CO$_2$ adsorption the numerical simulations and the controlling factors to low rank coal

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Abstract. Carbon Capture Sequestration (CCS) in unmineable coal seams questionably gives benefits for the commercial success through potential release of additional methane during the injection of CO$_2$ adsorbs into the coal seams, the process known as enhanced coalbed methane (ECBM) recovery. However, a significant concern lies in the loss of injectivity due to reduction in permeability by coal matrix swelling occurrences with CO$_2$ adsorption although this effect can be partially be offset with ‘huff and puff’ scheme of cyclic CO$_2$ injection followed by extraction of the released methane. The paper discusses the results of a numerical simulation study carried out with GEM compositional reservoir simulator to evaluate the effects of uncertainties in various reservoir parameters on the overall volume of CO$_2$ storage and additional methane recovery of low rank coalfield. A 12-15m thick seam at shallow depth, 50-75 m was considered for fluid flow simulation study. While some information on the reservoir setting was obtained through literature and personal communication with the CBM operators, the rest of the information was derived through laboratory studies. The reservoir parameters considered for the study are injection pressure, adsorption capacity, cleat permeability and porosity, and initial gas saturation. A 100-acre drainage area with 5-spot vertical well pattern was considered with one central injector and four producers on four corners of the study area. The maximum allowable injection pressure was estimated to be 7500 kPa at the reservoir setting. The injection pressure was varied from 1000 kPa to 7500 kPa in the simulation. A number of adsorption isotherms were established in the laboratory. The variations in the adsorption parameters observed through the isotherms were considered as uncertainty in the storage capacities. Significant variations were observed due to the variation in adsorption isotherms both for CO$_2$ storage and additional methane recovery. Fracture permeability was varied from 3 md to 200 md, which is the range of permeability observed in the coalfield is around 100-200 mD. The results of simulation indicate a strong influence of porosity on the CO$_2$ storage and ECBM recovery. Fluid flow simulation study shows that variation in sorption time has no significant effect for a low permeability situation while some marginal effect in high permeability situation. Cleat porosity was varied from 1 % to 10 %. Within this range of porosities, enhanced methane recovery varied from 1 % to 10 % relative to the primary recovery but the volume of stored CO$_2$ did not vary significantly. Lastly, the pore pressure, adsorption and gas saturation of CO$_2$ sequestered volume and additional methane recovery were found to increase substantially.

Keyword: Carbon Dioxide, Coalbed Methane, Enhanced Coalbed Methane, Carbon Capture Sequestration, Permeability, Porosity
1. Introduction
During the primary CBM production and ECBM through CO₂ injection, a series of complex physical and mechanical phenomena occur. The ability to represent the behavior of a coalbed reservoir as accurate as possible by computer simulations yields insight into the processes taking place and is an indispensable tool for the decision process of future operations. More specifically, the economic viability of projects can be assessed by predicting production: well performance can be maximized, drilling patterns can be optimized and, most importantly, associated risks with operations can be accounted for and possibly avoided.

However, developing representative computer models, simulating reservoir production and injection regimes are such a challenging process. A large number of input parameters are required, many of which data are uncertain even if they are determined experimentally or via in-situ measurements. Such parameters include, but are not limited to, seam geometry, formation properties, production constraints, etc.

Modelling of production and injection in multi-seam formations for hydraulically fractured wells is a recent development in coalbed methane/enhanced coalbed methane (CBM/ECBM) reservoir modeling, where models become even more complex and demanding. In such cases, model simulations are times become important.

The development of accurate simulation models that correctly account for the behavior of coalbeds in primary and enhanced production is a process that requires attention to detail, data validation, and model verification. A number of simplifying assumptions are necessary to run these models, where the user should be able to balance accuracy with computational time.

In this paper, a few analysis initiated by the pre- CO₂ injection simulation for A2 coalbed reservoir (as a preference coalbed) is carried out following by the reservoir base case model, and lastly charted by the preliminary reservoir parameters input from the previous experiment result. Each of assumption parameters which expected to be the controlling factors on the adsorption capacity will be validated in the sensitivity analysis. Then, numerical simulation with laboratory condition is combined as to minimize the uncertainties of the multiscale CBM/ECBM parameters in relation with CO₂ adsorption coupling factors.

2. Numerical Simulation of CO₂ Injection for Basecase Reservoir Model
The single-well analytical model (Figure 1) is designed specifically for CO₂ injection in coalbed reservoirs. This numerical simulation model is processed by using simple Darcy flow and gas adsorption input, as mechanisms to characterize the behavior of coalbed methane reservoirs. Due to limitation of subsurface data such as gas composition analysis, gas content analysis and methane (CH₄) adsorption isotherm analysis. Single phase of CO₂ gas component is used to forecast the capacity of CO₂ adsorption.

