DEVELOPMENT OF A 3D MODEL TO STUDY THE CO\textsubscript{2} SEQUESTRATION PROCESS IN DEEP UNMINEABLE COAL SEAMS.

M.S.A. Perera\textsuperscript{1}, P.G. Ranjith\textsuperscript{1}, S.K. Choi\textsuperscript{2}, D. Airey\textsuperscript{3}, A. Bouazza\textsuperscript{1} and J. Kodikara\textsuperscript{1}

\textsuperscript{1}Department of Civil Engineering, Monash University, Building 60, Melbourne, Victoria, 3800, Australia.

\textsuperscript{2}Australian Commonwealth Scientific and Research Organization (CSIRO), Locked Bag 10, Clayton South VIC 3169, Australia.

\textsuperscript{3} School of Civil Engineering, University of Sydney, Sydney NSW 2006, Australia.

Abstract
This paper presents a numerical model to study the carbon dioxide (CO\textsubscript{2}) sequestration process in deep coal seams and to investigate the factors that affect this process. A coal seam lying 1000 m below the ground surface was considered for the simulation. One injecting well was first inserted at the middle of the area under consideration and CO\textsubscript{2} was injected for a 10 year period. With one injection well, the storage capacity was calculated as $13 \times 10^7 \text{ m}^3$. The number of injecting wells was then increased to 4. It was found that the maximum storage capacity was observed at two well condition (an increment of 130\% of the single well condition). However, further increasing the number of wells (up to 4) reduced the storage capacity to $12.5 \times 10^7 \text{ m}^3$.

According to the model results, it is clear that CO\textsubscript{2} storage capacity in deep unmineable coal seams is dependent on the number of injecting wells and their location and porosity, the permeability of the coal seams, coal bed moisture content and temperature.

Keywords: Storage capacity, CO\textsubscript{2} sequestration, wells, moisture content, temperature, numerical modeling

1. Introduction
The world is currently facing the problem of global warming, the main cause of which has been identified as the release of green house gases such as carbon dioxide (CO\textsubscript{2}) into the atmosphere. CO\textsubscript{2} sequestration in deep coal seams has been recognised as a potential method of atmospheric CO\textsubscript{2} mitigation. In addition, it could produce large amounts of value-added energy products such as methane (CH\textsubscript{4}) as an outcome. According to Stevens et al.(2000), the coal mass can store a substantial amount of gases due to its large surface area and highly porous structure. For instance, it has been estimated that the combined Bowen and Sydney basins in eastern Australia can store 11.2 Gt of CO\textsubscript{2} (White et al. 2005).

Coal mass can be defined as a naturally-fractured reservoir for gas movement. The movement of gases through this highly complex coal mass structure depends on the permeability of the coal mass itself, which may be governed by Darcian Law/or non-linear laminar flow and the intrinsic permeability of the coal matrix, which is governed by Fickian FICKIAN\% diffusion. Therefore, the amount of CO\textsubscript{2} that can be stored in the coal mass is highly dependent on coal’s physical and chemical properties, the arrangement of injecting wells and their number. However, the process of CO\textsubscript{2} sequestration in deep coal seams remains in the experimental stage as many aspects need to be studied before it can be put into practice. Following a detailed review of the available studies related to CO\textsubscript{2} sequestration, White et al. (2005, p.? ) explain that “there is a fundamental lack of understanding concerning the physical, chemical and thermodynamic phenomena that occur when CO\textsubscript{2} is injected into a coal seam.”

Normally coal mass has "dual" porosities. It has inter-aggregate fractures (secondary porosity system) and intra-aggregate pores (primary porosity system). The interaction of these porosities can be complex and renders simple models inaccurate (Coll et al. 1994). Experimental and numerical modelling studies can help to provide a better understanding of the flow phenomenon in coal. To date, many field-scale models have been developed for flow in porous rock masses using different
computer codes, such as TOUGH 2 (Carneiro, 2009), COMSOL (Liu and Smirnov, 2009; Perera et al., 2010(a)) FEMLAB (Holzbecher, 2005) and COMET 3 (Pekot and Reeves, 2002; Perera et al., 2010(b)) which can be used to simulate gas and water flow in coal.

