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1**Modeling of CO₂ sequestration in coal seams: role of CO₂-**
2**induced elastic properties variation of coal on injectivity,**
3**storage efficiency and caprock deformation**

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35 **Abstract**

36 An effective and safe operation for sequestration of CO₂ in coal seams requires a clear understanding
37 of injection-induced coupled hydromechanical processes such as the evolution of pore pressure and
38 permeability as well as induced caprock deformation. In this study, CO₂ injection into coal seams
39 was studied using a coupled flow-deformation model with a new stress-dependent porosity and
40 permeability model that considers CO₂-induced elastic property variation. . Based on triaxial
41 compression tests of coal samples extracted from the site of the first enhanced coalbed methane field
42 tests in China, a substantial (one-order-of-magnitude) softening of Young's modulus and increase of
43 Poisson's ratio with adsorbed CO₂ content was observed. Such coal softening was considered in the
44 numerical simulation through an exponential relation between elastic properties (Young's modulus
45 and Poisson's ratio) and CO₂ pressure, considering that adsorbed CO₂ content is proportional to the
46 CO₂ pressure. The results of the numerical simulation show that the combination of softening of the
47 coal and enhancement of Poisson's ratio strongly affects the CO₂ sequestration performance, by
48 decreasing injectivity and stored volume (cumulative injection) during first ten days of injection,
49 and thereafter a softening mediated rebound in permeability tends to increase injectivity and storage
50 with time. A sensitivity study showed that hydromechanical characteristics including large softening
51 coefficient, high initial permeability and porosity, large initial Young's modulus and Poisson ratio
52 and high injection pressure all contribute synergistically to increase CO₂ injectivity and adsorption in
53 coal seams, but also result in larger caprock deformations. Overall, the study demonstrates the
54 importance of considering the CO₂-induced variations in elastic coal properties when analyzing the
55 performance and environmental impact of a CO₂-sequestration operation in unminable coal seams.

56 **Keywords:** CO₂ sequestration; Coal seams; Elastic modulus softening; Poisson's ratio rising; Caprock
57 deformations;

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711. Introduction

72CO₂ emitted during industrial burning of fossil fuels intensify the greenhouse effect that poses a
73serious long-term threat to the human living environment. Carbon capture and storage (CCS) is
74recognized as a promising approach to reduce CO₂ emission to the atmosphere and avoid further
75pollution of the natural environment ([Rubin, 2005](#)). CCS refers to a type of technology that captures
76CO₂ from the combustion of fossil fuels during industrial processes and store (or sequester) it deep
77underground. In geologic formations, CO₂ can be stored in oil and gas reservoirs, saline aquifers and
78coal seams ([Bachu, 2008](#); [Rutqvist and Tsang, 2002](#); [Van Bergen et al., 2004](#); [Haszeldine, 2009](#);
79[Ferronato et al., 2010](#); [Gou et al., 2014](#)). Among the geological sequestration options, storage of CO₂
80in deep and unminable coal seams has gained industrial attention because of its value added
81associated with Enhanced CoalBed Methane (ECBM) production ([White et al., 2005](#)).

82

83The storage of CO₂ in coal seams is a promising technology and a rational choice. In particular, the
84parts of coal seams that are not suitable for coal extraction offer a tremendous potential for
85sequestering CO₂ ([Gale, 2004](#)). The trapping mechanism for the storage of CO₂ in coal seams is
86different from those in saline aquifers and hydrocarbon reservoirs. Coal is a naturally fractured dual-
87porosity media consisting of cleat and matrix systems ([Warren and Root, 1963](#); [Gray, 1987](#)).
88Fractures and pores in cleat systems provide pathways for CO₂ seepage, while the micropores and
89grains in the matrix system act as the principal storage space where large quantities of CO₂ can be
90adsorbed. The CO₂ should stay adsorbed in the unminable coal as long as the reservoir pressure is
91above the desorption pressure ([Shukla et al., 2010](#)). Injection and storage of CO₂ in coal seams can
92also efficiently improve the production rate of coalbed methane (CO₂-ECBM) as have been observed
93in the field (e.g., [Zakkour and Haines, 2007](#)). Another important factor to consider related to storage
94of CO₂ in coal seams is that the adsorbed CO₂ can act as a type of plasticizer, which can alter the
95structure of a coal seam, which seems to improve the porosity and thereby increase the CO₂
96injectivity and storage capacity ([Goodman et al., 2006](#); [Shukla et al., 2010](#)).

97

98The plasticizing effect of adsorbed CO₂ can be expected to weaken the coal and thus result in a
99reversible decrease of elastic modulus and strength ([Ates and Barron, 1988](#); [Viete and Ranjith, 2006](#);
100[Masoudian et al., 2014](#)). For example, uniaxial compression testing by Viète and Ranjith (2006)
101showed that the elastic modulus could decrease by approximately 26%. Based on results from recent
102triaxial compression experiments, Masoudian et al. (2014) proposed a Langmuir-type relationship
103between the reduction in elastic modulus of bituminous black coal and adsorbed CO₂. However, in
104the study of Viète and Ranjith (2006), no obvious reduction in elastic modulus was found in
105experiments at high confining stress. This lack of weakening at high confining stress could be
106explained by decreased CO₂ adsorption at high confining stress ([Hol et al., 2011](#)).

