DEVELOPMENT OF A 3D MODEL TO STUDY THE CO_2 SEQUESTRATION PROCESS IN DEEP UNMINEABLE COAL SEAMS.

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Abstract

This paper presents a numerical model to study the carbon dioxide (CO_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_2 was injected for a 10 year period. With one injection well, the storage capacity was calculated as 13×10^7 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 conditions (an increment of 130% of the single well condition). However, further increasing the number of wells (up to 4) reduced the storage capacity to 12.5×10^7 m^3. According to the model results, it is clear that CO_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_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_2) into the atmosphere. CO_2 sequestration in deep coal seams has been recognised as a potential method of atmospheric CO_2 mitigation. In addition, it could produce large amounts of value-added energy products such as methane (CH_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_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 Fickain FICKIAN? diffusion. Therefore, the amount of CO_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_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_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_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).

$$\nabla.\left[b_g M_g\left(\nabla p_g+\gamma_g \nabla Z\right)+R_{sw} b_w M_w\left(\nabla_{pw}+\gamma_w \nabla Z\right)\right]_f+q_m+q_g=\left(\frac{d}{dt}\right)\left(\phi b_g S_g+R_{sw}\phi b_w S_w\right)_f \quad [1]$$

$$\nabla.\left[b_w M_w\left(\nabla p_w+\gamma_w \nabla Z\right)\right]_f+q_w=\left(\frac{d}{dt}\right)\left(\phi b_w S_w\right)_f \quad [2]$$

where b_n (n=g or w) is the gas or water bulking factor, γ_n (n=g or w) is the gas or water gradient, R_{sw} is the gas solubility in water, ϕ 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)) $= kk_m/\mu_n$, is the phase mobility, (*k*-permeability, k_m-matrix permeability, μ_n -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.

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

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.

$$q_{mi}=\left(V_m/\tau_i\right)\left[C_i-C_i\left(P_i\right)\right]\quad, i=1,2 \quad [4]$$

where, q_{mi} is the gas component flow, V_m is the bulk volume of the matrix element, τ_i 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.

$$\phi=\phi_i\left[1+c_p\left(P-P_i\right)\right]-c_m\left(1-\phi_i\right)\left(\frac{\Delta P_i}{\Delta C_i}\right)\left(C-C_i\right) \quad \textbf{[5]}$$

$$\frac{k}{k_i} = \left(\frac{\phi}{\phi_i} \right)^n \qquad [6]$$

where, c_p is the pore volume compressibility, c_m is the matrix shrinkage compressibility, ϕ is the coal mass porosity, ϕ_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.

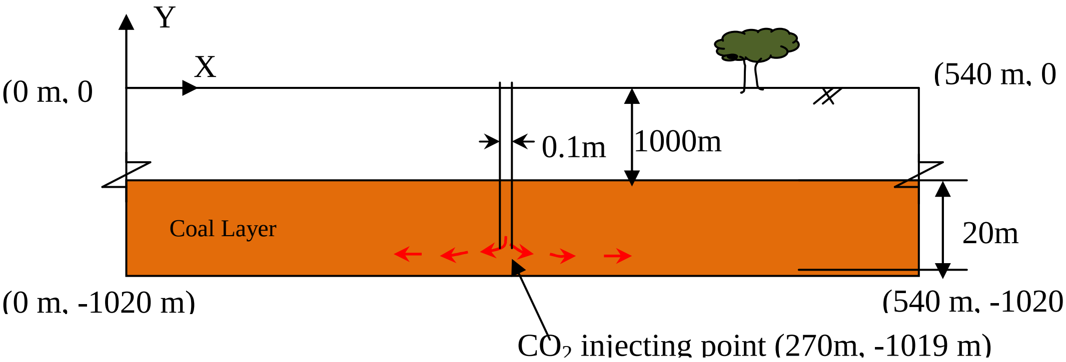

Figure 1. *Location of the coal layer.*

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

Table.1. *Model parameters*

Model Parameter	**Value**
Coal seam moisture content	0.5 (cm^3/cm^3)
Coal seam initial permeability	20 md
Coal seam porosity	0.1
Pore volume compressibility	$6.9e^{-5}$ (1/kPa)
Matrix shrinkage compressibility	$6.9e^{-7}$ (1/kPa)
Exponent of pressure dependent	3
Relative permeability variation	Cooray formula (Akin 2001), residual water and gas contents are 0.05 and 0.01 (cm^3/cm^3)
Temperature	30 ^0C
Langmuir volume for CO_2 adsorption	16 (m^3/m^3)
Langmuir pressure for CO_2 adsorption	1.56 MPa

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).

