



## A parametric study of coal mass and cap rock behaviour and carbon dioxide flow during and after carbon dioxide injection

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### HIGHLIGHTS

- ▶ Leakage of carbon dioxide is a major concern in carbon sequestration.
- ▶ COMSOL Multiphysics numerical simulator is used to model a deep coal seam.
- ▶ After some years of injection, CO<sub>2</sub> starts to move towards the cap rock layer.
- ▶ Cap rock may deform considerably due to CO<sub>2</sub> injection and CO<sub>2</sub> pressure built up along the cap rock.
- ▶ An existence of a fracture/s greatly increases the risk of CO<sub>2</sub> leakage into the atmosphere.

### ARTICLE INFO

#### Article history:

Received 3 May 2011

Received in revised form 3 October 2012

Accepted 23 October 2012

Available online 15 November 2012

#### Keywords:

CO<sub>2</sub> sequestration  
Cap rock deformation  
Rock fracture  
Back-migration

### ABSTRACT

In recent years, scientists have focused on processes which can be used to reduce greenhouse gas emissions, and CO<sub>2</sub> sequestration in deep coal seams and saline aquifers has been identified as a potential method. However, there is a fundamental lack of understanding concerning the flow and mechanical phenomena that occur when CO<sub>2</sub> is injected into coal seams. The main objective of this parametric study is to model the effect of CO<sub>2</sub> injection pressure on cap rock deformation and investigate the possibility of leakage or back-migration of CO<sub>2</sub> to the atmosphere through the cap rock. The COMSOL Multiphysics numerical simulator was used to investigate the effect of CO<sub>2</sub> injection on coal and other adjacent rock strata. For the purpose of the model, a 200 m long and 5 m thick coal seam was assumed to be lying below a 200 m long and 3 m thick cap rock layer 1000 m below the surface. According to the model's results, the cap rock deforms considerably just after injection in an upward direction due to the CO<sub>2</sub> movement, and the amount of deformation greatly depends on the injecting gas pressure. When the injecting gas pressure is increased from 10.2 MPa to 30 MPa, the cap rock is raised from 0.2 mm to 15 mm during the injecting period. Moreover, CO<sub>2</sub> first spreads and is stored in the coal mass and then after about 3–4 years it starts to move towards the cap rock layer. In the second stage of the study, a small rock fracture was inserted between the cap rock and the coal layer and a sudden increase in leakage of CO<sub>2</sub> to the cap rock through the fracture was observed. The existence of a rock fracture is highly possible, and may happen naturally in coal seams. This model shows that this kind of fracture greatly increases the risk of back-migration of CO<sub>2</sub> into the atmosphere. The model can be used to study general coal mass and cap rock behaviour and the back-movement of CO<sub>2</sub> flow to the atmosphere.

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### 1. Introduction

Carbon dioxide (CO<sub>2</sub>) sequestration in coal seams has been identified as a potential solution for reducing global warming. This

process can be used to reduce the large quantities of carbon dioxide in the atmosphere, and to produce an extensive amount of value-added product such as methane (CH<sub>4</sub>) as an outcome. In this process, CO<sub>2</sub> released from industrial activities such as power plants and steel plants is collected and separated for pumping into the underground coal mass and is stored by a sorption process. According to Stevens et al. [1], 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<sub>2</sub> [2].