107

108With CO₂ injection into coal seams, the free and adsorbed CO₂ could disturb the balance in the
109reservoir and induce changes in pore pressure and stress and cause heterogeneous swelling ([Reucroft
110and Patel, 1986](#)), which in turn, could significantly affect the permeability distribution within the
111coal seam. During CO₂ injection into a coal seam, the permeability is mainly controlled by the pore
112pressure and adsorption-induced swelling and their impact on the cleat system. An increase in pore

113pressure leads to a decrease in effective stress and thus enhances coal permeability. In contrast, the
114swelling of the coal matrix induced by the adsorption of CO₂ decreases the permeability ([Siriwardane](#)
115[et al., 2009](#); [Liu and Rutqvist, 2010](#)).

116
117A number of porosity and permeability models have been proposed to represent the effects of pore
118pressure and CO₂-adsorption-induced swelling on the evolution of permeability/porosity. The S&H
119model ([Seidle and Huitt, 1995](#)) assumes that permeability changes are only caused by coal matrix
120swelling. The P&M model ([Palmer and Mansoori, 1998](#)) includes a theoretical equation for porosity
121as a function of pore pressure, incorporating the effects of elastic properties and sorption-induced
122strain for low-porosity (less than 10^{-1}) coal seams under uniaxial stress conditions. Exponential
123forms are frequently used to formulate changes in porosity and permeability as a function of fluid
124pressure. Two well-known exponential permeability models, the S&D ([Shi and Durucan, 2004](#))
125model and C&B ([Cui and Bustin, 2005](#)) model, were developed for conditions of uniaxial strain and
126assuming that the horizontal stress and mean normal stress affect the permeability and porosity,
127respectively. In both of these models, the pore modulus is simplified to be constant, though pore
128modulus in coal actually varies with porosity and stress ([Detournay and Cheng, 1993](#)). Another
129exponential permeability model by Liu and Rutqvist (2010) considers fracture–matrix interaction
130during coal-deformation processes based on the concept of internal swelling stress, which can
131explain experimental data showing permeability decrease with CO₂ adsorption under constant
132confining stress.

133
134In this paper, a coupled flow-deformation model that employs a new stress-dependent porosity and
135permeability model and considers CO₂-induced coal softening and Poisson's ratio variation are
136applied to study CO₂ injection into coal seams. Though experimental evidence of substantial
137softening of coal and variation of Poisson's ratio with CO₂ content, such elastic property variations
138have generally not been considered in previous analyses of CO₂ sequestration operations in
139unminable coal. The objective of this study is to investigate the effects of such CO₂-induced coal
140softening and Poisson's ratio variation on the performance of CO₂ sequestration into coal seams. In
141this paper, we first provide the theoretical background and derive governing equations related to
142coupled fluid flow and mechanical deformations, including a new model for permeability evolution
143that considers coal swelling and CO₂-induced coal softening and Poisson's ratio variation. The
144governing equations are implemented and solved with the multi-physics software COMSOL, which
145is then applied for the study of coupled fluid flow and deformations during CO₂ injection into coal
146seams. The simulation results are presented to demonstrate the effects of elastic modulus softening
147and Poisson's ratio variation on permeability, injectivity, storage efficiency and deformations. In
148addition, the implications of the elastic property variations, hydraulic properties (porosity and
149permeability) and elastic properties (Young's modulus and Poisson ratio) of coal seams and injection
150pressure are studied in a sensitivity analysis. Overall, the study demonstrates the importance of
151considering the CO₂-induced softening when analyzing the performance and environmental impact of
152CO₂-sequestration in unminable coal seams.

153

1542. Governing and Constitutive Equations

1552.1. Coal seam deformation

156 On the basis of the constitutive relation of poroelasticity, stress equilibrium, effective stress law, and
157 considering CO₂-adsorption-induced volumetric strain (Cui and Bustin, 2005), the governing
158 equation for deforming coal seams can be expressed as follows (Rutqvist et al., 2001):

$$159 \quad \sigma = \sigma' - \alpha I p = D : (\varepsilon - \varepsilon_s \delta) - \alpha I p \quad (1)$$

160 where α is Biot's coefficient, σ and σ' are total and effective stress tensors, p is pore
161 pressure, D is the tangential stiffness matrix and ε_s is the sorption-induced volumetric strain
162 calculated by the Langmuir-type equation as:

$$163 \quad \varepsilon_s = \varepsilon_L \frac{p}{p + p_L} \quad (2)$$

164 where ε_L and p_L represent the Langmuir volumetric strain and Langmuir
165 pressure constants, respectively.

1652.2. Gas flow

166 The CO₂ mass balance equation for coalbed methane includes adsorption, diffusion and seepage and
167 is defined as:

$$168 \quad \frac{\partial m}{\partial t} + \nabla \cdot (\rho_g \vec{v}_g) = Q_s \quad (4)$$

169 where ρ_g is the gas density, \vec{v}_g is the Darcy velocity vector, t is time, Q_s is the gas
170 source, and m is the gas content, which includes the free and adsorbed CO₂ and is defined as
171 (Zhang et al., 2008):

$$172 \quad m = \rho_g \phi + \rho_{ga} \rho_c \frac{V_L p}{p + p_L} \quad (5)$$

173 where ϕ is the porosity of the cleat system, V_L is the Langmuir volume constant, ρ_c is coal
174 density and ρ_{ga} is CO₂ density under standard conditions.