(a) (b)

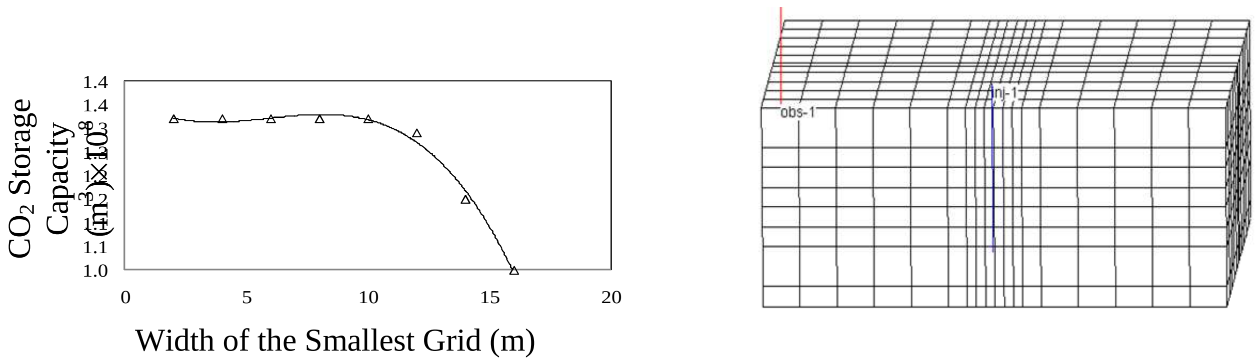

Figure 2. *(a) Effects of grid size on storage, and (b) selected model grid blocks for the coal seam.*

3. Model Simulation

After developing the model, the CO_2 migration rate along the horizontal distance was investigated for the bottom coal layer (Fig.3).

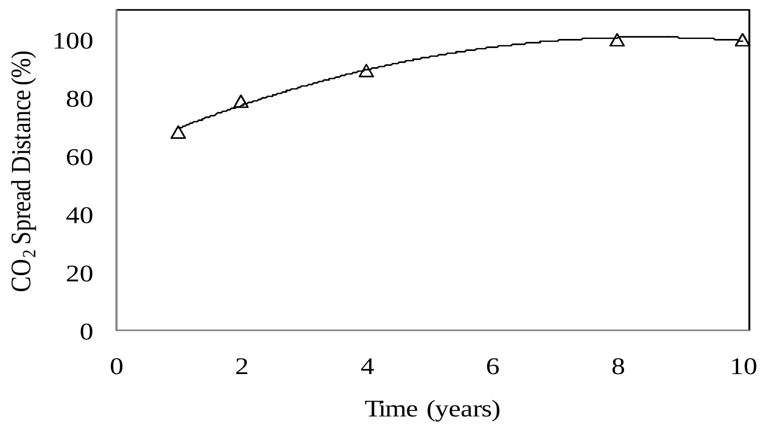

Figure 3. *Variation of CO_2 migration percentage with time.*

According to the above figure, after the first year CO_2 has spread through only around 65% of the coal layer and by the eighth year CO_2 has spread through the whole coal layer. It can also be seen that at the beginning the CO_2 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_2 and pores reduces, resulting in lower gas flow rate.

The effect of the injecting well operation on CO_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_2 storage capacity for 10 years of injection time with number of injecting wells is shown in Fig.4.

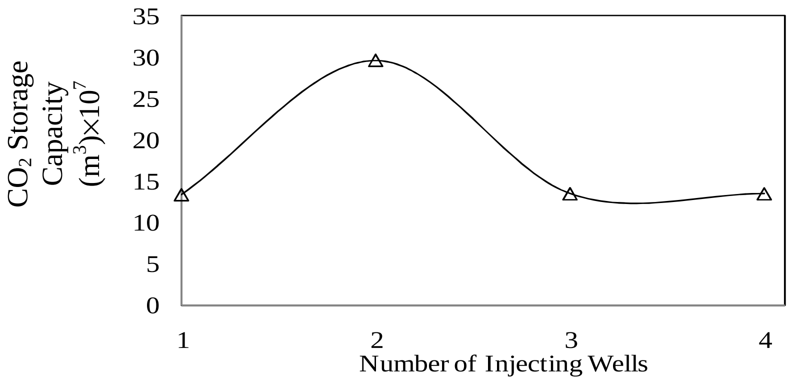

Figure 4. *Variation CO_2 storage capacity with number of injecting wells.*

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_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 number of injecting wells is increased from 1 to 4, 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_2 concentration contours was checked after 10 years of CO_2 injection for two and three injecting well conditions. The results are shown in Fig.5.

