Numerical analysis of dual porosity coupled thermo-hydro-mechanical behaviour during CO2 sequestration in coal

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Abstract

This study presents a coupled dual porosity thermal-hydraulic-mechanical (THM) model of non-isothermal gas flow during CO2 sequestration in coal seams. Thermal behaviour is part of the disturbed physical and chemical condition of a coal seam caused by CO2 injection, and must be understood for accurate prediction of CO2 flow and storage. A new porosity-permeability model is included for consideration of the fracture-matrix compartment interaction. The new model is verified against an analytical solution and validated against experimental measurements, before being used to analyse coupled THM effects during CO2 sequestration in coal. A simulation of CO2 injection at a fixed rate shows the development of a cooling region within the coal seam due to the Joule-Thomson effect, with the temperature in the vicinity of the well declining sharply before recovering slowly. The temperature disturbance further from the well is more gradual by comparison. Under the simulation conditions studied, CO2 injection increases coal matrix porosity and decreases the porosity and permeability of the natural fracture network, especially in the vicinity of the injection well, due to adsorption-induced coal swelling. Compared with the effects of gas pressure and temperature, the matrix-fracture compartment interaction plays an important role in changes of porosity and permeability. Considering the temperature disturbance caused by CO2 injection under the set of representative conditions studied, the coupled model can provide an insight into the associated effects on CO2 flow and storage during its sequestration in coal seams.

Keywords: CO2 sequestration; Gas flow; Coal; THM modelling; Dual porosity

1. Introduction

CO2 capture, utilisation and sequestration (CCUS) comprises a broad set of actions intended to reduce greenhouse gas emissions and mitigate climate change. Among the CCUS options is coal seam
sequestration [1, 2], which provides storage security by taking advantage of coal’s preference to adsorb CO₂ and can also enhance coalbed methane (CBM) recovery, either for electricity generation or as a feedstock for hydrogen production. Clearly the use of CBM should not lead to additional CO₂ emissions, which in most cases requires further CCUS. Coal seams have an excellent potential to handle these excess emissions, since it is well established that the CO₂ adsorption capacity of coal is around two times greater than for the naturally occurring CBM, depending primarily on coal rank [3, 4]. When CO₂ is injected into a coal seam, it disturbs the pre-existing physical and chemical condition and initiates coal-gas interactions [5-7]. For the successful storage of CO₂ in coal seams, factors influencing CO₂ injectivity, storage security, and CBM displacement should be better understood, including the role of non-isothermal behaviour explored in this paper.

CO₂ injection can lead to a dynamic temperature system within the coal seam and adjacent strata, which in turn affects the gas transport and adsorption behaviour [7-10]. As gas flows from high pressure to low pressure, the average distance between molecules increases and leads to growth of the potential energy due to intermolecular attraction. Since the expansion process is adiabatic and the total energy remains constant, the increase in potential energy implies a decrease in the kinetic energy and temperature, with this phenomenon being known as Joule-Thomas cooling (JTC) [11]. Zagorsčak and Thomas [8] observed that the high flow rate of CO₂ in a coal sample led to temperature drops of up to 6.8 °C during their experiments. Oldenburg [9] performed numerical simulations of CO₂ injection into depleted gas reservoirs to examine the importance of Joule-Thomson cooling, finding that the associated temperature drop can exceed 20 °C for a high injection rate into low permeability rock. Similarly, a coupled heat and mass flow model was developed by Ziabakhsh-Ganji and Kooi [12] to account for the pressure, temperature, and gas compositional influences on thermo-physical transport properties including density, viscosity, specific heat capacity, and Joule–Thomson coefficient. Whilst these studies do not concern the mechanical behaviour of coal during CO₂ sequestration, they show the importance of non-isothermal behaviour under similar conditions, which may be expected to have a broad impact on coal-gas systems considering the dependence of CO₂ sorption and coal swelling on temperature.

Coal swelling induced by CO₂ adsorption is a well-known phenomenon, which alters the stress state and pore pressure of a coal seam with consequent changes to its porosity and permeability. Experimental and theoretical studies have been performed to investigate the permeability changes of coal exposed to CO₂ and other gases, with detailed reviews provided by Pan and Connell [13]. Several authors have established coupled models to explore the thermal, hydraulic, and mechanical (THM) coupling mechanisms controlling coal seam behaviour. Qu et al. [14] presented a coupled model of non-isothermal gas flow and coal deformation to study coal permeability changes for different gas injection temperatures, while the effect of overburden was not considered. Their work focused on characterising internal and volumetric coal swelling and shrinking due to the competing influences of thermal and
sorption induced strains (i.e. the thermal expansion of coal is countered by a reduction in CO₂ sorption-swelling, and vice versa), with the latter found to be pre-dominant under the conditions considered. Non-isothermal behaviour has been considered in several other coupled models of CO₂ sequestration in coal [e.g. 6, 15], with the coal having been idealised as a single poroelastic medium when considering deformation. For example, Saliya et al. [6] used a single porosity model to investigate the influence of coal’s hydro-mechanical properties (Biot coefficient, bulk modulus), Langmuir adsorption parameters, and the initial pore pressure during CO₂ injection.

In this study, a coupled THM model is presented within the framework of dual poroelastic theory. The model consists of three main components; gas seepage in the dual porosity system, thermal transport under local thermal non-equilibrium, and the thermo-poroelastic mechanical model. The nonlinear governing equations are implemented in the COMPASS model and solved using the finite element method. In particular, this work builds upon previous works on dual porosity CO₂ flow and coal deformation presented by Hosking et al. [16] and Chen et al.[17, 18]. The enhanced numerical model is verified using analytical solutions for poro-thermo-elasticity in the absence of gas adsorption, before validation is pursued using experimental measurements as a benchmark. The coupled thermo-poroelastic dual porosity model is then used to predict the thermal, hydraulic, and goemechanical response of a coal seam to CO₂ injection.