175 According to the ideal gas law, gas density is given by:

$$176 \quad \rho_{ga} = \frac{p}{p_a} \rho_g \quad (6)$$

177 where p_a is the standard atmospheric pressure. In addition, gas-flow through the cleats according
178 to Darcy's law without the gravity effect is expressed as:

179 $\bar{v}_g = \frac{-k}{\mu} \nabla p$ (7)

180 where k is the permeability of the coal cleat system, and μ is the gas viscosity.

181 Substituting Eqs. (5), (6) and (7) into Eq. (4) gives the following governing equation for gas flow in
182 the cleat system:

183
$$\left[\phi + \frac{\rho_c p_a V_L p_L}{(p + p_L)^2} \right] \frac{\partial p}{\partial t} + p \frac{\partial \phi}{\partial t} + \nabla \cdot \left(\frac{-k}{\mu} p \nabla p \right) = Q_s$$
 (8)

184

185 From Eq. (8), the partial derivative of ϕ with respect to time is expressed as

186
$$\frac{\partial \phi}{\partial t} = S \left(\frac{-1}{K} \frac{\partial \sigma'}{\partial t} + \frac{\alpha - 1}{K} \frac{\partial p}{\partial t} \right)$$
 (14)

187 where $S = (\phi_0 - \alpha) \exp \left\{ \frac{-1}{K} [(\sigma' - \sigma'_0) + (1 - \alpha)(p - p_0)] \right\}$

188

189 Substituting Eq. (14) into Eq. (8), the governing equation yields

190
$$\left\{ \phi + \frac{\rho_c p_a V_L p_L}{(p + p_L)^2} + \frac{pS(\alpha - 1)}{K} \right\} \frac{\partial p}{\partial t} + \nabla \cdot \left(\frac{-k}{\mu} p \nabla p \right) = Q_s + \frac{pS}{K} \frac{\partial \sigma'}{\partial t}$$
 (15)

191 Eqs. (15) and (1) are the governing equations for gas flow and mechanics, respectively, that will be
192 solved considering various couplings, including those related to elastic property variations with CO₂
193 content and permeability variation with effective stress and swelling. These processes will be
194 described in detail in the next two subsections.

195

196

197 2.5 Elastic property variation with CO₂ content

198 In this paper, the results of triaxial compression tests on coal specimens are used to derive a
199 relationships for how elastic modulus and Poisson's ratio changes with CO₂ with adsorbed CO₂
200 content. Because adsorbed CO₂ is a function of CO₂ pressure, we directly relate elastic properties to
201 CO₂ overpressure, which is the gas pressure applied by injection minus the initial pressure in the coal
202 specimens. The initial pressure within the coal specimens was equal to atmospheric pressure, which
203 correspond to such a small CO₂ content that it has no significant influence on the elastic properties.
204 The dimension, test conditions and elastic modulus of the coal specimens are listed in Table 1.
205 Specimens with a diameter of about 50 mm and a height of about 102 mm were prepared from drill
206 cores obtained from a mine in the Qinshui Basin, which is the site the first CO₂ enhanced coalbed
207 methane (CO₂-ECBM) recovery single-well micro-pilot tests in China (Wong et al., 2010; Li and
208 Fang, 2014). The CO₂-saturated specimens were prepared by permeating CO₂ at different pressure
209 for 24 hours to ensure the desired saturation level. The triaxial tests were carried out with a loading
210 rate of 1 MPa/min until the confining pressure reached 5.0 MPa and then the specimens were loaded
211 axially to failure under a displacement rate of 0.005 mm/s.

212

213

214**Table 1**

215Dimension, test conditions, elastic modulus and Poisson's ratio of coal specimens

