Application of petrophysical shale gas model for CO_2 storage capacity assessment of coals

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Abstract. Carbon dioxide storage in unmineable coal seams is a potential solution for the reduction of GHG emissions. For the purpose of storage capacity estimations various static and dynamic models are applied and in this study a simple petrophysical model, originally designed for shale gas reservoirs, has been used. This model comprises of volumetric (free gas) and surface (adsorbed gas) component. Important input data for the model are Langmuir constants and other reservoirs parameters such as water saturation, porosity and rock density. Sorption isotherms on two distinct coals from the Upper Silesia Coal Basin were measured and calculated Langmuir constants with typical reservoir parameters were implemented into the model. It occurred that coal with higher ash content and higher sorption capacity for methane had a lower carbon dioxide sorption capacity. This was reflected in the overall carbon storage capacity which for the two coals varied from 31 m^3/t to approximately 42 m^3/t of coal at the storage pressure of 5.5-6 MPa where the majority of stored gas is the surface component (sorbed gas).

1. Introduction

Regulations on the GHG emissions in European Union are forcing countries where energy mix is based on fossil fuels to implement actions that would either allow for switching into other energy resources or reduce GHG (mainly CO_2) by other means. It occurs that even geothermal energy production contributes to CO_2 emissions reaching $330gCO_2$/kWh in case of Italy as opposed to $940gCO_2$/kWh emitted from coal fired power plants [1]. One of such solutions that could work for both the cases (emissions from fossil power plants and geothermal) is the Carbon Capture and Storage (CCS). In this technology CO_2 is captured in stationary emission source, transported and permanently stored underground in geological traps. This technology is well known and although not widely implemented to date, it has a huge potential and when taking into consideration the dominant role that fossil fuels continue to play in primary energy consumption, the deployment of CCS technologies is becoming increasingly urgent [2]. Concerning Europe, a considerable amount of studies has been conducted about the implementation of CCS in unmineable coal seams, with particular attention to Poland (particularly in the Upper Silesian Basin) where there are still considerable amounts of Coalbed Methane reservoirs. In order to assess CO_2 storage capacity the following parameters have to be taken into consideration:

- Sorption capacity of coal (Langmuir parameters)

- Water saturation of coal
- Coal porosity

In order to assess the dynamic properties of CBM reservoir, other parameters, such as permeability, are needed. Typical static models for the assessment of storage capacity take into consideration absolute sorption capacity and the volume of gas that could be stored in fractures and cleats of coals. In case of coals the vast amount of gas is adsorbed in coal matrix whereas only a minor fraction is the free gas in fractures and macropores.

In this study, we apply a petrophysical static model in order to assess the total storage capacity of coalbed. The model proposed by Ambrose [3] considers not only adsorbed gas measured in adsorption experiment and void volume space of fractures and macropores (porosity) but also subtracts from this sum the volume occupied by the adsorbed phase of gas.

2. Materials and methods

2.1. Materials

In the study two coal samples from the Upper Silesia Coal Basin (USCB) in Poland were used. They represented two types of steam coal i.e. good quality coal with low ash content (Coal A) and low quality coal with high ash content (Coal B). Prior to the start of the experiments the coals were dried and the data refer to the dry basis. Since the coal was acquired from active mine it was difficult to obtain data on water saturation. It was assumed that the coalbed will have two different values of water saturation i.e. 15% and 30% (see table 3), which represent typical values for the USCB. Technical analysis of coals used in the study is shown in table 1.

Table 1. Properties of coal used in the study.

Parameter	Coal A	Coal B
Ash content, %	4.66	11.33
Moisture content (as received), %	0.2	2.1
Moisture content (air dried), %	1.38	7.46
Higher heating value, KJ/kg	33376	22060

2.2. Methods

Typical method for assessing gas storage capacity is to conduct sorption experiment. Hence, a sorption isotherm can be established and, based on that, it is possible to calculate Langmuir parameters. For the purpose of the study a manometric sorption setup was used. Detailed description of experimental procedure can be found in [4]. Experiments were conducted in the following order:

1. Helium expansion – determination of void volume of the setup,
2. Gas evacuation – vacuum for 24 hours,
3. Methane adsorption experiment,
4. Gas evacuation – vacuum for 24 hours,
5. Carbon dioxide adsorption experiment.