![Figure 1. Base case reservoir model with single injector well.](image-url)
The coalbed model with 100 acres in area with pay thickness of 10 m is regulated at the shallow layer of 150 m. The base case option is based on constant 1000 m³/day of CO₂ injection volume assumption. The injection forecast is performed for 32 years period (year 2018 -2050). The input parameters used in the base case simulation is tabulated in Table 1. Listed parameters is obtained from the previous experimental test and assumption value. Every parameters will be reprocessed by ‘try and errors’ methods during the sensitivity analysis.

### Table 1. Base case input parameters.

| Parameter                          | Value | Unit |
|------------------------------------|-------|------|
| Area, A                           | 100   | Acres|
| Thickness, H                      | 10    | m    |
| Top of Reservoir, h               | 150   | m    |
| Coal Density, pb                  | 1435  | kg/m³|
| Clean Spacing, i                  | 1     | cm   |
| Initial Water Saturation, Swi     | 1     | %    |
| Reservoir Pressure, P_i           | 5000  | Kpa  |
| Reservoir Temperature, T_res       | 35    | degC |
| Coal Compressibility, B           | 1.476-07 | 1/KPa |
| Young Modulus, E                  | 1704  | Kpa  |
| CO₂ Langmuir volume constant, V_L | 1297  | scf/ton |
| CO₂ Langmuir Pressure constant, P_L | 4180 | Kpa |
| Matrix Porosity, φ_matrix         | 5     | %    |
| Fracture Porosity, φ_fracture      | 6.7   | %    |
| Matrix Permeability / direction, K_matrix | 10   | mD   |
| Matrix Permeability X direction, K_matrix | 10   | mD   |
| Fracture Permeability / direction, K_fracture | 100  | mD   |
| Fracture Permeability X direction, K_fracture | 100  | mD   |
| End-point relative permeability of water, k_w | 1 |   |
| End-point relative permeability of gas, k_g | 1  |   |

*Note: *¹ = Uncertainty parameters for sensitivity analysis

2.1. Base case scenarios

Referring to Figure 1, the base case of the square reservoir model demonstrates that both; the pore pressure and CO₂ adsorption volume of the models have increased affectedly to the 32 years of gas injection (refer to Figure 2). With the starting of the low initial reservoir pressure condition (P_i = 1000 Kpa), pore pressure at injection wellbore has noticed is increased very slightly starting from 1000 to 1407 Kpa the. However, pore pressure at initial reservoir pressure (P_i = 5000 Kpa) has increased gradually starting from 5000 Kpa to 6272 Kpa respectively, and pore pressure at initial reservoir pressure (P_i = 7500 Kpa) increased affectedly starting from 7500 Kpa to 9579 Kpa respectively (refer to Figure 8.4).

![Figure 2. Pore pressure increase during CO2 injection.](image)
CO₂ adsorption volume at injection wellbore has increased starting from 665 to 733 scf/ton at initial reservoir pressure (Pᵢ = 5000 kPa). Meanwhile, CO₂ adsorption volume at low initial reservoir pressure condition (Pᵢ = 1000 kPa) has also increased more significant starting from 229 to 299.5 scf/ton respectively.

Figure 3 shows the CO₂ adsorption isotherm capacity based on the laboratory experimental test has almost closely with the CO₂ adsorption capacity based on base case simulation result at pore pressure range from 0 kPa to 6000 kPa approximately. This imply that several parameters input obtained from Table 1 is acceptable. However, CO₂ adsorption isotherm curve from both measurement shows the difference at pore pressure range from 6000 kPa to 10,000 kPa. The difference of these adsorption isotherm curve may influence by controlled parameter input due to uncertainty of sorption kinetic parameters.

Several sensitivity analysis in the sub chapters below is performed to explain the uncertainties of sorption kinetic parameters that govern (controlling factors) to the CO₂ adsorption isotherm capacity between laboratory experiment test and numerical simulation result.

2.2. Sensitivity Analysis for Cleat Permeability

Cleat permeability values are varied in four values which are 3 mD, 50 mD, 100 mD and 200 mD. Figure 4 shows that cleat permeability values of 3 mD (too small) has the lowest CO₂ adsorption capacity while 50 mD, 100 mD and 200 mD lies on the same line which upheld that cleat permeability has no significant influencing the adsorption capacity.
2.3. Sensitivity Analysis for Matrix Permeability
Four matrix permeability values (1 mD, 5 mD, 25 mD and 50 mD) have been varied for the numerical runs. The numerical result in Figure 5 showed that matrix permeability that does not affect the CO$_2$ adsorption capacity. As said by Zhao et. al. [1] the flow of gas in the coal matrix is depending on non-Darcy flow that has significant influences by Klinkenberg effect and diffusion.