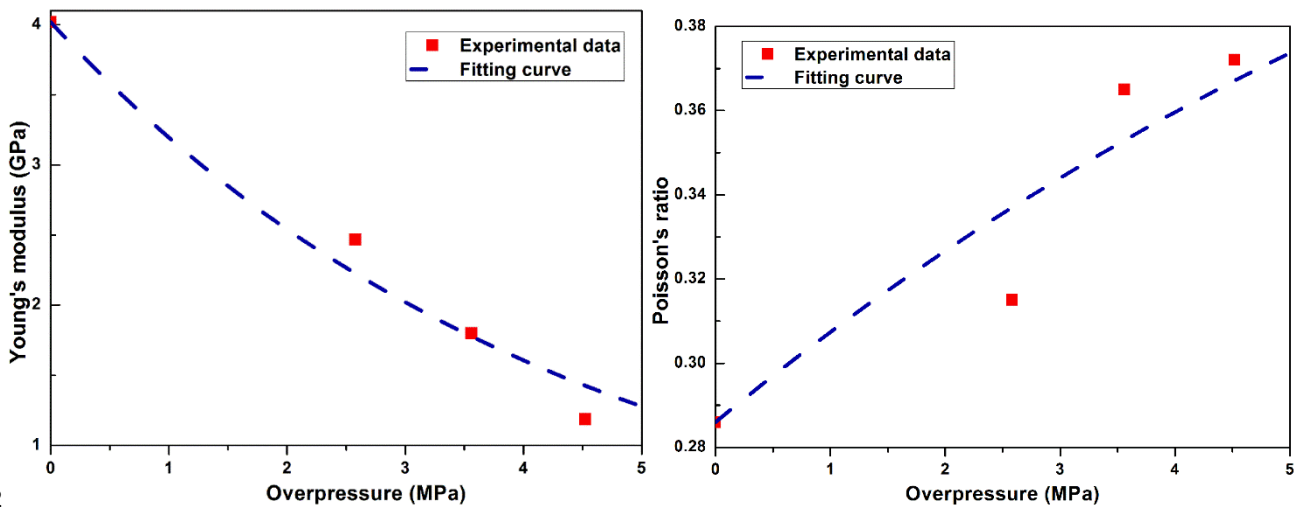
NO.	diameter (mm)	Height (mm)	Confining Pressure (MPa)	Overpressure (MPa)	Elastic Modulus (GPa)	Poisson's ratio
1	49.62	102.56	5.0	4.52	1.188	0.372
2	49.74	101.78	5.0	3.56	1.8	0.365
3	49.72	102.66	5.0	2.58	2.469	0.315
4	49.62	101.20	5.0	0	4.018	0.286

216

217The Young's modulus and Poisson's ratio versus overpressure for the experimental results are plotted
 218in Fig. 1 (red points). It can be clearly observed that the elastic modulus decreases and Poisson's ratio
 219increases with the increase in overpressure. The experimental data of Young's modulus is fitted to an
 220exponential relation written as

221 $E = E_{max} \exp(-a \times \Delta p)$ (9)

222



223 **Fig. 1. Exponential relationship between Young's modulus and Poisson's ratio, and overpressure**

224The Poisson's ratio is related to overpressure according to

225
$$u = u_m + \frac{m}{u_0 - u_i} \Delta p$$

226where Δp is the over pressure. E_{max} is the maximum/initial elastic modulus with no significant

227amount of CO₂ adsorbed in the coal, i.e. at low or atmospheric pressure. u_0 is Poisson's ratio at

228 zero overpressure and u_m is the limiting value of 0.5. The exponents a and b in Eqs. (9) and (10),
 229 are coefficients determining the rate of variability with increasing CO₂ overpressure. A larger a
 230 and b would result in more decrease of E and increase of u with overpressure. In this case,
 231 a and b are estimated to 0.2291 and 0.1054, respectively, by matching the exponential model
 232 to experimental data (Fig.1) using a least squares method with reasonable coefficients of
 233 determination ($R^2=0.9737$ and $R^2=0.8716$).

234 2.3 Evolution of porosity and permeability

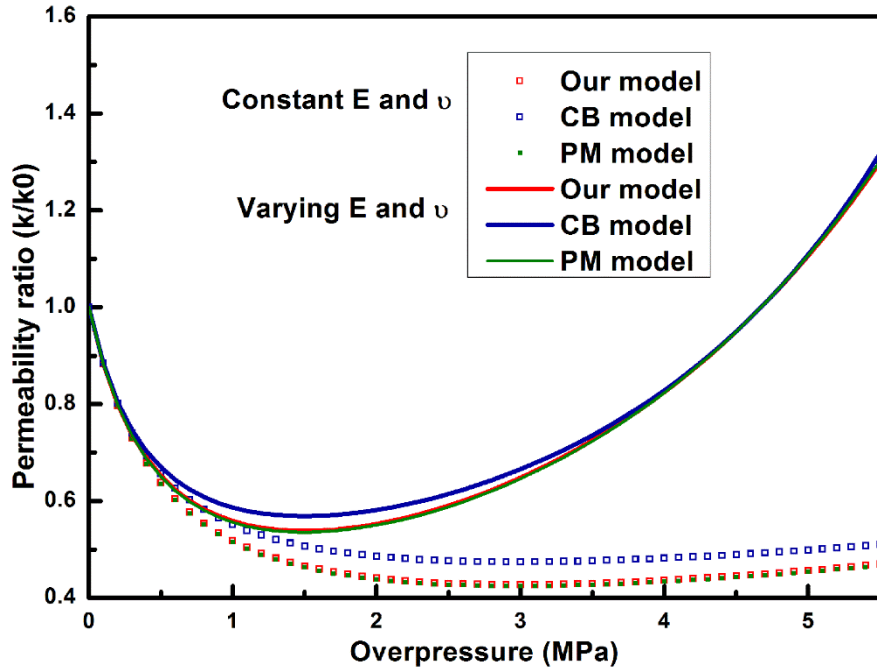
235 An increase of pore pressure during CO₂ injection will expand the pore volume resulting in increased
 236 porosity and permeability. While considering gas migration through a coal seam with desorption or
 237 adsorption, the changes in gas pressure (and gas concentration) induces coal swelling or shrinkage
 238 that in turn changes coal porosity and permeability. In this study, a new model relating porosity to
 239 mean effective stress is built based on the C&B model (**Appendix A**):

$$240 \quad \phi = \alpha + (\phi_0 - \alpha) \exp\left\{\frac{-1}{K} [(\sigma' - \sigma'_0) + (1 - \alpha)(p - p_0)]\right\} \quad (11)$$