Temperature of the experiments was kept constant at 35°C which was similar to in-situ conditions and the maximum pressure was approximately 15 MPa for methane experiment and approximately 10 MPa for carbon dioxide. In case of carbon dioxide experiment, the excess sorption values became negative near the supercritical point which is often observed for microporous adsorbent such as coal.

The numerical model chosen for the assessment of gas-in-place for carbon dioxide is a volumetric method proposed by Ambrose [3]. This model calculates the total gas in-place Gst (i.e. the total storage capacity of coal) in terms of:

- a volumetric component, Gf, which involves gas stored in the pore spaces of the coal matrix as free gas; and
- a surface component, Ga, which accounts for the gas physically adsorbed on large surface areas.

The total gas in-place can be calculated as:

$$Gst = Gf + Ga \qquad (1)$$

All three parameters are expressed in terms of sm³ of CO_2 per tonne of coal. Ga is quantified based on the sorption isotherm measurements and Langmuir isotherm model fitting, while Gf combines those results with physical parameters of the reservoir.

$$Ga = V_L \frac{p}{p+p_L} \qquad (2)$$

Where V_L is the Langmuir volume (sm^3/Mg), p is the equilibrium pressure (MPa) and p_L is the Langmuir pressure (MPa). The free gas component has the following formula:

$$Gf = \frac{32.0368}{Bg}\left[\frac{\varphi(1-Sw)}{\rho b} - \frac{1.318\times10^{-6}M}{\rho s}\left(V_L\frac{p}{p+pL}\right)\right] \qquad (3)$$

Where B_g is the gas formation volume factor (-), φ is the porosity of the rock (%), Sw is the water saturation (-), ρb is the bulk rock density (g/cm^3); M is the molar mass and ρs is the sorbed phase density (g/cm^3).

3. Results and discussion

In figure 1 results of excess sorption measurements (with Langmuir models fitted) of methane are shown. Figure 2 shows results of carbon dioxide excess adsorption and fitted Langmuir model. In table 2 a summary of the Langmuir parameters calculated for the coal samples is given.
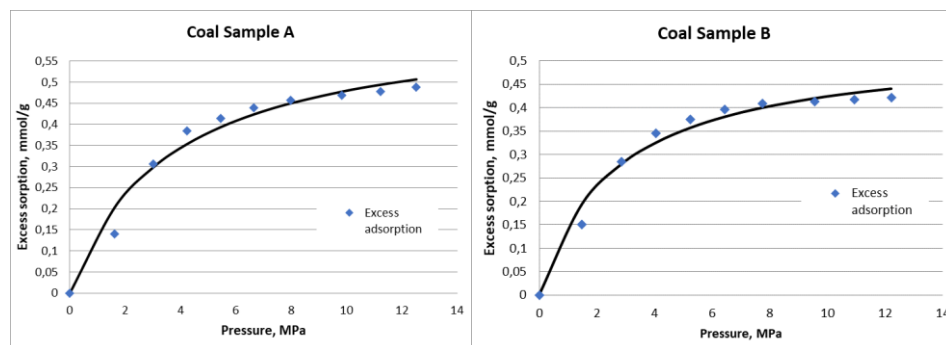

Figure 1. Results of methane adsorption on coal A and B. Black line represents Langmuir model fitting.
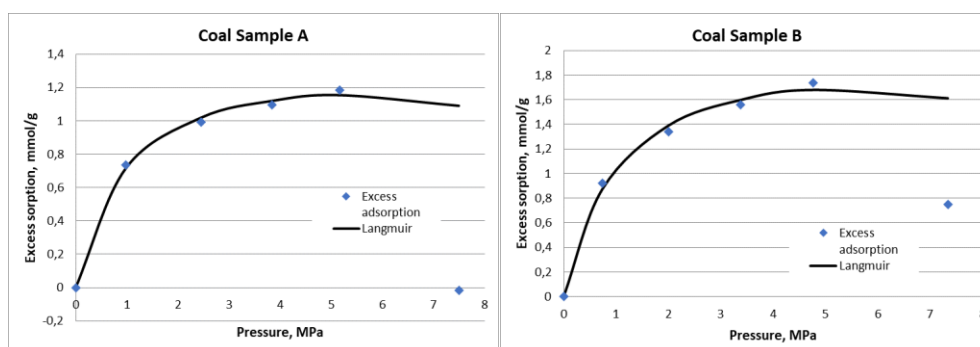

Figure 2. Results of carbon dioxide adsorption on coal A and B. Black line represents Langmuir model fitting.