2. Model development

Coal is treated as a dual porosity rock comprised of a porous matrix and a natural fracture network. Injected CO₂ flows through the fracture network before leaking into the coal matrix blocks and becoming adsorbed on the internal surfaces. In this section, a set of governing equations describing the fluid flow, thermal transport, and mechanical behaviour is presented for compressible fluid flow in a coal seam. For the purposes of the present work, it is assumed that the model generally applies to coal seams that are depleted of water and CBM following primary production; hence, only single phase, single component flow of CO₂ is considered. It is further assumed that coal seams are homogenous and isotropic, that coal deformation is small and linearly elastic, and that the coal is in local thermal non-equilibrium (LTNE).

2.1 Thermo-poroelastic mechanical model

A thermo-poroelastic mechanical model is developed to represent the deformation behaviour of coal. The convention of positive stress and strain in tension is used in this study, however, the fluid pressure is defined as positive in compression. For quasi-static conditions, the linear momentum balance equation for a representative elementary volume of a fractured porous medium can be reduced to the equilibrium equation for total stresses [19]:
\[ \sigma_{ij,j} + F_i = 0 \]  

(1)

where \( \sigma_{ij} \) is the component of the total stress tensor and \( F_i \) is the component of the body force vector. Following convention, a comma followed by subscripts denotes the differential with respect to spatial coordinates and repeated indices denote a summation over the range of the indices.

The total stress can be expressed in terms of the effective stress and the average pore pressure according to Biot’s effective stress law, as:

\[ \sigma_{ij}' = \sigma_{ij} - \alpha_m u_m \delta_{ij} - \alpha_f u_f \delta_{ij} \]  

(2)

where \( \sigma_{ij}' \) is the component of the effective stress tensor, \( \delta_{ij} \) is Kronecker’s delta tensor (\( \delta = 1 \) for \( i = j \), \( \delta = 0 \) for \( i \neq j \)), \( \alpha_f \) and \( \alpha_m \) are Biot coefficients, and \( u_m \) and \( u_f \) are pore gas pressures for the matrix and fracture continuum, respectively, given by:

\[ u_\beta = Z_\beta R T_\beta c_\beta \]  

(3)

where \( R \) is the universal gas constant, \( T_\beta \) is the temperature, \( c_\beta \) is the gas concentration, and \( Z_\beta \) is the gas compressibility factor. In this study, the equation of state (EoS) proposed by Peng and Robinson [20] is used to describe gas compressibility.

The constants \( \alpha_f \) and \( \alpha_m \) can be expressed in terms of physically measurable mechanical parameters, as [17]:

\[ \alpha_f = 1 - \frac{K}{K_m} \]  

(4)

\[ \alpha_m = \frac{K}{K_m} - \frac{K}{K_s} \]  

(5)

where \( K = E/3(1 - 2\nu) \) is the bulk modulus of the fractured rock with \( E \) being Young’s modulus, \( K_m = E_m/3(1 - 2\nu) \) is the modulus of the coal matrix with \( E_m \) being the respective Young’s modulus, which can be obtained from experiments performed on specimens that are devoid of fractures, \( K_s \) is the modulus of the solid constituent, and \( \nu \) is Poisson’s ratio.

The stress-strain constitutive relationship is:

\[ \sigma_{ij}' = 2G\varepsilon_{ij}^e + \lambda \varepsilon_{ij}^v \delta_{ij} \]  

(6)

where \( G = E/2(1 + \nu) \) is the shear modulus, \( \lambda = E\nu/(1 + \nu)(1 - 2\nu) \) is the Lamé constant, \( \varepsilon_{ij}^e \) represents elastic deformation, and \( \varepsilon_{ij}^v = \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33} \) is the elastic volumetric strain.
The total strain, \(\varepsilon_{ij}\), can be expressed as:

\[
\varepsilon_{ij} = \varepsilon_{ij}^e + \frac{1}{3} \varepsilon_T \delta_{ij} + \frac{1}{3} \varepsilon_{ad} \delta_{ij}
\]  

(7)

where \(\varepsilon_T\) is the thermal expansion-induced volumetric strain and \(\varepsilon_{ad}\) is the adsorption-induced swelling strain.

For a homogeneous, isotropic and elastic medium, the strain-displacement relation is given by:

\[
\varepsilon_{ij} = \frac{1}{2} \left( u_{i,j} + u_{j,i} \right)
\]  

(8)

where \(\varepsilon_{ij}\) is the component of the total stress tensor and \(u_i\) is the component of the solid displacement vector.

The thermal expansion-contraction strain is defined as:

\[
\varepsilon_T = \alpha_T (T_m - T_r)
\]  

(9)

where \(\alpha_T\) is the thermal expansion coefficient and \(T_r\) is the reference temperature.

The total adsorption-induced strain is calculated using a surface stress approach as [17, 21]:

\[
\varepsilon_{ad} = -\frac{\alpha_m u_a}{K}
\]  

(10)

\[
u_a = -\varphi \Gamma_{\text{max}} R T_m \ln(1 + b_L u_m)
\]  

(11)

where \(u_a\) is the swelling stress, \(\Gamma_{\text{max}}\) is a Langmuir adsorption constant, representing the adsorption capacity per unit adsorption surface, \(\varphi\) is a constant material parameter representing the correlation between changes in the adsorption area of the matrix pore and the porosity of the matrix, and \(b_L\) is the inverse Langmuir pressure constant. In this study, \(\Gamma_{\text{max}}\) and \(\varphi\) are lumped together as a coefficient related to adsorption induced swelling and obtained by matching experimental data.

2.2 Gas transport

For coal, there are two distinct scales for fluid flow in coal, namely, flow in the fracture network and transport in the porous matrix. Despite the discontinuous (fractured) nature of coal, in accordance with the convention of dual continuum modelling, it is assumed that each of these flow patterns is continuous.