241 Without consideration of the Klinkenberg effect, a cubic law is used to describe the relationship
 242 between the permeability and porosity of the porous media, which is shown as follows

$$243 \quad \frac{k}{k_0} = \left(\frac{\phi}{\phi_0}\right)^3 = \left\{\frac{\alpha}{\phi_0} + \frac{(\phi_0 - \alpha)}{\phi_0} \exp\left\{\frac{-1}{K} [(\sigma' - \sigma'_0) + (1 - \alpha)(p - p_0)]\right\}\right\}^3 \quad (12)$$

244 where ϕ_0 and k_0 represent the initial porosity at pressure p_0 and the initial effective stress.



245
 246 Fig. 2. Influence of elastic modulus on the proposed permeability model, C&B and P&M models. Poisson's ratio of
 247 0.35, an initial reference permeability of $1 \times 10^{-14} \text{ m}^2$, an initial reference porosity of 0.8%, an injection pressure

248 of 6 MPa and an initial coal-seam pressure of 0.5 MPa are assumed for all three models.
 249 Assuming that the coal-seams are under conditions of uniaxial strain, constant coal-seam loading and
 250 $\alpha=1$, our model, C&B model and P&M model are expressed as in Eqs. (A.18), (A.19) and
 251 (A.20), respectively. The permeability ratio versus pressure for the three models are plotted in Fig. 2.
 252 The red line is the model proposed in this paper, the green and the blue lines represent the C&B and
 253 P&M models, respectively. The solid lines are the evolution of the permeability ratio with a varying
 254 elastic modulus E and Poisson's ratio ν described in Eqs. (9) and (10), whereas the square
 255 symbols represent permeability evolution when assuming constant E and ν . The Langmuir-type
 256 relationship between pore pressure P and adsorption induced strain ϵ_s increases strongly at
 257 early time, while the change of ϵ_s is more flat at a higher injection pressure at later time. Thus, a
 258 clear decline in permeability is observed in all three models for both cases from its initial value with
 259 increasing pressure as a result of strong swelling of coal matrix. Then, it has no obviously rebound
 260 with a constant E and ν ($E=4.018 \text{ GPa}$, $\nu=0.286 \text{ GPa}$), but enhances up to a 1.3 times
 261 (solid lines) with the combination of a varying E and ν , as a result of reduced adsorption effect
 262 and dominance of pore pressure effect. The pressure where permeability starts to rebound is called
 263 as the rebound pressure (Shi and Durucan, 2004), which is given as (Cui and Bustin, 2005)

$$264 \quad p_{rb} = \sqrt{\frac{E \epsilon_s V_L p_L}{3\nu}} - p_L \quad (13)$$

265 From the equation, an increase of Poisson's ratio and a decrease of Young's modulus both reduce the
 266 rebound pressure that advances the permeability rebound. In two cases, permeability in C&B model
 267 predicts an obvious larger value than P&M and our model without consideration of the changes in
 268 the pore modulus. The value of permeability in our model is similar to the P&M model. This is

269because the P&M model can be deduced by Taylor expansion for the exponential function in our
 270model.
 271

2723. Numerical Implementation

273The governing Equations and constitutive relations described above are implemented within
 274COMSOL Multiphysics, which is an efficient visual platform for simulating and analyzing coupled
 275phenomena with finite elements method (<http://www.comsol.com/>). Two pre-arranged modules
 276named Geomechanics and Fluid Flow are selected to solve the partial differential equations (PDEs).
 277The schematic of solving coupled CO₂ flow and coal seam deformation in COMSOL, including
 278governing equations and coupling relations are illustrated in Fig. 3.

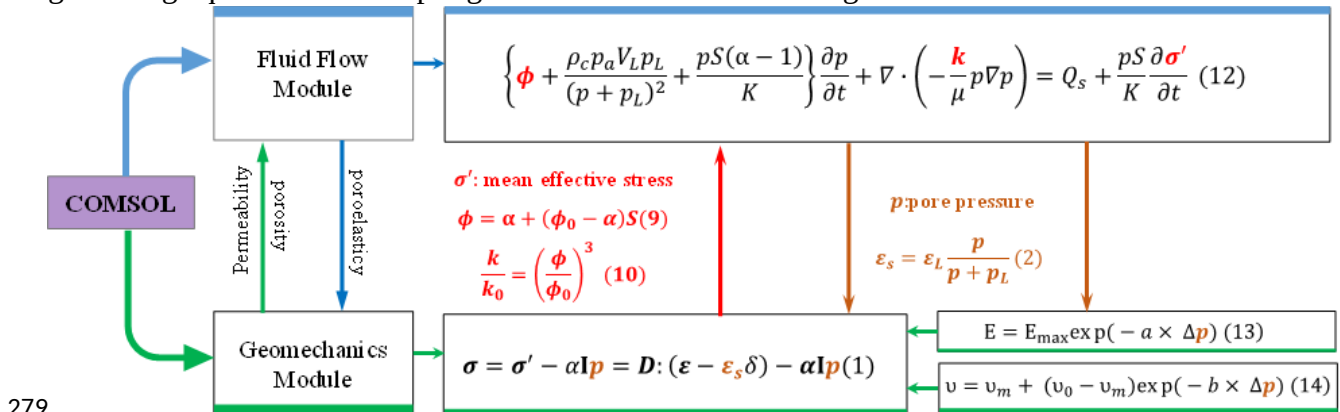


Fig. 3. Schematic of modeling coupled CO₂ flow and coal seam deformation in COMSOL