The main objective of this study is to develop a 3-D numerical model using COMET3 to simulate the CO$_2$ sequestration process in a deep unmineable coal seam. COMET 3 is a conventional and coal bed methane reservoir simulator, which can simulate single or two phase flow through single, dual or triple porosity reservoirs, such as coal or shale as well as conventional reservoirs (Pekot and Reeves, 2002).

1.1 Governing Equations Used in the Model

In COMET 3, fluid flow in the rock mass is modelled by using the mass conservation equations for water and gas as given in Eq.[1] and[2], respectively (Sawyer et al. 1990).

$$\nabla \left[ b_n M \left( \nabla p_n + \gamma_n \nabla Z \right) + R_{sw} b_w M_w \left( \nabla p_w + \gamma_w \nabla Z \right) \right]_f + q_m + q_g = \left( \frac{d}{dt} \right) \left( \phi_r S_n + R_{sw} \phi_{w, w} \right)_f$$

$$\nabla \left[ b_w M_w \left( \nabla p_w + \gamma_w \nabla Z \right) \right]_f + q_w = \left( \frac{d}{dt} \right) \left( \phi b_w S_w \right)_f$$

where $b_n$ (n=g or w) is the gas or water bulking factor, $\gamma_n$ (n=g or w) is the gas or water gradient, $R_{sw}$ is the gas solubility in water, $\phi$ is the fracture porosity, $Z$ is the elevation $q_g$ is the gas flow rate, $q_w$ is the water flow rate, $q_m$ is the matrix gas flow rate, $M_n$ (n=g (gas) or w(water)) = $k_n/\mu_n$, is the phase mobility, ($k$-permeability, $k_m$-matrix permeability, $\mu$ -phase viscosity). $S_n$ (n=g or w) is the gas or water saturation, and $P_n$ (n=g or w) is the gas or water pressure. Gas adsorption is calculated using the extended Langmuir model.

$$C_i \left( P_i \right) = \frac{V_{Li} P_i}{P_{Li} \left[ 1 + \sum_{j=1}^{3} \left( \frac{P}{P_L} \right)_j \right]}, \ i = 1, 2$$

where, $V_{Li}$ is the Langmuir volume, $P_{Li}$ is the Langmuir Pressure, $P_i$ is the partial pressure of the gas component, $C_i(P_i)$ is the adsorbed gas concentration at $P_i$, and $P$ is the total pressure. Gas flow through the matrix is modelled using Fick’s law of diffusion.

$$q_{mi} = \left( V_m / \tau_i \right) \left[ C_i - C_i \left( P_i \right) \right], \ i = 1, 2$$

where, $q_{mi}$ is the gas component flow, $V_m$ is the bulk volume of the matrix element, $\tau$ is the sorption time, and $C_i$ is the average matrix gas concentration of gas component $i$. Permeability is determined by the ARI (Advanced Resources International) model.

$$\phi = \phi_i \left[ 1 + c_p \left( P - P_i \right) \right] - c_m \left( 1 - \phi_i \right) \left( \frac{\Delta P_i}{\Delta C_i} \right) \left( C - C_i \right)$$
where, $c_p$ is the pore volume compressibility, $c_m$ is the matrix shrinkage compressibility, $\phi$ is the coal mass porosity, $\phi_i$ is the initial coal mass porosity, $P$ is the reservoir pressure, $P_i$ is the initial reservoir pressure, $C$ is the reservoir concentration, $C_i$ is the initial reservoir concentration, $P$ is the reservoir permeability, and $P_i$ is the initial reservoir permeability.

### 2. Model Development

For the purpose of modeling, a 540m×500m×20 m size coal seam, lying 1000 m below the ground surface, was considered. The location of the coal layer is shown in Fig. 1. CO$_2$ was injected at 14 MPa for 10 years from the bottom of the well as shown in the figure.

![Figure 1. Location of the coal layer.](image)

The model parameters used are shown in Table 1 (Balan and Gumrah 2009).