Table 2. Langmuir parameters calculated for the coal samples.

	Coal sample	Langmuir Volume (sm³/t)	Langmuir Pressure (MPa)
CH_4	A	14.56	3.57
	B	11.95	2.61
CO_2	A	33.46	1.04
	B	50.24	1.13

Sorption isotherms show that in case of methane sorption capacity is higher for sample A, which can be explained by lower ash and moisture content. For carbon dioxide this is not evident and the maximum sorption capacity of sample B is higher. It can be explained by a slightly higher moisture content since the solubility of CO_2 in water is much higher than of methane. Observation of sorption isotherms is proved by the calculated Langmuir parameters.

The total gas in-place (i.e. the maximum quantity of gas that can be stored in the coal) or CO_2 storage capacity is strictly related to the pressure and temperature of the gas at the moment of injection: for this matter, different injection pressures characteristics of CO_2 storage in coalbed were considered, but the temperature was assumed constant and equal to the one at which the sorption experiments were performed. For the calculation of the total gas-in-place the following parameters, shown in table 3 were used.

Table 3. Parameters used for the calculation of CO_2 storage capacity in coals.

Parameter	Coal A	Coal B
Porosity (ϕ, %	10	10
Water saturation (S_w), %	15	30
ρb g/cm^3	1.38	1.52
ρs, g/cm^3	0.706	
$\dot M$, g/mol	16.04	
V_L, sm^3/t	33.46	50.24
p_L, MPa	3.57	2.61

In table 4 results of the total CO_2 storage capacity for two coals used in the study are shown. The assessment was done for two ranges of pressures. Both ranges are considerably low in terms of recommended storage conditions (above 700 m) but could be considered valid for shallow unmineable coalbeds.

Table 4. CO_2 storage capacity results for selected coals.

Storage pressure	5.5-6 MPa		3.5-4 MPa	
	Coal A	Coal B	Coal A	Coal B
Gf, sm³/t	2,49	0,11	1,44	0,2
Ga, sm³/t	28,49	42,24	26,52	39,12
% Gf	8,0%	0,3%	5,1%	0,5%
% Ga	92,0%	99,7%	94,9%	99,5%
Gst, sm³/t	30,97	42,34	27,96	39,32

As could be expected, in both coals a higher amount of CO_2 can be stored with a higher pressure of injection/storage. Coal B accounts for a higher storage capacity at each pressure level compared to coal A, due to the lower adsorption of carbon dioxide in this last type of coal: the difference is

considerably high, with the coal B which can store on average 10 sm³/t more than coal A per each pressure range.