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## Nomenclature

$c$	CO <sub>2</sub> concentration of the fluid in the coal mass, kg m <sup>-3</sup>	$u_p$	pore pressure, Pa
$c_o$	the initial water concentration means initial CO <sub>2</sub> concentration in the moisture in in situ coal mass (before injecting CO <sub>2</sub> ), kg m <sup>-3</sup>	$V$	Darcy velocity, m s <sup>-1</sup>
$c_{CO_2}$	injecting supercritical CO <sub>2</sub> concentration, kg m <sup>-3</sup>	$V_L$	Langmuir volume, kg kg <sup>-1</sup>
$c_a$	adsorbed CO <sub>2</sub> concentration into the coal mass, kg m <sup>-3</sup>	$w$	fracture width, m
$C_m$	cohesion, Pa	$y$	depth, m
$C_p$	pore volume compressibility, Pa <sup>-1</sup>	$\nu$	Poisson's ratio
$c_m$	matrix shrinkage compressibility Pa <sup>-1</sup>	$\alpha$	volumetric swelling coefficient
$D$	vertical distance from the ground surface, m	$\sigma$	stress, Pa
$D_L$	hydrodynamic dispersion tensor, m <sup>2</sup> s <sup>-1</sup> (function of tortuosity, diffusivity and dispersivity of the coal mass)	$\alpha_b$	biot poro-elastic constant
$E_F$	fracture Young's modulus, Pa	$\rho$	fluid density in the coal mass, kg m <sup>-3</sup>
$E$	coal mass Young's modulus, Pa	$\rho_o$	initial coal moisture density (before mixing with the CO <sub>2</sub> flow, kg m <sup>-3</sup>
$F$	vector that contains the fluid pressure gradient (includes the fluid flow and structure coupling term and other available body forces, Nm <sup>-3</sup>	$\rho_{CO_2}$	injecting supercritical CO <sub>2</sub> density, kg m <sup>-3</sup>
$F_x$	edge load in $x$ direction, Nm <sup>-2</sup>	$\rho_r$	rock density, kg m <sup>-3</sup>
$F_y$	edge load in $y$ direction, Nm <sup>-2</sup>	$\theta$	porosity
$F_b$	body forces in $x$ and $y$ direction, Nm <sup>-3</sup>	$\theta_i$	initial porosity
$g$	gravitational acceleration, m s <sup>-2</sup>	$\theta_s$	fluid volume fraction in the coal mass pore space (equal to porosity in this study)
$k$	coal cleat permeability, m <sup>2</sup>	$\phi$	anti-clockwise angle of any plane from the horizontal axis
$k_o$	coal cleat initial permeability, m <sup>2</sup>	$\phi_f$	friction angle
$k_f$	fracture permeability, m <sup>2</sup>	$\eta$	viscosity of the fluid in the coal mass, Pa s
$n$	directional vector component	$\eta_o$	initial water viscosity (before mixing with the CO <sub>2</sub> flow) in the coal mass, Pa s
$p$	pressure, Pa	$\eta_{CO_2}$	injecting supercritical CO <sub>2</sub> viscosity, Pa s
$p_F$	pressure in the coal cleats, Pa	$\tau_a$	allowable shear strength, Pa
$\Delta p$	change of applied pressure in $z$ direction, Pa	$\tau$	shear stress, Pa
$P_L$	Langmuir pressure, Pa	$\tau_{xy}$	shear stress in $x$ - $y$ plane, Pa
$\Delta S$	change of adsorbed CO <sub>2</sub> mass, mg kg <sup>-1</sup>	$\sigma_n$	normal stress, Pa
$S$	storage coefficient, s <sup>2</sup> m kg <sup>-1</sup>	$\sigma_x$	stress in $x$ direction, Pa
$t$	time, s	$\sigma_y$	stress in $y$ direction, Pa
$u$	total displacement, m		

Natural coal beds normally exist at deep locations (800–1000 m below the surface). Therefore the pressures in these locations are greater than the critical values of most of the gases in coal seams, such as CO<sub>2</sub> or CH<sub>4</sub>, which therefore exist at their supercritical states [3–6]. For instance, the critical temperature for CO<sub>2</sub> gas is 304.8 K and the critical pressure is 7.38 MPa. In deep coal beds both factors exceed their critical values and CO<sub>2</sub> gas exists in its supercritical state. CO<sub>2</sub> density increases with pressure and at 313 K temperature and 20 MPa pressure, pure CO<sub>2</sub> density is closer to water density (around 900 kg/m<sup>3</sup>). Akgerman and Giridhar [7] explain that supercritical fluids have liquid-like densities and solvent powers while having “gas-like” viscosities. Therefore, the supercritical CO<sub>2</sub> in deep coal seams preferably mixes with moisture in the coal pore structure, depending on the equation of state, such as pressure and temperature. The 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 is governed by Darcian law and also the intrinsic permeability of the coal matrix, which is governed by Fickian diffusion.

However, CO<sub>2</sub> sequestration in deep coal seams process remains in the experimental stage as many aspects need to be studied before being put into practice. After a detailed review of the available studies related to CO<sub>2</sub> sequestration, White et al. [2] explained that “there is a fundamental lack of understanding concerning the physical, chemical and thermodynamic phenomena that occur when CO<sub>2</sub> is injected into a coal seam.” The effects of CO<sub>2</sub> injection on the cap rock and the possibility of remigration of the injected CO<sub>2</sub> into the atmosphere through the cap rock are important

aspects to be studied [8]. Moreover, rock faults or fractures may be present in the cap rock and coal seams and may cause injected CO<sub>2</sub> to leak to the atmosphere [9,10]. Numerical models play an important role in identifying the effect of the CO<sub>2</sub> sequestration process on the coal mass structure [11], and its effect on the cap rock and the back-migration of injected CO<sub>2</sub> into the atmosphere. In the present study the COMSOL Multiphysics numerical simulator was used to develop a numerical model to simulate the CO<sub>2</sub> sequestration process in a deep coal seam.

COMSOL Multiphysics is a partial differential equations (PDEs) and finite element analysis (FEM)-based numerical software, which can be used to model and solve a wide range of scientific and engineering problems. This simulator is available as a graphical user interface (GUI) or as a script programme in the MATLAB language. Of these, the former is easier and more user-friendly as models can be developed by giving several parameters, such as material properties, loads, constraints and sources. In this case, the user can easily select the equations necessary for the particular problem as the software itself contains a large number of PDEs. Moreover, in the COMSOL Multiphysics GUI, any type of equation can be introduced as a material parameter, boundary condition, load, constraint or source. However, since COMSOL Multiphysics is a basic type of numerical software which contains a large number of PDEs, the user must select the appropriate equations to solve their problem. COMSOL Multiphysics consists of several types of modules, including acoustics, chemical engineering, earth science, heat transfer and structure mechanics. The user can use one of these modules or several modules can be coupled using PDEs to develop the model. Of the modules, the heat transfer module has

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