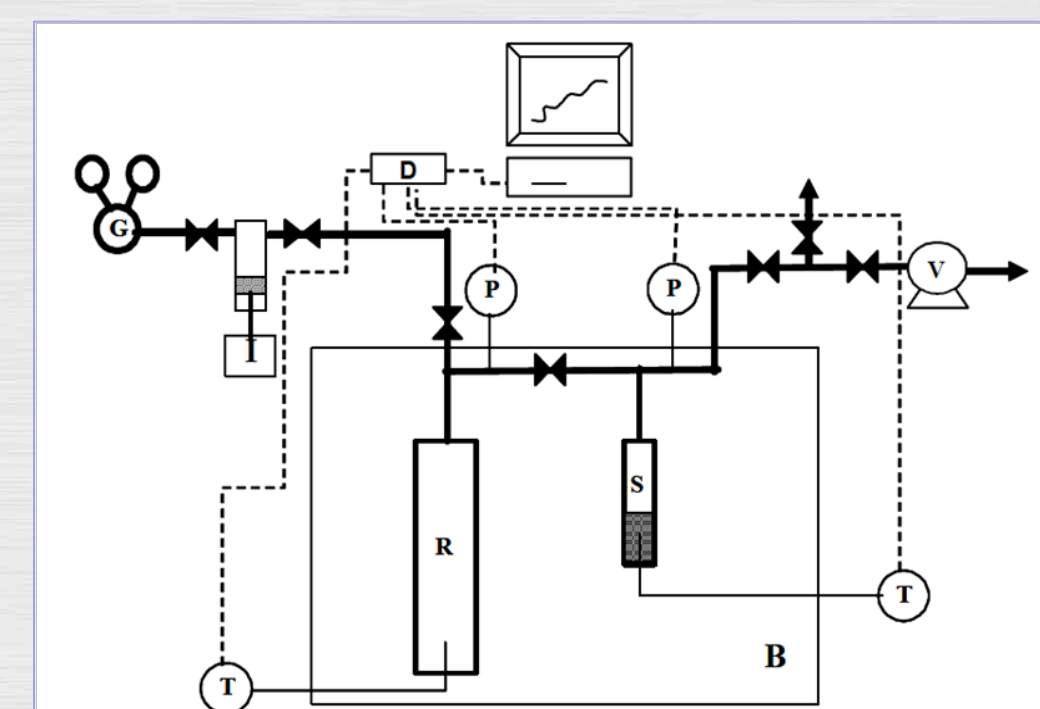


Fig.2. The construction of CO<sub>2</sub> sorption isotherms by using manometric method. The image and schematic illustration of manometric apparatus.

*Major difficulties: the actual density of adsorbed phase, void volume in sample cell, and reliability of apparatus.*