281First, the model geometry is built in the COMSOL graphic window. Thereafter, various material
 282properties are assigned, including density and viscosity of CO₂ and permeability, porosity, density,
 283elastic modulus and passion's ratio of the coal seam and surrounding rock The boundary and initial
 284conditions are also set in the two modules. For CO₂ flow, pressure and no flow boundary conditions
 285are defined:

$$286 \quad p = p_0 \quad \text{on} \quad \partial\Omega \quad ; \quad -n \cdot \rho u = 0 \quad \text{on} \quad \partial\Omega \quad (16)$$

287Here p_0 is the specified CO₂ pressure on the boundary $\partial\Omega$, n is the vector normal to the
 288boundary, ρ is gas density and u is the velocity vector. The initial condition for flow is:

$$289 \quad p(0) = p \quad \text{in} \quad \Omega \quad (17)$$

290For geomechanics module, displacement and stress conditions are specified on the boundary as

$$291 \quad u = u_0 \quad \text{on} \quad \partial\Omega \quad ; \quad s \cdot n = F_A \quad \text{on} \quad \partial\Omega \quad (18)$$

292where u_0 and F_A are the prescribed displacement and stress on the boundary $\partial\Omega$ and S

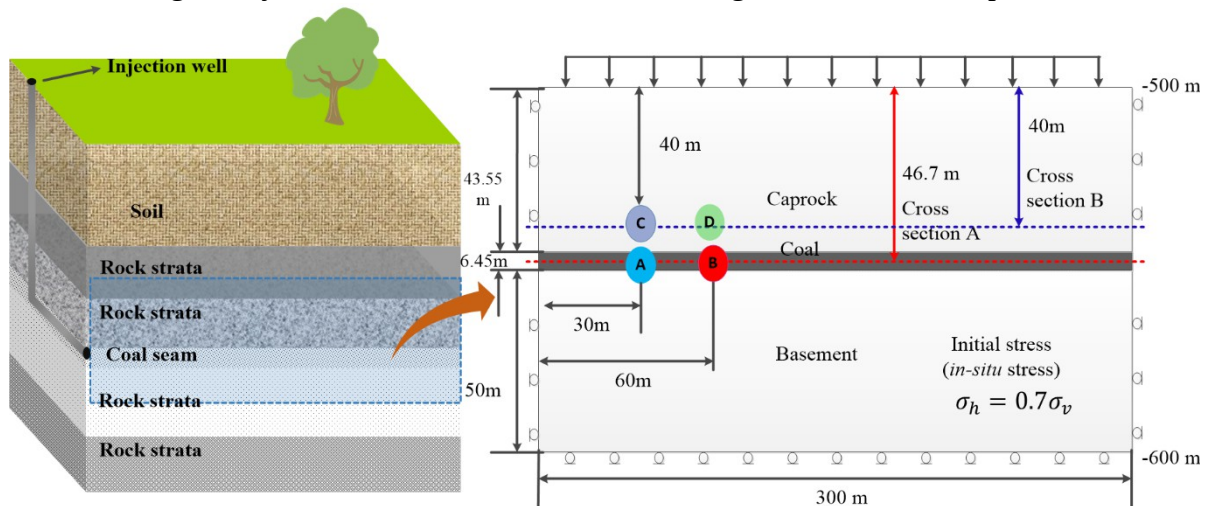
293is stress symbol in COMSOL. The initial conditions for displacement and *in-situ* stress in the domain
 294are described as

$$u(0)=0 \in \dot{\Omega} ; \quad s(0)=s \in \dot{\Omega} \quad \Omega \quad (19)$$

296 Finally, in the simulation conducted in this paper a default MUMPS solver was employed to solve all
 297 the equations in a fully coupled (monolithic) mode. Note that in this modeling we selected a
 298 relatively small absolute and relative tolerance (compared to default settings) for a stringent and
 299 accurate solution. It makes the model run slightly slower, but it is an efficiency method to stabilize
 300 convergence and improve the precision of the calculation.