Based on the treatment of flow mechanisms within the porous matrix block, dual porosity models can be grouped into at least two categories, namely, dual porosity-single permeability (DPSP) models and
dual porosity-dual permeability (DPDP) models. The key difference is that the DPSP model only considers bulk fluid flow within the fracture continuum with the porous matrix acting as a sink or source for fluid flow within the adjacent fractures. By comparison, in the DPDP model, the matrix is also assumed to be permeable [21]. The mass balance equations are derived in this section using the framework of the generalised DPDP model, whilst they can be transformed for the purposes of DPSP modelling simply by ignoring bulk flow in the matrix. Based on the principle of conservation of mass, single phase gas flow in each of the continua is defined as:

$$\frac{\partial \rho_\beta n_\beta}{\partial t} = -\nabla \cdot (\rho_\beta \mathbf{v}_\beta) + Q_{s\beta} + \omega \Gamma$$

(12)

where $n_\beta$ is the porosity of continuum $\beta$, $\mathbf{v}_\beta$ is the gas velocity, $Q_{s\beta}$ is a gas sink-source term for adsorption-desorption, $\Gamma$ represents the mass transfer between the fracture and matrix continua, and the parameter $\omega = -1$ if $\beta = f$, otherwise $\omega = 1$.

Expanding the left-hand side of equation (12) produces:

$$\frac{\partial \rho_\beta n_\beta}{\partial t} = n_\beta \frac{\partial \rho_\beta}{\partial t} + \rho_\beta \frac{\partial n_\beta}{\partial t}$$

(13)

where $\rho_\beta$ is the gas density in continuum $\beta$, given by:

$$\rho_\beta = M c_\beta$$

(14)

where $M$ is the gas molar mass.

The temporal derivative of fluid density can be expanded to give:

$$\frac{\partial \rho_\beta}{\partial t} = \frac{\partial \rho_\beta}{\partial u_\beta} \frac{\partial u_\beta}{\partial t} + \frac{\partial \rho_\beta}{\partial T_\beta} \frac{\partial T_\beta}{\partial t} = \rho_\beta C_{c\beta} \frac{\partial u_\beta}{\partial t} - \rho_\beta \alpha_{T\beta} \frac{\partial T_\beta}{\partial t}$$

(15)

where $C_{c\beta} = \frac{1}{\rho_\beta u_\beta}$ is the fluid compressibility and $\alpha_{T\beta} = -\frac{1}{\rho_\beta T_\beta} \frac{\partial \rho_\beta}{\partial T_\beta}$ is the thermal expansion coefficient.

Gas flow in the fracture network is assumed to be laminar and viscous, and is governed by Darcy’s law. Neglecting gravity, this gives:

$$\mathbf{v}_\beta = -\frac{k_\beta}{\mu} \nabla u_\beta$$

(16)

where $k_\beta$ is the permeability of continuum $\beta$ and $\mu$ is the gas viscosity.
Gas storage in coal seams is typically dominated by the adsorbed phase within the porous matrix, where the majority of internal surface area is found. It is therefore assumed that no adsorbed gas is present in the fracture continuum, i.e. $Q_{sf} = 0$. The sink-source term in the matrix continuum is given by:

$$Q_{sm} = -\frac{dR_{ad}}{dt} \quad (17)$$

$$R_{ad} = M\rho_s c_s \quad (18)$$

where $c_s$ is the adsorbed concentration and $\rho_s$ is the coal density.

The adsorption behaviour of gas in coal is generally described by a Langmuir isotherm, as:

$$c_s = \frac{V_L b_L u_m}{b_L u_m + 1} \quad (19)$$

where $V_L$ is the Langmuir volume constant. Considering the thermal effect, Tang and Ripepi [22] presented the following temperature dependent form of the inverse Langmuir pressure constant, $b_L$:

$$b_L = b_{L0} \exp\left(\frac{E_i}{RT_m}\right) \quad (20)$$

where $b_{L0}$ is the temperature-independent Langmuir constant and $E_i$ is the interaction energy between the adsorbate and the adsorbent.

Mass exchange between the dual continua is derived in this work based on the assumption that a quasi-steady state pore gas concentration distribution prevails in the matrix blocks. This assumption allows the inter-porosity gas transfer rate to be expressed as a linear function of the difference between the average pore gas concentration in the fracture and matrix continua [16]. Considering the geometric effect of coal matrix, the resulting mass exchange term for the pore gas component is expressed as [17, 18]:

$$\Gamma = aDM(c_f - c_m) \quad (21)$$

where $a$ is a matrix block geometric factor and $D$ is the gas diffusion coefficient in the coal matrix.

Generally, Arrhenius' law is used to describe the correlation between gas diffusion and temperature [23]. However, when the temperature change is not sufficiently large, the effect of temperature on gas diffusion may be regarded as negligible [23]. Therefore, to simplify the mass exchange, a constant sorption time, $\tau$, is introduced to approximate the diffusivity of the coal matrix [e.g. 5], given as:
\[ \tau = \frac{1}{aD} \quad (22) \]

### 2.3 Heat transfer

A LTNE approach is applied for separate parameterisation of the fractures and matrix pores, considering heat transfer between the continua linked with mass transfer. The slow rate of gas flow in the coal matrix means that the gas and solid grains achieve thermal equilibrium relatively quickly. In effect, it can be said that each continuum remains at local thermal equilibrium, with the potential for a non-equilibrium condition to exist between the continua. Several thermal responses may develop as a result of geological CO\textsubscript{2} sequestration [e.g. 7, 11]; notable among these are the Joule-Thomson effect and conductive heat exchange due to a difference in temperature between the injected CO\textsubscript{2} and the surrounding fluids and rock.