## Sorption isotherms on coals

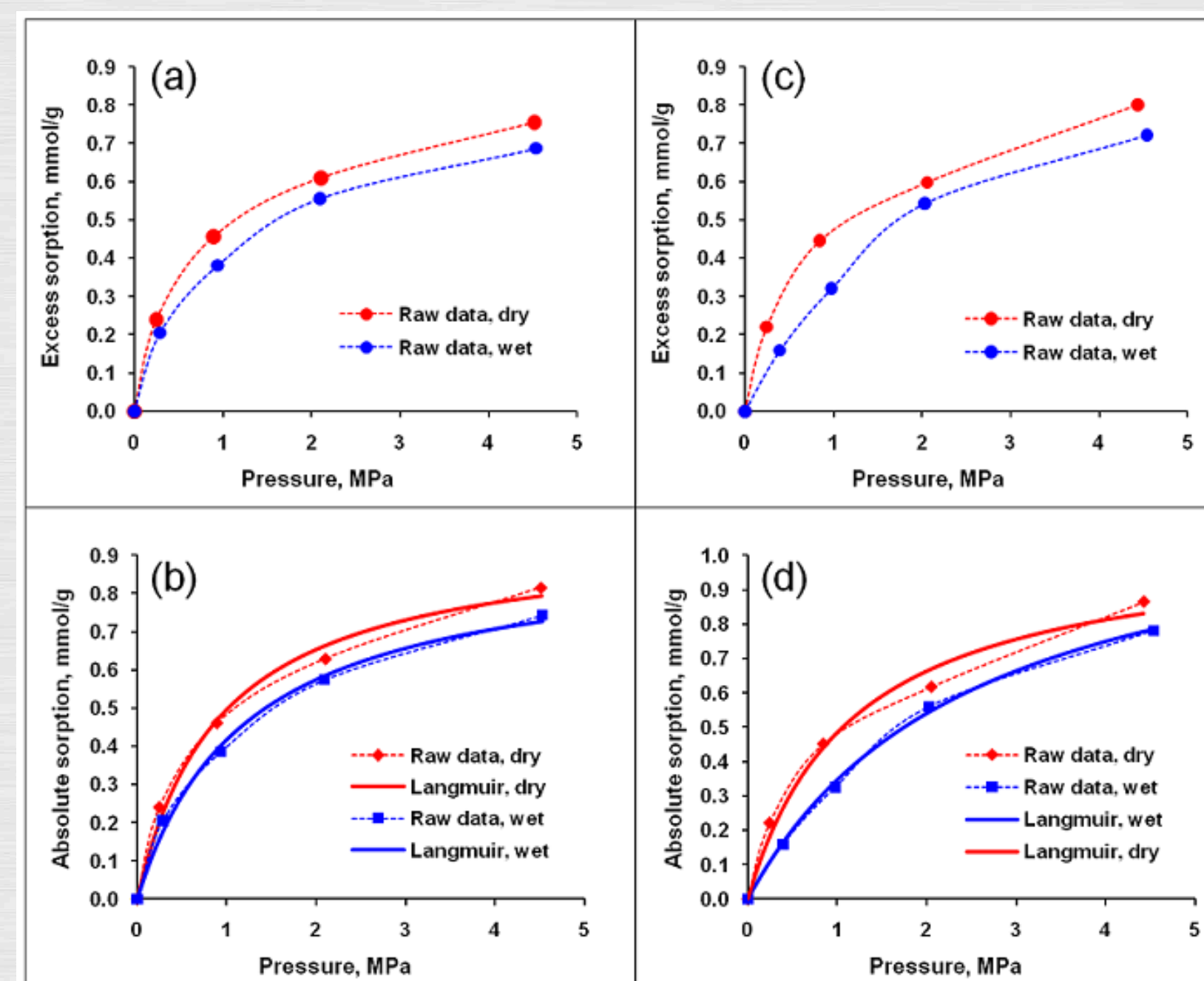


Fig.3. Carbon dioxide excess and absolute adsorptions (dry basis). (a), (b) Pocahontas #9. (c), (d) Pocahontas #3. (b), (d) solid lines indicate the best fits.

Definitions and gas law to calculate the Gibbs excess adsorption:

$$n^{ex} = n_{total} - V_{void} \rho_{gas} \quad n^{abs} = n_{total} - V_{gas} \rho_{gas} \quad V_{void} = V_{gas} + V_{adsorbed}$$

$$\Delta n^{ex} = \left( \frac{P_{Ri}}{z_{Ri}} - \frac{P_{Rf}}{z_{Rf}} \right) \frac{V_R}{wRT} - \left( \frac{P_{Si}}{z_{Si}} - \frac{P_{Sf}}{z_{Sf}} \right) \frac{V_o}{wRT}$$

$$n^{ex} = \Delta n_1^{ex} + \Delta n_2^{ex} + \Delta n_3^{ex} + \dots + \Delta n_i^{ex}$$

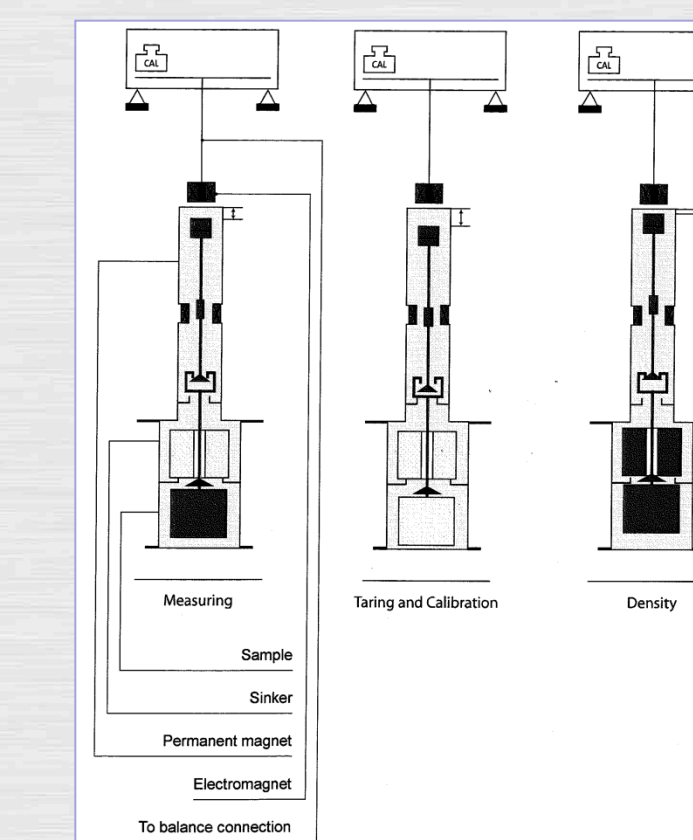
$n^{ex}$ : the total amount of Gibbs excess adsorbed gas



Fig.4. Constructing a gravimetric apparatus that has a visual window cell. It may improve an accuracy of sorption isotherms and provide feasibility for the observation of structural deformation of coal.