![Figure 4](image4.png)

**Figure 4.** CO$_2$ adsorption capacity for various of cleat permeability values.

![Figure 5](image5.png)

**Figure 5.** CO$_2$ adsorption capacity with different matrix permeability value.

2.4. Sensitivity Analysis for Cleat Porosity
1 %, 5 % and 10 % of cleat porosity are selected for numerical runs. The numerical result displayed in Figure 6 describes that there is no significant stimulously on the adsorption at early stage of injection, but it noticeably diverge starting at 5500 kPa until to the last stage of injection period. With the increasing of the pore pressure value, the highest cleat porosity shows the highest adsorption capacity, to prove that cleat porosity is one of the governing behaviour for adsorption capacity.
2.5. Sensitivity Analysis for Matrix Porosity
Conversely, coal with lowest matrix porosity value (matrix pore = 1%) have a largest excess swelling volume rather than other coal with highest matrix porosity (matrix pore = 10 %). Figure 7 illustrates that the coal with matrix porosity 10 % has the lowest CO\textsubscript{2} adsorption capacity rather than other values 1 % and 5 % respectively. Figure 7 shows that matrix porosity gives large impact in affecting the adsorption capacity.

![Figure 6. CO\textsubscript{2} adsorption capacity at different cleat porosity value.](image)

![Figure 7. CO\textsubscript{2} adsorption capacity with variations of matrix porosity value.](image)

2.6. Sensitivity Analysis for Initial Water Saturation
Just like other sensitivity parameters, initial water saturation parameter is also performed at initial reservoir pressure of 5000 kPa. This initial water saturation describe the initial water filled into cleat/fracture and micropore. Three initial water saturation value (25 %, 50 % and 100 %) have been selected for numerical runs. The numerical result displayed in Figure 8 characterise that the coal with initial water saturation 100 % has the highest CO\textsubscript{2} adsorption capacity rather than other values. Interaction and exchange of the CO\textsubscript{2} molecule with H\textsubscript{2}O molecule in the pore structure area (cleat)
may control this phenomena. The mechanism by which CO₂ and water interact in coal remain uncertain and these are key questions for understanding ECBM processes and defining the long-term behaviour of CO₂ injection.

According to Sun et al. [2], micro-capillary of water molecule gradually decreased while macro-capillary and bulk water increased with time after the injection of CO₂. They assume that the CO₂ molecules diffuse through and/or dissolve into the capillary water to access the coal matrix interior, which promotes desorption of some water molecules from the surface of the coal micropores and mesopores. Thus, the adsorbed water in coals can be replaced by CO₂.

Figure 8 shows that the difference of initial water saturation in cleat/ fracture has significantly influenced the adsorption capacity.

![Figure 8. CO₂ adsorption capacity at different initial water saturation.](image)

2.7. Sensitivity Analysis for Cleat Spacing

Figure 9 illustrates that there is no significance between the variance value of 1 cm, 3 cm and 5 cm of cleat spacing and CO₂ adsorption capacity.

![Figure 9. CO₂ adsorption capacity at different cleat spacing value.](image)
2.8. Sensitivity Analysis for Well Spacing
In this sensitivity analysis study, five spots of injector well scenarios are set to perform the dynamic of sorption kinetic parameters based on well spacing design. Figure 10 shows different model of numerical simulation settings. Reservoir block with 100 acres drainage area and 500 meter well spacing has applied in the first model. While reservoir block with 500 acres drainage area and 1000 meter well spacing has applied in the second model. Both of these model has treated by injecting 200 m³/day of CO₂ gas into each injector wellbore during 32 years.

![Figure 10](image_url)

**Figure 10.** Two option of reservoir block model with 500 meter well spacing (left) and 1000 meter well spacing (right).

The difference between the well spacing scenarios have significant impact in changes of pore pressure buildup, CO₂ adsorption capacity and gas saturation. Figure 10 illustrate the evolution of pore pressure grid, CO₂ adsorption capacity grid and gas saturation in cleat by using both well spacing scenario.
Well spacing 500 meter

Well spacing 1000 meter

**Figure 11.** 3D grid evolution after CO2 injection. (a) Pore pressure evolution 100 acres drainage area (left) and 500 acres drainage area (right) (b) CO2 adsorption evolution 100 acres drainage area (left) and 500 acres drainage area (right) (c) Gas saturation evolution 100 acres drainage area (left) and 500 acres drainage area (right).
The numerical result displayed in Figure 12 describe the reservoir with 500 meter well spacing that has a significant increment in pore pressure buildup and CO$_2$ adsorption capacity rather than reservoir with well spacing 1000 meter. Meanwhile, reservoir with well spacing 500 meter also have a rapid increment in gas saturation that filled in cleat / fracture due to smallest drainage area.