Another interesting insight of the results is the breakdown of the total gas in-place value into the volumetric (Gf) and surface components (Ga). The ratio of the first one, which is related to the free gas stored in the pores of the coal, is higher under the same pressure conditions in coal A than in coal B, due to the lower water saturation of the first type of coal. It can also be noticed that the volumetric component tends to increase in coal A with increasing of the pressure, while in coal B it tends to decrease: the reason of these different behaviours is that coal B, adsorbing more CO_2, has a higher increase of the surface component (which is related to the gas physically adsorbed in the coal) with the increase of the pressure than coal A. This proves that in coals a significant part of gas is stored in adsorbed phase rather than in macropores, cleats or fractures. Even considerably higher water saturation of Coal B did not contribute significantly to the lowering of storage capacity. In figure 3 a graphical comparison of results shown in Table 4 is presented. It is evident that volumetric component (Gf) does not have a significant contribution to the overall storage capacity.
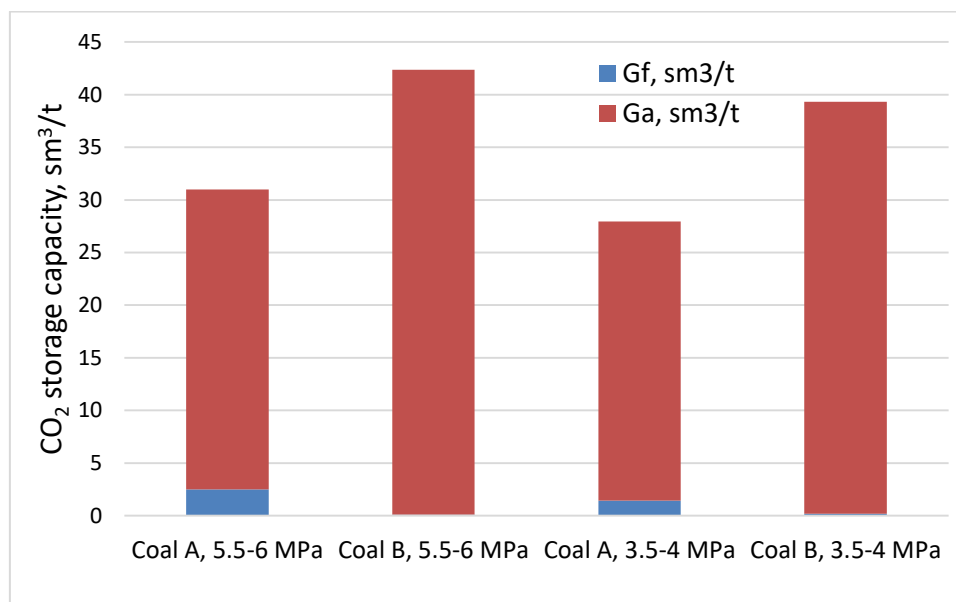

Figure 3. Graphical comparison of calculated CO_2 storage capacity of coals.

In general, the total potential storage capacity can be considered as rather high, reaching over 40 sm³/t of coal at the pressure of 6 MPa. This high amount results from the method of sorption measurement, which considers ideal conditions and full coal saturation with gas. In practice it is unlikely to achieve such conditions hence obtained data should be treated with caution. The results calculated with the Ambrose model can be used to assess the storage capacity of the reservoir in terms of total sm³ of CO_2 that can be stored. This can be recalculated by multiplying the storage capacity from Ambrose by the density and volume of the coal seam [5]. As density value, the bulk rock density can be considered, while the volume of the reservoir can be assessed by multiplying the area of its surface by its thickness. The area and thickness of the reservoirs were assumed in accordance with typical values for coal seams and assumed equal for both type of coal. In table 5 reservoir parameters and storage capacity expressed in terms of sm³ and tonne of CO_2 are shown.

Results show that a maximum of about 2.5 Gsm³ of CO_2 can be stored in reservoir of coal B at 5.5-6 MPa, while a maximum of about 1.7 Gsm³ of CO_2 can be stored at the same pressure in a coalbed composed by the coal A.

Table 5. Reservoir parameters and storage capacity expressed in terms of sm³ and tonne of CO_2.

	5.5-6 MPa		3.5-4 MPa	
	Coal A	Coal B	Coal A	Coal B
Area, m²	4000000			
Thickness, m	10			
ρb t/m^3	1.38	1.52	1.38	1.52
Gst, sm³	1 709 782 733	2 574 517 421	1 543 128 914	2 390 574 710
ρs t/m^3	1.936			
Gst, t	3 310 891 676	4 985 398 515	2 988 176 554	4 629 204 491

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By multiplying those results by the adsorbed phase density, it is possible to convert the results in terms of tonne of CO_2 stored. Hence, in coal A reservoir a maximum of 3.3 Gt of CO_2 can be stored at 5.5-6 MPa, while in a coal B reservoir under the same pressure conditions approximately 4.9 Gt of CO_2 can be stored.

4. Conclusions
The intention of this study was to perform a simple carbon dioxide storage capacity assessment based on the petrophyscial model designed primarily for shale gas reservoirs. The following conclusions can be drawn based on the obtained results:

- Sorption isotherms show that, as expected, carbon dioxide sorption capacity is higher than for methane; however for the Coal B of lower quality the maximum CO_2 sorption capacity was higher than for coal A,
- In general, the calculated CO_2 storage potential is relatively high and it seems that the model is overestimating the storage potential,
- In order to obtain more credible results it is necessary to conduct additional analysis of coalbed reservoir parameters such as water saturation and, above all, the porosity.

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