

# Geomechanical Modelling of Coalbeds used for CO<sub>2</sub> Sequestration

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## Abstract

While evaluating carbon capture and storage processes, coal seams are chosen. Furthermore a general approach is conducted on methodologies, existing projects and associated problems.

In order to show a conducting line, Parameter changes, technical e scientific challenges are identified to characterize the technological evolution. Regarding coal matrix strain and the potential associated risks due to the stress state change, mechanical and flow behaviours, for different coal seams the physical and chemical properties alterations are summarized. The production technologies and meaningful projects are observed in order to demonstrate practicability.

For the purpose of conducting a future adequate geomechanical simulation, regarding Portuguese coal reservoirs, Douro's carboniferous basin is chosen as a potential target for continuous study. For the purpose of an "in-situ" sampling campaign a geological description is made on the study area.

The lack of data and the insufficient knowledge on the variation relation of the parameters, needed for an adequate simulation

A search is made for the best approach on implementing a Geomechanical simulation that translates the effects and that prevents the risks associated with carbon dioxide sequestration in coal reservoirs, taking into account the effect of CO<sub>2</sub> on the "surrounding middle" properties.

Proceeds to the establishment of a set of requirements for laboratory research that objective knowledge of the thermo-hydro-mechanical behavior.

**Keywords:** Carbon, Coal, Injection, Sequestration

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## 1. Introduction

CCS (Carbon Capture and Storage) is a technology or set of technologies that consist of carbon dioxide (CO<sub>2</sub>) capture and storage in underground formations. CO<sub>2</sub> is considered harmful to the atmosphere when in excess, contributing to the greenhouse effect.

Several technical options have been investigated but consensus has only been achieved in terms of goals and best practices. Amongst the various options tried and studied, CO<sub>2</sub> sequestration and storage in coal formations, as a means to achieve the reduction of emissions of such a greenhouse gas, have been the focus of the scientific community.

### 1.1. Objectives

This dissertation aims to review the process of capture and storage of carbon dioxide, more specifically in coal reservoirs, without disregarding other methodologies of underground geologic sequestration (UGS- Underground Geological Sequestration).

It does not intend, to monitor legislative developments. Instead, the goal is to address the technical and scientific aspects of these procedures. This process, based on CO<sub>2</sub> adsorption mechanism on the coal's surface and the incorporation of carbon in its mineral structure (carbonation), should lead to higher safety and reliability in long-term storage (Gomes, A.I.M, 2010).

In addition it tries to analyse past, present and future developments of this subject.

A brief description of the Portuguese coal formations, with a higher emphasis on the Douro's coal basin in the Northern area of the

country, is performed in an attempt to assess the viability of this CCS option.

## 2. CO<sub>2</sub> Sequestration

It is important to address the technical and social challenges that hinder proper modelling of CCS. In addition to the constant political and social changes, economic uncertainty and environmental constraints, CO<sub>2</sub> storage in coal reservoirs is far from being consensual. Advances in this field are debatable.

The cost of CO<sub>2</sub> injection in a highly complex geological environment, hampers the feasibility of a CCS project.

Even with the possibility of methane production, the attractiveness of this process has yet to be fully recognised by the energy markets, rendering this CSS option to be strictly a theoretical exercise.

Coal will be the focal point of this study, due to its reservoir properties. Furthermore, coal is still the largest source of energy when compared to other fossil fuels (BP, 2014), being also one of the main responsible for CO<sub>2</sub> emissions. Coal is a fossil fuel formed in geological conditions similar to those of oil and gas. It is ranked according to its Carbon content (table 1).