![Figure 12](image)

**Figure 12.** (a) Sensitivity pore pressure at different well spacing (b) Sensitivity CO$_2$ adsorption capacity at different well spacing (c) Sensitivity gas saturation at different well spacing.

2.9. Sensitivity Analysis for Coal Density

The numerical simulation of CO$_2$ adsorption capacity are divided into two different part. The part one perform the different of CO$_2$ adsorption capacity based on different coal density. In this study, three coal density scenario (1.2 gr/cc, 1.300 gr/cc and 1.435 gr/cc ) is selected for the numerical runs. In total there are 18 runs were conducted following by the different initial reservoir pressure (1000 kPa, 5000 kPa and 7500 kPa).

The numerical result displayed in Figure 13 describes that coal with density 1.200 gr/cc have a highest CO$_2$ adsorption capacity rather than other higher density. However, coal density parameter is not significantly influence to the CO$_2$ adsorption capacity at low injection pressure. CO$_2$ adsorption capacity of coal density 1.435 gr/cc related closely with CO$_2$ adsorption isotherm based experimental test at pore pressure range from 0 kPa to 5000 kPa.
In order to compare the capacity of CO$_2$ adsorption based on simulation results with the experimental data, the images is used for coal A2 sample to re-construct the core for numerical testings (Figure 14). The virtual core representing the sample is cylindrical with a diameter of 6 cm and a length of 13 cm. The initial porosity and permeability of fracture system are calculated from CT image as shown also in Fig. 5.4. Because this is a couple parameter between the coal deformation and gas flow, boundary and initial conditions are required for each component model. Initial properties such as initial pressure and temperature was set in the laboratory condition (1 atm, 25°C).

A several scenarios (Table 2) is varied purposely to extend the CO$_2$ adsorption isotherm curve in different pore pressure condition. In different way, to perform additional sensitivity analysis it is compulsory to try to ensure this coupling factors that controlled CO$_2$ adsorption capacity in laboratory measurement.

**Figure 13.** CO$_2$ adsorption sensitivity based on different coal density input.

**Figure 14.** Core dimension drawing for numerical testing.
Based on the case scenarios, 0.005 m³/d amount of CO₂ is injected during 10 days. The evolution of core sample during CO₂ saturated illustrated in Figure 15.

Another controlling factor to be considered in the CO₂ adsorption capacity is the coal matrix moisture. So three coal matrix moisture scenario (0 % moisture, 50 % moisture and 94 % moisture) have been selected for the numerical runs. In total of 18 runs were conducted with following different pore pressure case as shown in Table 2.

The numerical result displayed in Figure 15 describe that coal with 0 % moisture (dried treatment) has the highest CO₂ adsorption capacity rather than other values. However, the moist sensitivity simulation to the experimental CO₂ adsorption isotherm is illustrated below.

Shear dilation may affect directly in CO₂ adsorption capacity for Coal A2 sample. It can be observed with high slope increment area (Figure 16). Shear dilation regime occurred at pore pressure ranging from
5000-6000 kPa. Shear dilation may create a new pore network pathway, allow isolated matrix pore re-opening, and causing expanding in diffusion capacity, which explained below (Figure 17).

Cuss et al.,[3] studies clearly explained that as gases started to move, the core sample underwent mechanical dilation. Under in situ conditions, the onset of dilation (micro-fissuring) is a necessary precursor for the advection/diffusion movement of gas. Gas propagation occurred along shear dilation pathways and exploit the pore network of the material. While dilation continues, indicating that gas pathways have increased.

![Figure 17. Model of main processes of gas movement in sediment rock during injection (modified after Marschall et al. [4]).](image)

4. Conclusion
Maximum swelling zone is difficult to interpret by numerical CMG simulation, because ideally, entire decrement of permeability has interpreted as swelling regime. However, by using alternative method by calculating new adsorption isotherm using acoustic derived time, CO₂ saturated sample and its’ swelling capacity of each samples can be compared. Further, the maximum swelling zone can be described. Unfortunately, numerical simulation such as CMG simulator is not powerful for this issue. Moreover, the result of sensitivity analysis by using both base case reservoir model and core dimension model shows that coal density is the most significant parameter that controlling CO₂ adsorption capacity, successively followed by drainage area, initial water saturation, matrix porosity, cleat permeability and cleat porosity. Meanwhile, matrix permeability and cleat spacing has evidently not influencing the CO₂ adsorption capacity.

Dramatically increment of CO₂ adsorption capacity refer to comparation both of laboratory experiment and numerical simulation result has an advantage to perform the shear dilation regime. Also, other method such as AE test and static model are not recommended for shear dilation mapping purpose.

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