The governing equations for heat transfer through the fracture and matrix continua can be obtained by applying the principle of conservation of energy. Ignoring the heat supply due to thermal expansion of the solid skeleton, heat transfer in the fracture continuum can be written as:

\[
\begin{align*}
&n_f \rho_f C_{pg} \frac{\partial T_f}{\partial t} - n_f (\rho_g C_{pg} \mu_{JT} + 1) \frac{\partial u_f}{\partial t} = \nabla \cdot (\lambda_g \nabla T_f) - \rho_f C_{pg} \nu_f \cdot (\mu_{JT} \nabla u_f - \nabla T_f) - q_{fm}
\end{align*}
\]

and in the matrix continuum as:

\[
\begin{align*}
&\left(\rho_m C_{pm}\right)_{eff} \frac{\partial T_m}{\partial t} - n_m (\rho_m C_{pg} \mu_{JT} + 1) \frac{\partial u_m}{\partial t} = \nabla \cdot (\lambda_{em} \nabla T_m) - \rho_f C_{pg} \nu_m \cdot (\mu_{JT} \nabla u_m - \nabla T_m) + q_{fm}
\end{align*}
\]

where:

\[
\begin{align*}
&\left(\rho_m C_{pm}\right)_{eff} = (1 - n_m - n_f)(\rho_s C_{ps} + \rho_a C_{pa}) + \rho_g C_{pg} \\
&\lambda_{em} = (1 - n_m - n_f)(\lambda_s + \lambda_a) + n_m \lambda_g
\end{align*}
\]

where \(C_{pg}\) and \(\lambda_g\) are the specific heat capacity and thermal conductivity of gas, \(C_{ps}\) and \(\lambda_s\) are the same for the coal solids, \(C_{pa}\) and \(\lambda_a\) are the same for adsorbed gas, \(\rho_a\) is the adsorbed phase density, \(\mu_{JT}\) is the Joule–Thomson coefficient, and \(q_{fm}\) represent the heat transfer between the dual continua. \(C_{pg}\) and \(\mu_{JT}\) are calculated using the Peng and Robinson EoS. Due to limited information on \(C_{pa}\) and \(\lambda_a\) for gas adsorption in coal, it is assumed that they are equivalent to \(C_{pg}\) and \(\lambda_g\).
The heat transfer term, $q_{fm}$, is separated into two processes according to the main heat transfer mechanisms, namely, conduction across the fracture surfaces and advection via mass flow between the continua [24, 25]. This can be expressed mathematically as:

$$q_{fm} = h_{TR} A_{fm} (T_f - T_m) + \Gamma C_{pg}(T_f - T_m)$$

(25)

where $h_{TR}$ is the heat transfer coefficient between the fracture and matrix continua, and $A_{fm}$ is the interfacial fracture-matrix specific area, which can be estimated based on the geometric relation of the fractures and matrix blocks.

The first term on the right-hand side of equation (25) represents the heat exchange between the fracture and matrix continua by conduction across the fracture surfaces, and the second term represents heat transfer by advection through the mass exchange term. Both $h_{TR}$ and $A_{fm}$ are important parameters influencing the fracture-matrix interactions. The heat transfer coefficient is typically calculated by harmonic averaging of the fracture and matrix thermal conductivities [25]:

$$h_{TR} = \frac{2\lambda_{em}\lambda_{ef}}{l\lambda_{ef} + w\lambda_{em}}$$

(26)

where $\lambda_{ef}$ is the effective thermal conductivity of the fracture continuum; in this work, $\lambda_{ef} = \lambda_g$.

The interfacial fracture-matrix specific area can be obtained using geometrical considerations for an aperture, $w$, and a matrix block length, $l$ [24]:

$$A_{fm} = \frac{4l}{(l+w)^2}$$

(27)

2.4 Porosity and permeability evolution

Generally, the relationship between porosity and permeability is given by the cubic law, written as:

$$\frac{k_{\beta}}{k_{\beta0}} = \left(\frac{n_{\beta}}{n_{\beta0}}\right)^3$$

(28)

where $k_{\beta0}$ and $n_{\beta0}$ are the permeability and porosity at a reference state.

The porosity at the current state can be defined as:

$$n_{\beta} = n_{\beta0} + \Delta n_{\beta}$$

(29)

where $\Delta n_{\beta}$ is the change in porosity from the reference state.
For non-adsorbing gas flow in isothermal fractured rock, the fracture and matrix pore volume change per unit of bulk volume is due to three components [17], namely, (i) a change in pore volume with a change in bulk volume of the porous medium, (ii) a change in pore volume due to compression of the solid phase by fluid pressure occupying the pore space, and (iii) a change in pore volumes due to fracture-matrix interaction driven by a pressure difference between the pore regions. When adsorption and thermal effects are involved, the influence of adsorption-induced and thermal deformation should also be considered.

Recent studies have shown that the effect of deformation resulting from adsorption-induced swelling on the fracture and matrix pore volumes is characterised by both global and local strains [26]. Before global (volumetric) deformation occurs, adsorption-induced swelling is contained in the vicinity of a fracture as a local strain, whereby matrix expansion narrows the fracture opening. It is worth pointing out that when global deformation takes place, a fracture-matrix compartment interaction may still exist if there is a pressure difference between the pore regions. It is assumed that the effect of global swelling strain on porosity evolution is analogous to that of pore pressure. Considering the influence of multiple coupled processes after reaching a final equilibrium state, a porosity change can be expressed as:

\[
\Delta n_f = (\alpha_f - n_f) \Delta \varepsilon_v + \frac{(\alpha_f - n_f)}{K_s} \Delta u_f - (\alpha_f - n_f) \left( \frac{1}{K_m} - \frac{1}{K_s} \right) \Delta (u_m^a - u_f) - \Delta \varepsilon_{al} \quad (30a)
\]

\[
\Delta n_m = (\alpha_m - n_m) \Delta \varepsilon_v + \frac{(\alpha_m - n_m)}{K_s} \Delta u_m^a - (\alpha_f - n_f) \left( \frac{1}{K_m} - \frac{1}{K_s} \right) \Delta (u_f - u_m^a) + \Delta \varepsilon_{al} \quad (30b)
\]

where \( u_m^a = u_m - u_a \), \( \varepsilon_v \) is the bulk volumetric strain, expressed as a combination of strain due to effective stress, adsorption, and thermal expansion, giving:

\[
\Delta \varepsilon_v = \Delta \varepsilon_e + \Delta \varepsilon_{ad} + \Delta \varepsilon_T \quad (31)
\]