Coal Rank	Proximate Analysis (wt % ar)				Ultimate Analysis (wt % maf)					Net Heating Value (maf) (MJ/kg)
	Fixed carbon	Volatile matter	Moisture	Ash	C	H	O	N	S	
Anthracite	81.8	7.7	4.5	6.0	91.8	3.6	2.5	1.4	0.7	36.2
Bituminous	54.9	35.6	5.3	4.2	82.8	5.1	10.1	1.4	0.6	36.1
Subbituminous	43.6	34.7	10.5	11.2	76.4	5.6	14.9	1.7	1.4	31.8
Lignite	27.8	24.9	36.9	10.4	71.0	4.3	23.2	1.1	0.4	26.7

**Notes:**  
 • wt % = percent by weight ar = as received maf = moisture and ash free  
 • C = Carbon H = Hydrogen O = Oxygen N = Nitrogen S = Sulfur  
 • Multiply Net Heating Values in MJ/kg by 430.11 to convert to Btu/lb.

Source: Chris Higman and Maarten van der Burgt (2008). Coal Gasification, 2nd Edition. Gulf Professional Publishers.

Table 1 - Coal Classification

After sinking and sedimentation (subduction) and other processes, is transformed into coal by geological processes including high temperatures and pressures. Thicknesses of commercially exploited deposits can be thinner than 1m or larger than 100 meters. Many of these deposits also contain natural gas both within coal seam and the rock in which it is enveloped.

This confined gas (methane, CH<sub>4</sub>), is sometimes released into the atmosphere during mining operations while exploiting coal. The gas diffuses from the micropores to the larger and the debate exists, if the micropores aren't actually nanopores on macromolecular structure of organic matter. (Flores, R. M., 2013). Coal, an organic rock, has its own characteristics that change make it difficult to make an exact prediction of its behaviour when mechanical and chemical changes are imposed due to the injection of a gas as CO<sub>2</sub>. In addition to the possible economic return from the sale or use of the methane produced, mechanisms have been created to encourage reduction of CO<sub>2</sub> released into the atmosphere. Since most of the CO<sub>2</sub> is adsorbed to the coal's surface with a density similar to that of a liquid, it is expected to be a means to hijack CO<sub>2</sub> per million years, making it the preferred option and more attractive than all other subsuperficial means. ECBM also allowed progress in storing mechanisms. However, there are technical challenges such as unexploitable reserves definition, evaluation of storage capacity, storage and site characterisation, methods for CO<sub>2</sub> injectivity optimisation. Researchers generally believe that the adsorption of each component in the mixture of gases is not independent and there is competition between the different gases.

The isotherm of a binary gas lies between the high gas adsorption and low gas adsorption isotherms. Different gas mixtures result in different isotherms, being the isotherms of multi-component gases even more complex. Although there is a significant difference between the multi-component gas adsorption and pure gases the Langmuir equation was fit for mixture of gases as for pure gases. The experimental result of adsorption isotherm shows that the concentration of gas is not constant during each step of adsorption, however, decreases over time due to adsorption on internal porous surfaces. Additionally, the trend is the concentration decrease of CO<sub>2</sub> in five pressure stages. The experimental result of adsorption isotherm shows that the coal rank determines its adsorptive properties and its physical and chemical behaviour.

The swelling induced by CO<sub>2</sub> adsorption on coal results in permeability and injectivity reduction, observed in field trials. (Yang, y., Zoback, m., 2014)

Comparative studies between powdered and block coal samples showed that adsorption caused a higher expansion (8%) for coal powder than for block coal (7%). (Romanov, v., Soong, y., et al., 2008). Coal Bed Methane (CBM), is considered a nuisance by the extractive industry, being related to many accidents in mines.

Unconventional methane besides being used in the form of CH<sub>4</sub> to produce energy can also be dissociated into H<sub>2</sub> and CO<sub>2</sub> and hydrogen used as fuel. It is considered that the use of coal methane (CBM) and CO<sub>2</sub> sequestration is a contribution to a lower CO<sub>2</sub> emission, contributory gas for global warming and climate long-term instability. The ECBM

method consists in CO<sub>2</sub> injection which is adsorbed by the coal staying on its porous matrix, releasing the methane gas trapped there. The process results in the imprisonment of a noxious gas, responsible for the greenhouse effect, freeing another and that can be used as fuel, hence profitable, if sufficient in order to be marketed. Hopefully the future will eventually proceed on projecting self-sustaining energy production infrastructure and free of harmful emissions into the atmosphere. CO<sub>2</sub> is a gas that is produced as a product of respiration by living beings, it can also be produced through the complete burning of organic material as fuel oils, coal, natural gas, etc. The use of these fuels has contributed to a big increase in emissions as can be seen in figure 1.