301 4. Geometry and material properties

302 Fig. 4 illustrates a conceptual model of CO₂-injection from a horizontal well (on the left) and the
 303 two-dimensional computational model geometry for the analysis of CO₂ injection into a coal seam.
 304 The choice of a horizontal well configuration is a pragmatic one, simplifying the model geometry to
 305 a two-dimensional plane strain model. However, in the field a horizontal well configuration could be
 306 beneficial by accessing a larger reservoir area and being able to take advantage of known anisotropic
 307 permeability and thereby help alleviate permeability reduction and injectivity loss in a CO₂-ECBM
 308 and/or CO₂ storage project ([Durucan and Shi, 2009](#)). The injection formation (coal seam) has a
 309 thickness of 6.45 m and the model extends 300 m horizontally, which ensures that the overpressure
 310 does not reach the right boundary over the time scale of the simulation. The coal seam is bounded by
 311 a 50-m thick basement and a 43.55-m thick caprock, and half of a horizontal well is modeled at the
 312 symmetry plane of the left lateral boundary. The permeability of the caprock and basement was
 313 assumed to be small enough so that the injected CO₂ is completely confined within the coal seam. In
 314 other words, the gas only flows within the coal seam and no gas leaks into the caprock and basement.



315

316

Fig. 4. 3D conceptual model and geometric configuration and

317

2D computational model domain with initial and boundary conditions

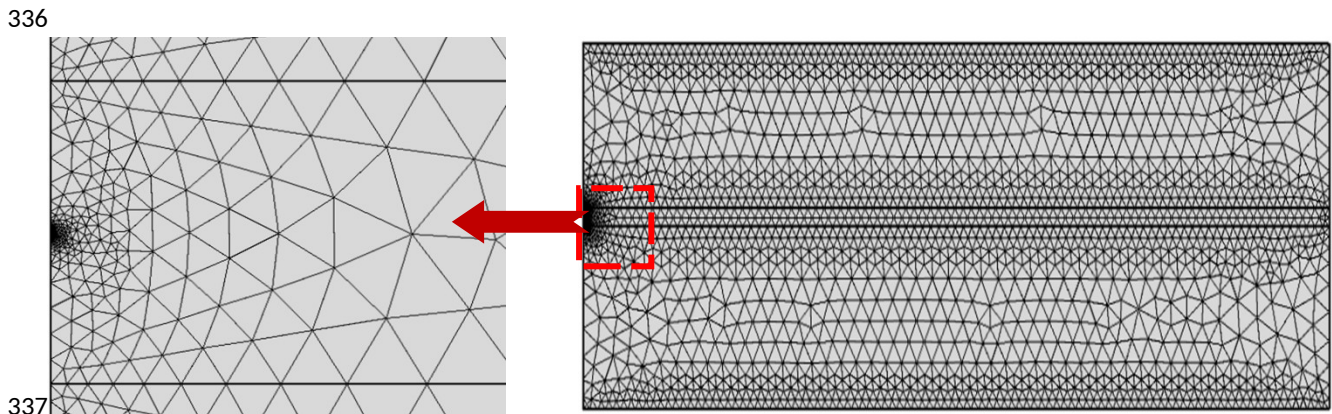
318 In the simulations, CO₂ was injected from the simulated wellbore located at the mid elevation of left
 319 boundary of the coal seam. The injection pressure was linearly increased to 6 MPa in the first two
 320 days and then kept constant. The initial pore pressure of CO₂ in coal-seam was assumed to be 0.5
 321 MPa, which assumes that CO₂ injection commences into a coal seam previously pressure depleted by
 322 primary production and is gas saturated ([Kumar et al., 2014](#)). In this model, the top of the caprock is
 323 located at the depth of 500 and has a vertical boundary loading of 11.3 MPa corresponding to the

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324 weight of the overburden for an average overburden rock density of 2300 kg/m^3 . An extensional
 325 stress regime ($\sigma_h = 0.7 \sigma_v$) was assumed. Displacement constraints were assigned normal to the
 326 left, right and bottom boundaries. First, a stationary study was carried out to ensure equilibrium and
 327 correct *in-situ* and effective stress vertical gradients at the start of the coupled simulation of the CO₂
 328 injection. All of the simulation cases were meshed with the dense triangular element discretization
 329 shown in Fig. 5 to minimize interpolation errors. The coal and CO₂ properties listed in Table 2 are
 330 taken from the results of history matching of a micro-pilot test at Qinshui (Wong et al., 2007). In
 331 addition, The Biot's coefficient α for the coal seam is assumed to be 0.57 calculated by Eq. (A3)
 332 with coal grains Young's modulus of 8.14 GPa (Zhang et al., 2008), fluid viscosity is 1.6×10^{-5} .
 333 The caprock and basement are assumed impermeable having Young's modulus of 25 and 30 GPa and
 334 Poisson's ratio of 0.339 and 0.25. That is the rock units above and below the coal seam is
 335 significantly stiffer than the coal seam.



338 Fig. 5. Finite element mesh in COMSOL (on the right). The figure on the left shows a close-up view of mesh near
 339 the injection boundary.
 340

341 Table 2

342 Parameters for the coal seam from history matching of a micro-pilot test at Qinshui (Wong et al., 2007)

Parameter	Value
Young's modulus (GPa)	8.14
Poisson's ratio	0.339
Permeability (D)	1.0E-12
Porosity	0.25
Fluid viscosity (Pa·s)	1.6E-5
Biot's coefficient	0.57
Rock density (kg/m ³)	2300
Caprock Young's modulus (GPa)	25
Basement Young's modulus (GPa)	30
Caprock Poisson's ratio	0.339
Basement Poisson's ratio	0.25

3445. Simulation results and discussion

345To explore the effects of coal softening on CO₂ sequestration into coal seams, the following two
346numerical simulation cases were defined:

347

348Case A: The elastic modulus of coal softens during CO₂ injection as a result of overpressure (and
349CO₂ concentration), as described by Eq. (13).