The first terms on the right-hand side of equations (30a) and (30b) represent the change in pore volume with a change in bulk volume, with the second terms representing the contribution of compression of solids. Interactions between the fracture and matrix continua are represented by the third and fourth terms; the former being due to the pressure difference and the latter due to local swelling. With small deformation, it is assumed that local swelling is linearly proportional to global swelling, as:

\[
\varepsilon_{al} = \gamma \varepsilon_{ad} \quad (32)
\]

where \( \gamma \) is the ratio of local to global swelling, which can be obtained by matching the experimental results of coal swelling and permeability.
Substitution of equation (30) into equation (29) with rearrangement based on the assumption of small strain yields:

\[ n_f = n_{f0} + \alpha_f \Delta \varepsilon_v + \frac{\alpha_f}{K_s} \Delta u_f - \alpha_f \left( \frac{1}{K_m} - \frac{1}{K_s} \right) \Delta (u_m^a - u_f) - \Delta \varepsilon_{al} \]  

(33a)

\[ n_m = n_{m0} + \alpha_m \Delta \varepsilon_v + \frac{\alpha_m}{K_s} \Delta u_m^a + \alpha_f \left( \frac{1}{K_m} - \frac{1}{K_s} \right) \Delta (u_m^a - u_f) + \Delta \varepsilon_{al} \]  

(33b)

### 2.5 Governing equations

Substituting the relationships developed above into the stress equilibrium and transport equations yields a system of coupled governing equations expressed in terms of five primary variables, namely, the displacement vector \( \mathbf{u} \), the gas concentrations in the fracture \( c_f \) and matrix \( c_m \) continua, and the temperature in the fracture \( T_f \) and matrix \( T_m \) continua.

For thermo-poroelastic displacement:

\[ C_{uu} du + C_{uf} dc_f + C_{um} dc_m + dT_m + dF = 0 \]  

(34)

where:

\[ C_{uu} = PD^T \]

\[ C_{ucf} = P I \alpha_f Z_f RT_f \]

\[ C_{ucm} = -P D I \frac{1}{3} \frac{\partial \varepsilon_{ad}}{\partial c_m} + P I \alpha_m Z_m RT_m \]

\[ C_{utm} = -P D I \frac{1}{3} \frac{\partial \varepsilon_{ad}}{\partial T_m} + \varepsilon_T \]

where \( P \) is the strain matrix, \( D \) is the elasticity matrix, and \( I = [1,1,0]^T \) for plane strain problems and \( I = [1,1,1,0,0,0]^T \) for three dimensional problems.

For gas transport in the fracture continuum:

\[ C_{cf} \frac{\partial c_f}{\partial t} + C_{cf} \frac{\partial c_m}{\partial t} + C_{cf} \frac{\partial T_f}{\partial t} + C_{cf} \frac{\partial T_m}{\partial t} + C_{cf} \frac{\partial u}{\partial t} = \nabla \cdot \left( K_{cf} \nabla c_f \right) + \nabla \cdot \left( K_{cf} \nabla T_f \right) + K_{cf} c_{cf.f} + K_{cf} c_{cf.m} \]  

(35)

where:

\[ C_{cf} = n_f + \frac{\alpha_f u_f}{K_m} \]
\[C_{cf c_m} = -c_f \alpha_f \left( \frac{1}{K_m} - \frac{1}{K_s} \right) (Z_m R T_m - \frac{\partial u_a}{\partial c_m}) - c_f \frac{\partial \varepsilon_{al}}{\partial c_m} \]

\[C_{cf T_f} = \frac{\alpha_f Z_f R c_f}{K_m} \]

\[C_{cf T_m} = -c_f \alpha_f \left( \frac{1}{K_m} - \frac{1}{K_s} \right) (Z_m R c_m - \frac{\partial u_a}{\partial T_m}) - c_f \frac{\partial \varepsilon_{al}}{\partial T_m} \]

\[C_{cf u} = c_f \alpha_f ^T P \]

\[K_{cf f} = c_f Z_f R \frac{k_f}{\mu} \]

\[K_{cf T_f} = c_f ^2 Z_f R \frac{k_f}{\mu} \]

\[K_{cf f, f} = -\frac{1}{\tau} = -K_{cf f, m} \]

For gas transport and adsorption-desorption in the matrix continuum:

\[C_{cm c_m} \frac{\partial c_m}{\partial t} + C_{cm c_f} \frac{\partial c_f}{\partial t} + C_{cm T_m} \frac{\partial T_m}{\partial t} + C_{cm T_f} \frac{\partial T_f}{\partial t} + C_{cm u} \frac{\partial u}{\partial t} = \nabla \cdot \left( K_{cm c_m} \nabla c_m \right) + \nabla \cdot \left( K_{cm T_m} \nabla T_m \right) + K_{cm c_m, f} + K_{cm c_m, m} \]  

(36)

where:

\[C_{cm c_m} = n_m + c_m \alpha_f \left( \frac{1}{K_m} - \frac{1}{K_s} \right) (Z_m R T_m - \frac{\partial u_a}{\partial c_m}) + \rho_s \frac{\partial c_s}{\partial c_m} + c_m \frac{\partial \varepsilon_{al}}{\partial c_m} \]

\[C_{cm c_f} = -c_m \alpha_f \left( \frac{1}{K_m} - \frac{1}{K_s} \right) Z_f R T_f \]

\[C_{cm T_m} = c_m \alpha_f \left( \frac{1}{K_m} - \frac{1}{K_s} \right) (Z_m R c_m - \frac{\partial u_a}{\partial T_m}) + \frac{\partial c_s}{\partial T_m} + c_m \frac{\partial \varepsilon_{al}}{\partial T_m} \]

\[C_{cm T_f} = -c_m \alpha_f \left( \frac{1}{K_m} - \frac{1}{K_s} \right) Z_f R c_f \]

\[C_{cm u} = c_m \alpha_m ^T P \]

\[K_{cm c_m} = c_m Z_m R T_m \frac{k_m}{\mu} \]

\[K_{cm T_m} = c_m ^2 Z_m R \frac{k_m}{\mu} \]

\[K_{cm c_m, f} = \frac{1}{\tau} = -K_{cm c_m, m} \]