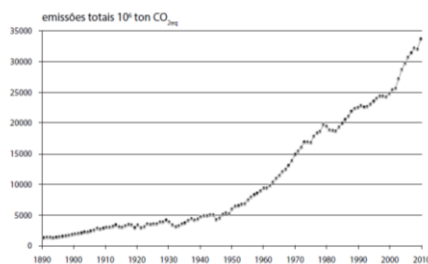


Figure 1 - CO<sub>2</sub> emissions released to the atmosphere from the combustion of fossil substances. Curve constructed with data obtained from the CDIAC database – Carbon Dioxide Information Analysis Center (Boden, Marland et al., 2012)

After the CO<sub>2</sub> recovery processes with the necessary purification, depending on the source of carbon dioxide and impurities contained therein, is further compressed. Activated carbon towers and/or molecular sieves, are used. After compression, the carbon dioxide is liquefied by heat exchange with refrigerants such as ammonia, then sent to storage tanks. Besides being inert, CO<sub>2</sub> is also considered a gas easily operable. Additionally, the existence of pipeline type

infrastructures for gas and oil could be an asset for this type of projects, since the costs of adaptation for the transport of CO<sub>2</sub> would be smaller than the construction of a new transmission line specific for CO<sub>2</sub>. Numerous studies demonstrate that adsorption of CH<sub>4</sub> and other gases in coal are a physical process of monolayer adsorption isotherms and suited to the Langmuir model. "Coal can be treated as a double porosity system, highly complex consisting of micro-pores and macro-pores" (Perera, 2011). The micro-pores are in the matrix while the macro-pores are defined by the natural fractures in the coal that constitute the cleat system.

The fluids move inside the coal bed driven by Fickian diffusion due to the concentration gradient of fluids in the micro porous structure. While accessing the macro-porous structure the flow responds to the pressure gradient and flows according to Darcy's law. The flow in the cleat system, according to Darcy, occurs significantly faster than the flow by Fickian diffusion through the coal matrix cleat system. Intact coal presents low permeability values and the duration of the tests necessary to observe the flow is time-consuming. For this reason naturally fractured samples are selected, in order to analyze the flow rate for pressures close to the critical pressure of CO<sub>2</sub> (7.38 MPa) (Perera, 2011).

Thus, the existing numerical simulators, developed for CBM primary recovery processes, must account for several important characteristics such as:

- (1) A dual porosity system;
- (2) The Darcy flow in the natural fractures system;
- (3) pure gas Diffusion and adsorption in the primary porosity system;
- (4) Coal Contraction (shrinkage) due to desorption.

The process becomes even more complex with the injection of CO<sub>2</sub>. It is necessary to take into account other important characteristics, such as: (1) Expansion of coal due to adsorption. (2) Adsorption of mixed gases. (3) Mixed gases diffusion. (4) Non-isothermal effect for gas injection.

### 3. Pilot/demonstration projects

Overview and data for several demonstration projects around the world, since the nineties to date. Operating mainly in the United States, Canada, Poland, Japan and China.

### 4. CO<sub>2</sub> Sequestration Technologies

It's assumed that Coal reservoirs chosen to be used for storing CO<sub>2</sub> should be left untouched after injection.

Unilateral or multilateral horizontal wells such as those used in the "APP-CO<sub>2</sub> ECBM project" (Figure 2) may be an effective method to increase CO<sub>2</sub> injectivity when compared with conventional vertical wells.