<table>
<thead>
<tr>
<th>Model Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal seam moisture content</td>
<td>0.5 (cm$^3$/cm$^3$)</td>
</tr>
<tr>
<td>Coal seam initial permeability</td>
<td>20 md</td>
</tr>
<tr>
<td>Coal seam porosity</td>
<td>0.1</td>
</tr>
<tr>
<td>Pore volume compressibility</td>
<td>6.9e$^{-3}$ (1/kPa)</td>
</tr>
<tr>
<td>Matrix shrinkage compressibility</td>
<td>6.9e$^{-7}$ (1/kPa)</td>
</tr>
<tr>
<td>Exponent of pressure dependent</td>
<td>3</td>
</tr>
<tr>
<td>Relative permeability variation</td>
<td>Cooray formula (Akin 2001), residual water and gas contents are 0.05 and 0.01 (cm$^3$/cm$^3$)</td>
</tr>
<tr>
<td>Temperature</td>
<td>30 °C</td>
</tr>
<tr>
<td>Langmuir volume for CO$_2$ adsorption</td>
<td>16 (m$^3$/m$^3$)</td>
</tr>
<tr>
<td>Langmuir pressure for CO$_2$ adsorption</td>
<td>1.56 MPa</td>
</tr>
</tbody>
</table>
After developing the model, the effect of mesh size on storage capacity was examined by changing the width of the smallest grid block from 2 m to 14 m at 2 m intervals. The obtained CO2 storage capacity for 10 years and for 14 MPa gas injecting pressure is shown in Fig.2. According to the figure, when the grid width reduces from 14 m to 10 m, corresponding gas CO2 storage capacity increases from 1.108 m3 to 1.32×108 m3 and thereafter reduction of grid size does not change the storage. This is due to the fact that, when analysing the gas flow rate through a coal layer and it is a function of pressure gradient calculated using the mesh size, resulting a mesh size dependant outcome. This problem can be minimised by selecting smaller grid size, which gives more consistent results. However, a reduction of grid size causes an increase in the time required for the calculation (Nam et al. 2008). Therefore, the selection of optimum mesh size is important in any kind of finite element analysis. Considering all these factors, the size of the smallest grid block was taken as 10 m for the model. The final grid system selected for the coal layer is shown in Fig.2 (b).

![Figure 2](image)

**Figure 2. (a) Effects of grid size on storage, and (b) selected model grid blocks for the coal seam.**

### 3. Model Simulation

After developing the model, the CO2 migration rate along the horizontal distance was investigated for the bottom coal layer (Fig.3).

![Figure 3](image)

**Figure 3. Variation of CO2 migration percentage with time.**

According to the above figure, after the first year CO2 has spread through only around 65% of the coal layer and by the eighth year CO2 has spread through the whole coal layer. It can also be seen that at the beginning the CO2 spread at a fast rate. This is because at the beginning there are more
pores available and the pore pressure in the reservoir is lower. Therefore, the advective flux rate is higher. However, as the pore pressure increases over time, the pressure difference between the injecting CO\textsubscript{2} and pores reduces, resulting in lower gas flow rate.

The effect of the injecting well operation on CO\textsubscript{2} storage capacity was investigated. The number of injecting wells was changed from 1 to 4, which changed the distance among the injecting wells. The variation of CO\textsubscript{2} storage capacity for 10 years of injection time with number of injecting wells is shown in Fig.4.

\begin{figure}[h]
\begin{center}
\includegraphics[width=0.5\textwidth]{fig4}
\end{center}
\caption{Variation CO\textsubscript{2} storage capacity with number of injecting wells.}
\end{figure}

According to Fig.4, the maximum storage capacity is obtained by having two injection wells and the addition of further injecting wells into the coal seam does not increase the CO\textsubscript{2} storage capacity by a significant amount. This may be due to the fact that further increasing the number of injecting wells after the two injecting well condition causes pressure contours to coincide, resulting in increased pore pressure and consequently reduced storage capacity. This arises because, when the distance among the injecting wells reduces, such that for 2, 3 and 4 injecting well conditions the distances among the wells are 680m, 528m and 500 m respectively. In order to check this, the spread of CO\textsubscript{2} concentration contours was checked after 10 years of CO\textsubscript{2} injection for two and three injecting well conditions. The results are shown in Fig.5.

\begin{figure}[h]
\begin{center}
\includegraphics[width=0.5\textwidth]{fig5}
\end{center}
\caption{CO\textsubscript{2} concentration contour cutting patterns}
\end{figure}

According to Fig.5 (a), under the two injecting well condition, concentration has spread throughout the coal layer. However, as shown in Fig.5 (b), for more than two wells, CO\textsubscript{2} concentration is mainly limited to the surrounding areas of the injecting wells. This is because, with increased numbers of injecting wells, the distance between the injecting points is reduced, resulting in
the pressure contours produced by each CO\textsubscript{2} injecting well meeting each other within a shorter time. This causes the pore pressure to increase and consequently the injecting capacity to reduce.