For heat transfer in the fracture continuum:

\[C_{T_f T_f} \frac{\partial T_f}{\partial t} + C_{T_f c_f} \frac{\partial c_f}{\partial t} = \nabla \cdot \left( K_{T_f T_f} \nabla T_f \right) + A_{T_f T_f} \nabla T_f + A_{T_f c_f} \nabla c_f + K_{T_f T_f, f} + K_{T_f T_f, m} \]  

(37)
where:

\[ C_{T/T_f} = n_f \rho_f C_{pg} - n_f (\rho_{gf} C_{pg} \mu_{JT} + 1) Z_f R c_f \]

\[ C_{T/c_f} = -n_f (\rho_{gf} C_{pg} \mu_{JT} + 1) Z_f R T_f \]

\[ K_{T/T_f} = \lambda_g \]

\[ A_{T/T_f} = -\rho_f C_{pg} v_f + \rho_f C_{pg} v_f \mu_{JT} Z_f R c_f \]

\[ A_{T/c_f} = \rho_f C_{pg} v_f \mu_{JT} Z_f R T_f \]

\[ K_{T/T_f,f} = -h_f A_{fm} - \Gamma_{mf} C_{pg} = -K_{T/T_f,f,m} \]

For heat transfer in the matrix continuum:

\[ C_{T/m} \frac{\partial T_m}{\partial t} + C_{T/cm} \frac{\partial T_m}{\partial t} = \nabla \cdot \left( K_{T/m} \nabla T_m \right) + A_{T/m} \nabla T_m + A_{T/cm} \nabla c_f + K_{T/m,f} + K_{T/m,m} \] (38)

where:

\[ C_{T/m} = (\rho_m C_{pm})_{eff} - n_f (\rho_{gf} C_{pg} \mu_{JT} + 1) Z_m R c_m \]

\[ C_{T/cm} = -n_m (\rho_m C_{pg} \mu_{JT} + 1) Z_m R T_m \]

\[ K_{T/m} = \lambda_{em} \]

\[ A_{T/m} = -\rho_m C_{pg} v_m + \rho_m C_{pg} v_m \mu_{JT} Z_m R c_m \]

\[ A_{T/cm} = \rho_f C_{pg} v_m \mu_{JT} Z_m R T_m \]

\[ K_{T/m,f} = h_f A_{fm} + \Gamma_{mf} C_{pg} = -K_{T/m,m} \]

### 3. Computational approach

A numerical solution of the coupled governing equations is achieved using the finite element method. The Galerkin weighted residual method is employed to spatially discretise the governing equations and an implicit mid-interval backward-difference time-stepping algorithm is used for temporal discretisation. A sequential implicit numerical approach is used to couple fluid flow with geomechanics. The solution procedure follows the works on coupled THCM behaviour for fractured porous media presented in detail by Thomas and co-workers [21, 27, 28]. Both systems of equations are simultaneously solved by iteration until convergence is achieved. Time dependent matrix and fracture properties like coal porosity and permeability are updated in each time step based on the numerical
results of the previous time step. This process continues until the specified simulation time is reached. Fig. 1 shows the implemented numerical solution procedure.

4. Model verification and validation

In the following sub-section, a verification test is used to provide confidence that the governing equations have been correctly implemented in the model, which is achieved by using an analytical solution as a benchmark. The test problem considers the coupled THM response of rock under thermal loading. This is followed by a validation test aimed at providing confidence in the ability of the proposed model to predict the behaviour of a coal-gas system based on published experimental measurements. More verification and validation tests on the developed model can be found in Chen [21].

4.1 THM response of rock under thermal loading

An analytical solution is only available for the coupled THM behaviour of a single porosity medium and so it is assumed that the fracture continuum is absent, which is realised by considering fracture porosity and permeability to be zero. This verification test considers a one-dimensional fully saturated poroelastic column restrained at its base and sides, such that only vertical (uniaxial) displacement is allowed, as shown in Fig. 2. Zero fluid pressure boundaries are imposed to the top surface, where fluid may exit freely from the column, and no flow boundaries are prescribed to both sides. A constant temperature of 273 K is applied to the top surface, the initial temperature is uniform at 323 K, the initial pressure is 0 Pa, and the initial equilibrium stress is fixed at zero. The analytical solution and parameters used in this verification test are taken from Selvadurai and Suvorov [29], as listed in Table 1.

Figs. 3 show the distributions of temperature, pore pressure and displacement along the column at selected times. It can be seen that there is a good agreement between the analytical solutions and the numerical results, which provides further confidence that the coupled model developed in this work has been accurately implemented in the COMPASS code.

4.2 Validation test for CO2 flow and coal deformation

Pini et al. [30] performed gas injection experiments on a high volatile bituminous coal core under hydrostatic confinement. Upstream and downstream pressures were measured and are now used as benchmarks to test the validity of the model developed in this work. The coal core was 2.54 cm in diameter and 3.6 cm long and was tested for He, N2 and CO2 injection at pressures ranging from 1 MPa to 8 MPa under constant and varying confining pressure. In this section, the results for CO2 injection under a constant confining pressure provide a benchmark for testing the performance of the numerical model in terms of the gas flow and coal deformation behaviour. Due to the highly heterogeneous pore
structure of coal, the permeability for fluid flow in coal seams is predominantly attributed to the fracture network, with the porous matrix typically making a negligible contribution. However, the coal matrix is predominantly micro-porous, which provides a large number of sites for gas adsorption. Hence, most gas stored in coal is adsorbed onto the surfaces of micropores and a DPSP model can reasonably be applied to describe the flow behaviour. A schematic of the coal core used by Pini et al. is shown in Fig. 4a, which can be simplified to the domain shown in Fig. 4b by taking advantage of axisymmetry.