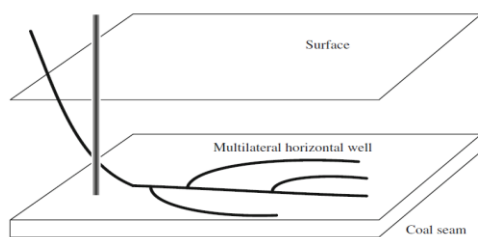


Figure 2 – Depiction of a multilateral completion well for ECBM (source: Pan, 2012; (Li, X., Fang, Z., 2014)

Wells are the major sources of potential CO<sub>2</sub> exhaust problems as they connect reservoir to surface so, special care on cementing operations may be carried out to avoid this unwanted migration. Cement bonds are critical

to seal the borehole from faults or drilling induced cracks through where the migration might occur.

After the extraction of water and methane, the pressures tend to decrease causing a decrease in volume by contraction of the coal mass.

Changes in the tension state with depth, may cause displacements along faults and discontinuities present in the formations or cavities (e.g. caused by rock dissolution) leading to hole instability and hence, damaging the bonds between the well completion and the formation.

As a contingency, techniques as secondary cement jobs are often carried out (i.e. squeeze cement job) obtaining a higher degrees of bonding and sealing off small fractures and cavities around the borehole.

Pilot tests in Canada and Japan showed that injecting a mixture of N<sub>2</sub> with CO<sub>2</sub> increased injectivity and reservoir permeability due to coal contraction (shrinkage) resulting in an increase of micro-fracturation.

#### 4.1 Importance of chemical and physical properties on CCS methodology implementation

Thorough special core analysis (SCAL) is often performed in order to fully characterize the reservoir petrophysical properties both with and without the presence of CO<sub>2</sub>.

Masoudian (2014), while analyzing the effect of CO<sub>2</sub> on mechanical properties of coal, found similarities with the behavior of polymers when added a plasticizer. Polymers show a reduction in mechanical strength when such a compound is present. This transition from a vitrified state to an elastic state, is widely regarded as an explanation for the expansion process with the

adsorption of CO<sub>2</sub> changing its molecular structure (Masoudian et al., 2014).

According to Ian Palmer (2008) coal is a weak rock, with low resistance to shear stresses, which denotes shear ruptures while/after injection. The induced micro-fractures lead to micro-seismic phenomena (i.e. bursts). Laboratory testing showed a permeability increase during the process of rupture, counterbalancing the expandability of the resulting coal CO<sub>2</sub> adsorption, resulting in higher CO<sub>2</sub> injectivities. Other phenomena that influence permeability of coal porous media impacting gas production and injection, are: creation of fine grains and their migration (permeability reduction); and localized coal expansion/dilatancy (permeability increase).

With CO<sub>2</sub> injection, there is a tendency for the coal to swell. At the same time, displaced methane, evicted from the pores and fissures by the injected fluid, will cause coal to shrink due to pressure reduction by desorption. The balance between swelling and shrinkage will depend on the mass balance between the injected and produced fluid. Volumetric variations however, are due to coal compressibility, its thickness and the stress state of the surrounding formations.

#### 4.2 Risks

Risks vary deeply according to the reservoir location. A thorough risk assessment should take into account all geological characteristics, mechanical resistance of the Massif, existence of faults, formation isotropy and radius of influence between wells. Other risks involved in CO<sub>2</sub> underground storage are: Heterogeneity of the Massif as a whole (stratigraphic heterogeneities, existence of discontinuities); Correct injection system that

considers biogeochemical properties (mineral dissolution by microbiological activity, acidification and clay/shale dehydration); Dynamic geomechanical state.

#### 4.3 Future Developments

Expandability of the coal matrix due to CO<sub>2</sub> adsorption will depend on the conditions of the adsorbed phase. Super-critical state of CO<sub>2</sub> doubles coal expansion when compared with the expansion induced by CO<sub>2</sub> in sub-critical state near boundary conditions. The use of N<sub>2</sub> has the potential to reverse some areas of expansion caused by the adsorption of CO<sub>2</sub>. Due to a better developed cleat system, black coal has superior mechanical properties than brown coal. In brown coal, CO<sub>2</sub> adsorption in sub-critical phase, decreases the uniaxial compressive strength and Young's modulus in approximately 10% and 16%, respectively. The reduction of uniaxial compressive strength and Young's modulus, black coal, is 53% and 36%, respectively. (Perera, 2014)