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- Resolution: 10μg ~ 1μg
- The system-affecting forces:  
 $S_{MP} \cdot g = F_g + F_{ads} - F_b$
- $S_{MP}$ : measurement signal detected by the balance
- $F_g$ : gravity affecting the system
- $F_{ads}$ : force resulting from the adsorption of gas molecules
- $F_b$ : buoyancy force

Fig.5. Simultaneous sorption and density measurement by using the three-position magnetic suspension balance. It measures the density of adsorbing fluids directly.

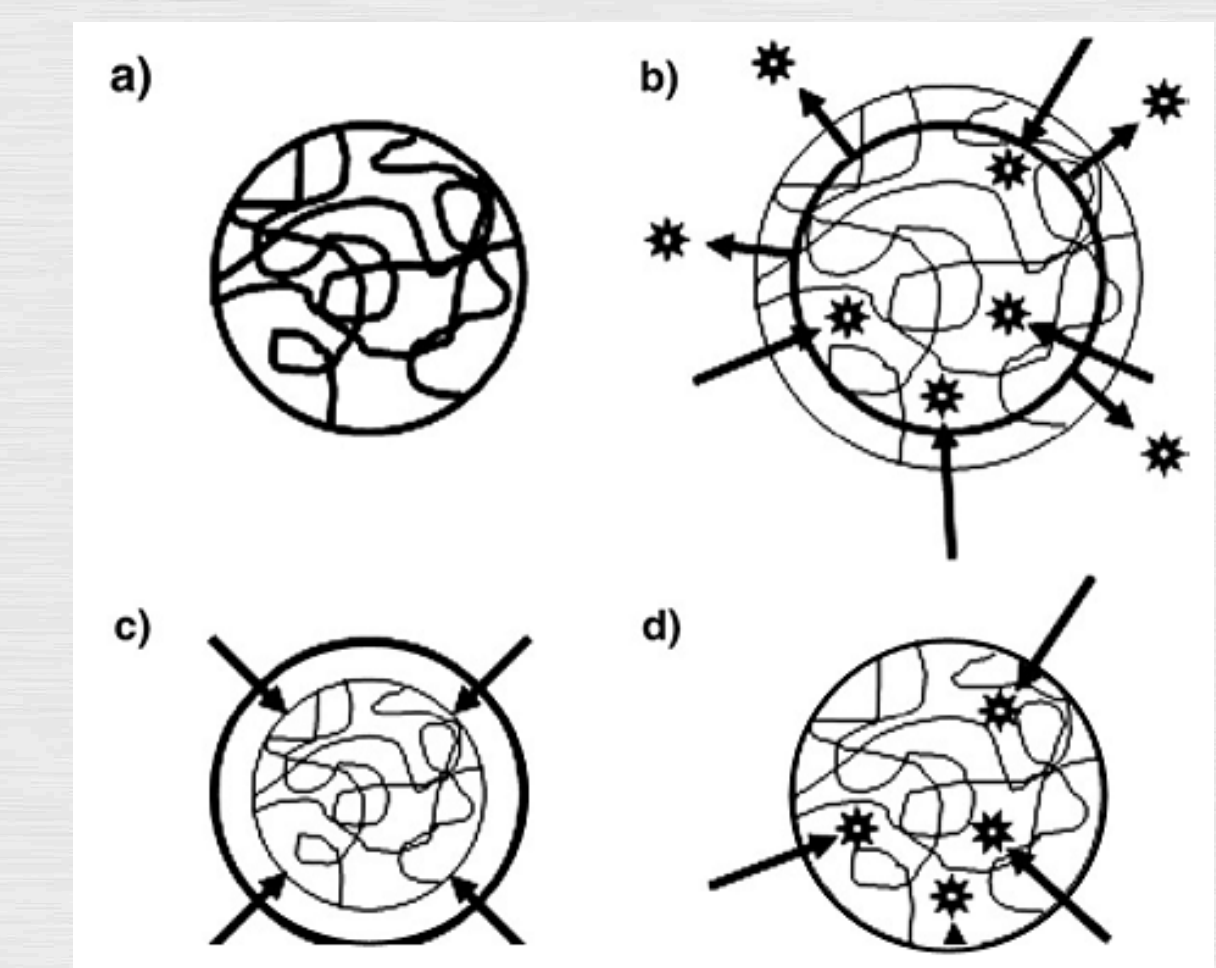


Fig.6. Schematic illustration of the structural deformation of coal sample that might be happening under high CO<sub>2</sub> pressure. a) initial coal sample, b) swelling, c) shrinkage, d) gas molecule penetration without change in volume[R2].

## References:

- [R1] U.S. Department of Energy-NETL, *Carbon Sequestration Atlas of the United States and Canada*, third edition, 2010  
[R2] V. Romanov and Y. Soong, *International Journal of Coal Geology* 77, (2009) 10-15