Fig. 4b shows that no flow boundaries are used along the left- and right-hand sides of the domain. A time-dependent upstream CO2 injection pressure is prescribed, whilst for coal deformation a vertical constraint is applied to the upstream and downstream boundaries with a constant confining stress at the right-hand boundary. The left-hand side of the domain is fixed horizontally and the initial pressure is 1 MPa in both continua. The material parameters used for this test are provided in Table 2, many of which are taken from Pini et al.[30], with $\Gamma^{max}$ and $\varphi$ lumped together and obtained by fitting the swelling strain, as shown in Fig. 5. The internal swelling ratio comes from calibrating against the experimental data on permeability, as shown in Fig. 6. The fracture permeability used in Table 2 was selected from experimental test on Sulcis Coal presented in the work by Pini et al. [30]. A similar value of permeability can also be found in work of Zang et al. [31].

Comparisons of transient steps recorded in the experiment with those predicted by the model are shown in Fig. 7. It can be seen that the numerical model successfully predicted the CO2 flow dynamics in coal at the laboratory scale under the conditions considered, which provides confidence that the developed model may be applied in the simulation of CO2 sequestration in coal.

5. Analysis of THM behaviour during CO2 sequestration in coal

This section presents an application of the coupled model to study the non-isothermal behaviour of a 890 m deep and 5 m thick coal seam during CO2 injection. The coal seam is assumed to be homogenous, isotropic, and axisymmetric with a radius of 200 m around the injection well, as shown in Fig. 8a. To consider the interaction between the coal seam and adjacent rock strata, an analysis region is formed that runs 25 m vertically, comprising a 10 m thick caprock, the 5 m thick coal seam, and a 10 m thick underlying stratum. The system is assumed to be dry following primary CBM production with a uniform initial gas pressure and temperature of 0.1 MPa and 313 K, respectively. The caprock and underlying stratum are considered to be impermeable. A constant stress of 21 MPa is applied to the top surface of the caprock, corresponding to an overburden density of around 2450 kg/m$^3$, and displacement at the lower boundary and injection well is constrained. Due to different Poisson’s ratios for the rock strata and coal seam, radial stresses of 5.6 MPa and 11.2 MPa are assigned at the external boundary of the
rock strata and coal seam, respectively. For fluid flow, CO₂ is injected at a fixed injection rate of 0.2 kg/s at 313 K and it is assumed that no CO₂ permeates the caprock or underlying stratum.

The domain is discretised using 4-node isoparametric quadrilateral elements with a varying mesh size that gets finer towards the injection well, as shown in Fig. 8b. Table 3 shows the parameters used in this simulation; it is assumed that the thermophysical properties of coal and rock are constant. The ratio of local swelling to global swelling is evaluated by fitting the experimental results with parameters from the literature [17]. Analysis points are located 5 m, 20 m and 40 m radially from the injection well.

5.1 Gas pressure distribution within the coal seam

Figs. 9 and 10 show the predicted spatial and temporal changes of gas pressure in the fracture and matrix pore regions of the coal seam. Gas pressure in the fractures remains larger than in the coal matrix, although the size of this difference reduces with time and distance from the injection well. The higher transmissivity of the fractures means that gas pressure near the injection well increases rapidly, which in turn promotes mass transfer into the coal matrix. Further from the injection well, the gas pressure changes are slower and there is less distinction between the pore regions. The rate of equilibration between the pore regions strongly depends on the matrix block length, \( l \), taken here as a relatively small value of 0.01 m. Larger values of \( l \) will generally result in a larger and more sustained pressure difference between the pore regions than can be seen in Figs. 9 and 10.

5.2 Temperature distribution within the coal seam

Similar to the discussion of gas pressure given above, thermal equilibrium between the pore regions is established relatively quickly. Fig. 11 shows a temperature drop of more than 10 K that advances into the coal seam upon CO₂ injection, despite the temperature of the injected gas being the same as the initial coal seam temperature. This change in temperature results from Joule-Thomson cooling and can have a significant impact on CO₂ injectivity since CO₂ adsorption increases as temperature reduces, which may in turn increase the magnitude of coal swelling. Fig. 12 displays the temperature variation at radial distances of 5 m, 20 m and 40 m from the injection well. As a result of the larger changes in gas pressure near to the injection well, the temperature profile in this region shows the sharpest decline and then gradually recovers as injection continues. In contrast, temperature changes further from the injection well are more gradual as a result of the smoother changes in gas pressure.

5.3 Porosity and permeability changes within the coal seam

Fig. 13 shows the loss of fracture porosity resulting from CO₂ adsorption-induced coal swelling. This porosity loss is greatest near to the injection well early in the simulation, after which it becomes more
gradual as conditions tend towards equilibrium. In contrast, Fig. 14 shows that matrix porosity increases as a result of CO$_2$ injection, with this change again being most apparent near to the injection well. Porosity changes occur as a result of competitive mechanisms depending on the gas pressure, temperature, and CO$_2$ adsorption. Whilst the increase in gas pressure can increase fracture porosity by reducing the effective stress, the temperature decrease shown in Figs. 11 and 12 has a competing effect by increasing CO$_2$ adsorption and coal swelling. The net effect under the simulation conditions studied here was a loss of fracture porosity. In addition, CO$_2$ adsorption in the coal matrix increases the pressure difference between the pore regions and local swelling and leads to a large fracture-matrix compartment interaction. By comparing the porosity changes of both pore regions, it can be inferred that the fracture-matrix interaction plays an important role in the variation of coal porosity and can constrain the temperature effect.

The changes in fracture permeability caused by CO$_2$ injection are shown in Fig. 15; only the fracture permeability is shown since the fractures provide the principal pathways for fluid flow in coal seams. It can be seen that there is around a 90% reduction of permeability in the vicinity of the injection well relative to the initial permeability. This again highlights the predominant role of CO$_2$ adsorption-induced coal swelling, which overcomes the competing influence of elevated pore pressures that would tend to increase fracture permeability. Moreover, it has been shown that Joule-Thomson cooling led to a significant drop in temperature under the simulation conditions considered, which further strengthened coal swelling by increasing the CO$_2$ adsorption capacity.