Figure 3 Depicts CO<sub>2</sub> phase diagram (envelope)

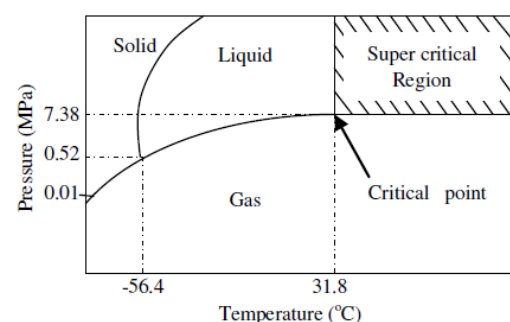


Figura 3. Diagrama de fase para o CO<sub>2</sub> (Perera, 2014)

CO<sub>2</sub> adsorption when in supercritical phase has a much greater influence on the mechanical properties of coal compared with

what happens in the subcritical phase. In this case the uniaxial compressive strength and Young's modulus can achieve a 78% and 71% decrease, respectively. Field scale models predict that the storage capacity increases with the decrease in water content in the reservoir, increased temperature and injection pressure. Although higher injection pressure improve results, these will gradually be reduced by the effect of the expansion of the coal matrix.

The deformation caused in the upper layers are considerable and upwards due to the CO<sub>2</sub> injection pressure and the expansion will depend on the type of gas, pressure and duration of injection. Thus, high pressure injection may return the CO<sub>2</sub> to the atmosphere.

Permeability variation of coal deposits depends on the CO<sub>2</sub> injection conditions, hence the possibility of sudden increases in depth tensions, due to the cumulative effect, which increases the possibility of fractures in the enveloping rock.

There is a clear increase in permeability with a rise in temperature under any type of containment when CO<sub>2</sub> injection pressure is higher than 10MPa. On the contrary, temperature has little influence in permeability when CO<sub>2</sub> injection pressure is lower than 9MPa. Coal's permeability is significantly reduced due to volumetric deformation (expandability) as soon as in the first hour of CO<sub>2</sub> Injection (Perera, 2014).

## 5 Geomechanical Case-study

In order to evaluate the possible implementation of a sequestration project in Portugal, major coal occurrences are described.

This CO<sub>2</sub> injection project focuses on Douro's coal basin as a preferred target.

Germunde was selected from Douro's basin, not only by the knowledge of the area but, mainly, for existence of the largest coal amount that could be used as a preferred means for storing CO<sub>2</sub>.

Since the elastic modulus variation is due to CO<sub>2</sub> adsorption on coal matrix, these can be correlated. It is assumed that the reduction of the modulus will have a Langmuir type curve. It doesn't, necessarily, mean that this is a linear function of adsorption.

The association of computational tools requires the implementation of 3 major relations:

Update of porosity which depends on the mechanical stress (stress and pressures) and adsorption. (The permeability is updated by TOUGH2 through porosity-permeability);

Computation of pressure in gas pores;

Computation of strain induced by adsorption.

The supervisor (python) intermediates computation for CODE\_ASTER® (mechanics) and TOUGH2.

(Loschetter, a. et al., 2012).

## 6 Conclusions

It is necessary to conduct laboratorial tests to assess the elastic modulus, permeability and mechanical resistance variation, from samples collected in the presence of CO<sub>2</sub>, in tri-axial confinement, with gas injection for different pressures and temperatures. For better understanding of samples and subsequent correlation, the following tests should be carried out: Petrographic analysis and isothermal adsorption of CO<sub>2</sub>, by volumetric method. It is necessary to make in-situ trials

with different levels of pressure and flow rates for better monitoring and assessment.

Without "in-situ" testing, given the anisotropy and the swelling/shrinkage phenomena, resulting from injection and temperature, it is not possible to establish the estimation of constants required for modeling (either numerical or analytic). Social, environmental and political interest are key factors for a successful project.

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