After checking the injecting well effect, the effect of coal mass physical properties on CO\textsubscript{2} storage capacity was investigated. The effect of coal bed moisture content on CO\textsubscript{2} storage capacity was investigated by changing the coal-bed moisture content from 0.1 to 0.5 (cm\textsuperscript{3}/cm\textsuperscript{3}). The variation of CO\textsubscript{2} storage capacity with the bed moisture content is shown in Fig.6 (a). Here, the gas injecting pressure and the coal mass temperature were maintained at 14 MPa and 30 °C, respectively. Next, the coal bed temperature on storage was changed from 20 °C to 60 °C to investigate the temperature effect on total amount of CO\textsubscript{2}, that can be injected into the coal mass (Fig.6(b)). According to Fig.6(a), up to around 0.45(cm\textsuperscript{3}/cm\textsuperscript{3}) moisture content the storage capacity significantly reduces with moisture content and hereafter moisture content does not affect the CO\textsubscript{2} storage capacity. The reduction of CO\textsubscript{2} storage is 99% when moisture content changes from 0.1 to 0.45. The amount of CO\textsubscript{2} that can be stored in the coal mass is highly dependent on the available pore space, and the presence of water causes the coal mass pore space available for the CO\textsubscript{2} movement to largely reduce (Skawinski et al. 1991). However, according to Anderson et al. (1956), before reaching the critical moisture content (around 0.45(cm\textsuperscript{3}/cm\textsuperscript{3}) in this study), the water molecules adsorb into the coal pore surface and obstruct the gas molecules adsorption into the surface. After the saturation point, the excess water (more than 0.45(cm\textsuperscript{3}/cm\textsuperscript{3}) in this study) in the coal mass moves into the mobile phase and therefore does not affect the gas sorption. If the effect of coal bed temperature on CO\textsubscript{2} storage capacity is considered, according to Fig.6 (b), it can be seen that the increase of temperature causes the amount of CO\textsubscript{2} that can be injected into the coal mass to significantly reduce. This may be due to the fact that, when the coal mass temperature increases, the gas molecules start to be released from the coal mass surface by the breakage of the bond between the molecules and the coal surfaces. As the temperature increases, this causes the kinetic energy of the gas molecules to increase and accordingly the rate of diffusion also to increase, resulting in reduction of the adsorption capacity (Levy et al. 1997). This may reduce the CO\textsubscript{2} storage capacity as the amount of CO\textsubscript{2} that can be captured inside the coal mass is totally dependent on its adsorption capacity.

![Figure 6. Variation of CO\textsubscript{2} storage capacity of coal mass for 10 years of injection with the (a) coal bed moisture content and (b) coal bed temperature.](image)

4. Conclusions

The carbon dioxide (CO\textsubscript{2}) sequestration process in deep unmineable coal seams can be successfully modelled using the COMET 3 numerical simulator. According to the results of this study, the number of injecting wells is a critical parameter, which should be investigated using an appropriate model before any field investigation. The reason is that according to the model results, CO\textsubscript{2} storage capacity in the coal seam cannot be increased by simply increasing the number of injecting wells. In fact, for a 500×540×20m coal seam, the two injecting well operating condition provides the optimum storage
capacity and any further increase in injecting wells significantly reduces the storage capacity. When more than one injecting well is present in the coal seam, the CO$_2$ storage capacity is controlled by the pressure contours induced by all the available injecting wells. Coal mass temperature and the moisture content significantly control coal’s CO$_2$ storage capacity. According to the developed model, the amount of CO$_2$ that can be injected into the coal mass reduces with both coal bed temperature and the moisture content, whereas the reduction of the storage capacity with moisture content occurs only up to the critical moisture content of the coal mass.

References


"*International Journal of Fuel*.