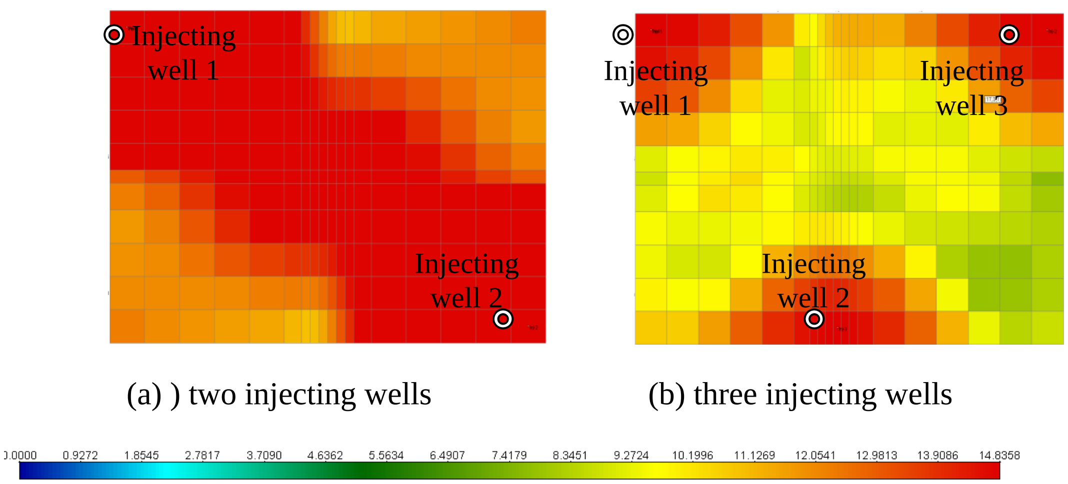

Figure 5. *CO_2 concentration contour cutting patterns*

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_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_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_2 storage capacity was investigated. The effect of coal bed moisture content on CO_2 storage capacity was investigated by changing the coal-bed moisture content from 0.1 to 0.5 (cm^3/cm^3). The variation of CO_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 ^oC, respectively. Next, the coal bed temperature on storage was changed from 20 ^oC to 60 ^oC to investigate the temperature effect on total amount of CO_2, that can be injected into the coal mass (Fig.6(b)). According to Fig.6(a), up to around 0.45(cm^3/cm^3) moisture content the storage capacity significantly reduces with moisture content and hereafter moisture content does not affect the CO_2 storage capacity. The reduction of CO_2 storage is 99% when moisture content changes from 0.1 to 0.45. The amount of CO_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_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^3/cm^3) in this study), the water molecules adsorb into the coal pore surface and obstruct the gas molecules adsorbtion into the surface. After the saturation point, the excess water (more than 0.45(cm^3/cm^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_2 storage capacity is considered, according to Fig.6 (b), it can be seen that the increase of temperature causes the amount of $CO_{2,}$ 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_2 storage capacity as the amount of CO_2 that can be captured inside the coal mass is totally dependent on its adsorption capacity.