6. Conclusions

In order to investigate the coupled response of coal to CO$_2$ injection, this study has presented a coupled thermal, hydraulic and mechanical (THM) model within the framework of dual thermo-poroelastic theory. A numerical solution for the system of governing equations is achieved using the finite element method. Model verification and validation tests have been pursued by comparing the numerical predictions with an analytical solution for a problem of thermo-poroelasticity and experimental results of CO$_2$ flow through a coal core. The model has then been applied to analyse THM behaviour during CO$_2$ sequestration in a coal seam.

Under the simulation conditions considered, the numerical results did not indicate a significant distinction between the gas pressures and temperatures in the fracture and coal matrix pore regions, which has been attributed to the input of a relatively small matrix block thickness. As expected, differences between the pressure and temperature of the two pore regions were largest nearer to the injection well and reduced with time and radial flow distance. Despite CO$_2$ being injected at the same temperature as that of the coal seam, a region of Joule-Thomson cooling was formed, whereby
temperatures in the vicinity of the injection well declined sharply before slowly recovering. The severity of this cooling zone reduced as the CO$_2$ advanced into the coal seam. CO$_2$ injection decreased the fracture permeability, especially near the injection well, highlighting the predominance of coal swelling caused by CO$_2$ adsorption. Moreover, the development of the cooling region further strengthened the coal swelling response since more gas adsorption occurs at lower temperatures. Based on the findings presented in this work, it is recommended that care is taken when assuming isothermal conditions in the computational study of problems of CO$_2$ sequestration. Whilst the development of a cooling region is not exclusive to the conditions found in coal seams, the temperature change can have a considerable influence on the flow regime due to the coupling with CO$_2$ adsorption and the associated coal swelling. The influence of non-isothermal behaviour therefore needs to be recognised, especially when making practical plans for CO$_2$ injection.

Acknowledgments

The first author gratefully acknowledges the financial support provided by the Welsh European Funding Office (WEFO), through the FLEXIS project. The financial support from the China Scholarship Council for the PhD studentship of the second author is also gratefully acknowledged.

References


Figures

Specify initial information

Calculate the coefficient matrices and build systematic stiffness matrix

Solve the governing flow equations and deformation process (COMPASS)

Check for convergence against tolerance limits on primary variables

Converged

Calculate the stress field

Update the fracture and matrix properties

No

End of analysis ?

End

Yes

Update mid-interval value

Loop through time step

Fig. 1 Numerical solution procedure of the coupled model.
Fig. 2 Schematic of the domain with the initial and boundary conditions used for the verification test.
Fig. 3. Comparisons between the numerical results and analytical solutions for (a) temperature, (b) pressure, and (c) displacement.
Fig. 4 Geometry and boundary conditions for the numerical simulation of an experiment performed by Pini et al. (37).

Fig. 5 Comparison of swelling strains predicted by the model with the experimental data.
**Fig. 6** Comparison of the permeability ratio predicted by the model with the experimental data.

**Fig. 7** Comparisons between the predicted results (lines) and experimental measurements (symbols) for the upstream and downstream pressure under a constant confining pressure.
Fig. 8 (a) Axisymmetric geological model and boundary conditions, and (b) mesh geometry for the numerical analysis performed to analyse coupled THM behaviour during CO$_2$ sequestration.
**Fig. 9** Radial pressure profiles within the coal seam outward from the injection well at selected times.

**Fig. 10** Temporal change of pressure at radial distances of 5 m, 20 m and 40 m from the injection well.
Fig. 11 Radial temperature distribution profiles within the coal seam at selected times.

Fig. 12 Temporal change of temperature at radial distances of 5 m, 20 m and 40 m from the injection well.
Fig. 13 Temporal changes of fracture porosity at radial distances of 5 m, 20 m and 40 m from the injection well.

Fig. 14 Temporal changes of matrix porosity at radial distances of 5 m, 20 m and 40 m from the injection well.
Fig. 15 Temporal changes of fracture permeability at radial distances of 5 m, 20 m and 40 m from the injection well.
## Tables

**Table 1** Material parameters used for the verification test (36).

<table>
<thead>
<tr>
<th>Material parameters</th>
<th>Value</th>
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<tbody>
<tr>
<td>Bulk modulus, $K$ (GPa)</td>
<td>5</td>
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<tr>
<td>Poisson's ratio, $v$ (-)</td>
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<tr>
<td>Permeability, $k_m$ (m²)</td>
<td>$6 \times 10^{-19}$</td>
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<td>Porosity, $n_m$ (-)</td>
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<tr>
<td>Fluid viscosity, $\mu$ (Pa·s)</td>
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<td>Modulus of solid constituent, $K_s$ (GPa)</td>
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<td>Fluid compressibility, $C_{cm}$ (GPa⁻¹)</td>
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<td>Effective specific heat capacity, $(\rho C_p)_eff$ (J/K·m³)</td>
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<td>Thermal expansion coefficient of solid, $\alpha_T$ (1/K)</td>
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<td>Thermal expansion coefficient of fluid, $\alpha_{Tm}$ (1/K)</td>
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**Table 2** Material parameters used for the validation test against the experiment by Pini et al. (37).

<table>
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<th>Material parameters</th>
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<td>Young's modulus of coal, $E$ (GPa)</td>
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<td>Matrix modulus, $K_m$ (GPa)</td>
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<td>Initial fracture porosity $n_{f0}$ (-)</td>
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<td>Density of coal, $\rho_c$ (kg/m³)</td>
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<tr>
<td>Viscosity of gas, $\mu_g$ (Pa·s)</td>
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<td>Langmuir volume constant, $V_L$ (mol/kg)</td>
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<td>Gas constant, $R$ (J/mol·K)</td>
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Table 3 Input parameters used for the numerical simulation of CO2 sequestration in coal.

<table>
<thead>
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<th>Material parameters</th>
<th>Value</th>
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<tr>
<td>Bulk modulus of rock, $K$ (GPa)</td>
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<td>Thermal conductivity of rock, $\lambda_r$ (W/m/K)</td>
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