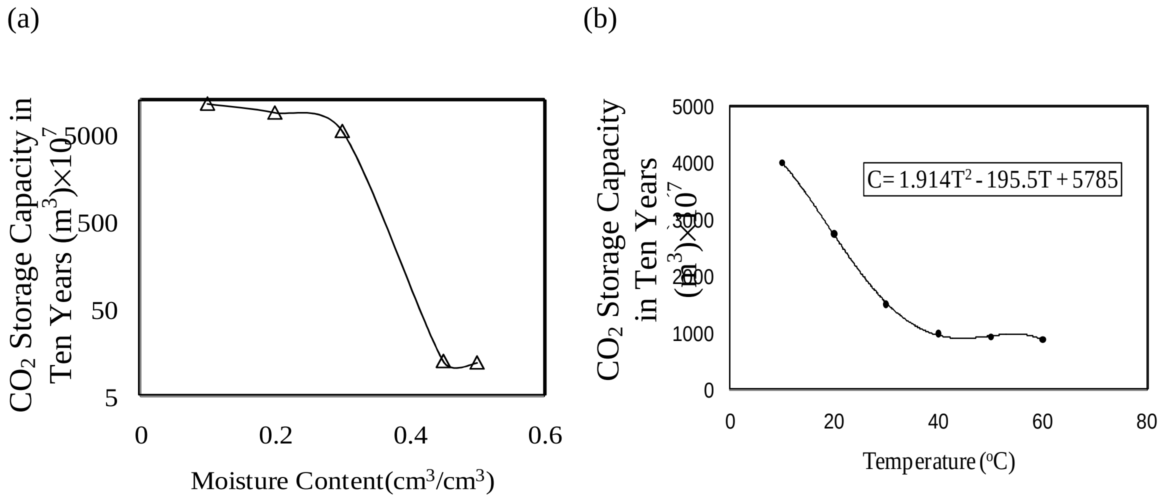

Figure 6. *Variation of CO_2 storage capacity of coal mass for 10 years of injection with the (a) coal bed moisture content and (b) coal bed temperature.*

4. Conclusions

The carbon dioxide (CO_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_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

Akin, S. (2001). "Estimation of fracture relative permeabilities from unsteady state corefloods." *Journal of Petroleum Science and Engineering*, 30(1), 1-14.

Anderson, R. B., Hall, W. K., Lecky, J. A., and Stein, K. C. (1956). "Sorption Studies on American Coals." *The Journal of Physical Chemistry*, 60(11), 1548-1558.

Balan, H. O., and Gumrah, F. (2009). "Assessment of shrinkage-swelling influences in coal seams using rank-dependent physical coal properties." *International Journal of Coal Geology*, 77(1-2), 203-213.

Carneiro, J. F. (2009). "Numerical simulations on the influence of matrix diffusion to carbon sequestration in double porosity fissured aquifers." *International Journal of Greenhouse Gas Control*, 3(4), 431-443.

Coll, M. C., Cortiula, B., Toledo, A., and S.A, M. (1994). "Identification of Productivity Problems in Clastic Sandstone Reservoirs of the Eocene Lower C Group, Block III, Lake Maracaibo, Western Venezuela using Well Log Data." SPE Latin America/Caribbean Petroleum Engineering Conference, Society of Petroleum Engineers Inc., Buenos Aires, Argentina.

Holzbecher, E. "*FEMLAB performance on 2D porous media variable density benchmarks* " *FEMLAB Konferenz 2005. Proceedings.*, Göttingen, 203--208.

Levy, J. H., Day, S. J., and Killingley, J. S. (1997). "Methane capacities of Bowen Basin coals related to coal properties." *Fuel*, 76(9), 813-819.

Liu, G., and Smirnov, A. V. (2009). "Carbon sequestration in coal-beds with structural deformation effects." *Energy Conversion and Management*, 50(6), 1586-1594.

Nam, J., Kim, J.-H., Kim, S., Yi, N., and Byun, K. (2008). "A study on mesh size dependency of finite element blast structural analysis induced by non-uniform pressure distribution from high explosive blast wave." *KSCE Journal of Civil Engineering*, 12(4), 259-265.

Pekot, L. J., and Reeves, S. R. (2002). "Modeling coal shrinkage and differential swelling with CO_2 injection for enhanced coal bed methane recovery and carbon sequestration application."

Perera, M. S. A., Ranjith, P.G. Choi, S.K., Bouazza , A. Kodikara, J. (Under Review). "A Parametric Study of Coal Mass and Cap Rock Behaviour and Carbon Dioxide Flow during and after Carbon Dioxide Injection " *International Journal of Petrolium Science*.

Perera, M. S. A., Ranjith, P.G. Choi, S.K., Airey, D. (Accepted). "Numerical Simulation of Gas Flow through Porous Sandstone and Its Experimental Validation
" *International Journal of Fuel*.

Sawyer, W. K., Paul, G. W., and Schraufnagel, R. A. "Development and application of a 3D coalbed simulator." *Paper CIM/SPE, Calgary* 90-119.

Skawinski, R., Zolcinska, J., and Dyrga, L. (1991). "Experimental investigations of the permeability in gas flow in coal with various water content." *Archives of Mining Sciences*, 36(3), 227-238.

Stevens, S. H., Kuuskraa, V. A., Gale, J. J., and Beecy, D. (2000). "CO (sub 2) injection and sequestration in depleted oil and gas fields and deep coal seams; worldwide potential and costs." *AAPG Bulletin*, 84(9), 1497-1498.

White, C. M., Smith, D. H., Jones, K. L., Goodman, A. L., Jikich, S. A., LaCount, R. B., DuBose, S. B., Ozdemir, E., Morsi, B. I., and Schroeder, K. T. (2005). "Sequestration of Carbon Dioxide in Coal with Enhanced Coalbed Methane Recovery A Review." *Energy & Fuels*, 19(3), 659-724.