350

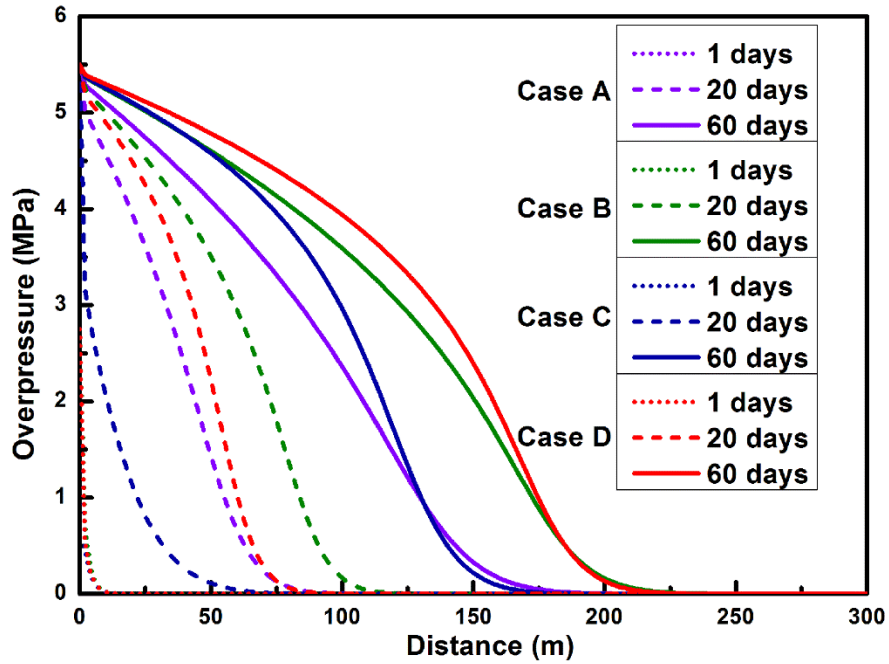
351Case B: Elastic modulus is assumed to be constant and equal to the initial elastic modulus of 3.5
352GPa.

353

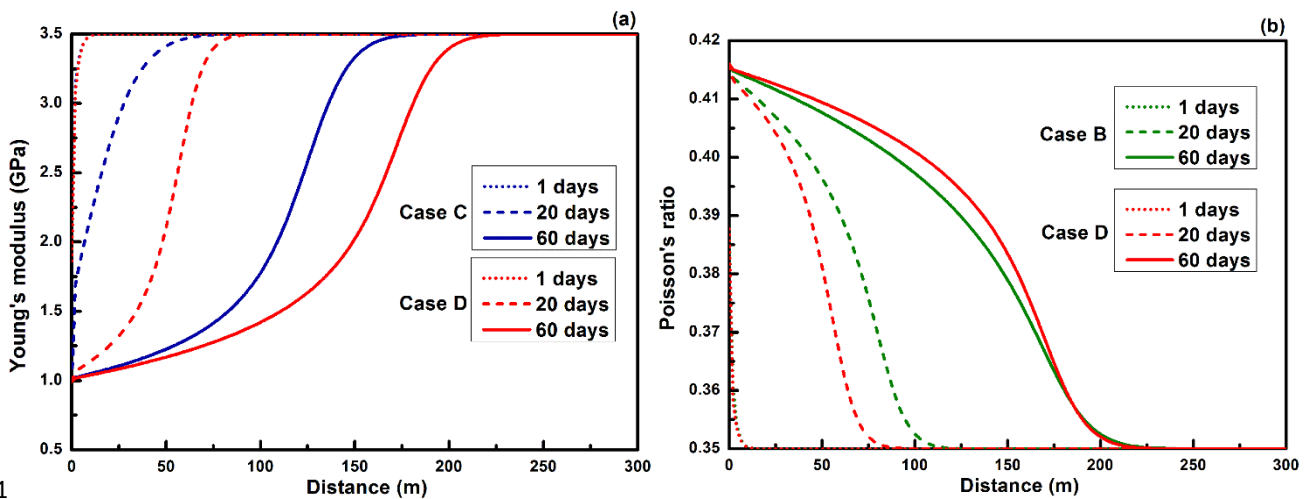
354We consider Case A, including modulus softening as the base case and by comparing the simulation
355results for Case A and Case B we can study the effect of coal softening on the CO₂ injection
356performance.

3575.1 Simulation results

358Fig. 6 shows the distributions of overpressure along cross-section A in the coal seam after 1, 20 and
35960 days of injection for four the different cases. The overpressure range of the coal seam with
360increasing pore pressure keeps expanding away from the gas injection well. After 60 days of
361injection, gas pressure has already propagated approximately 180 m for case A and C (purple and
362blue solid lines) and 220 m for case B and D (green and red solid lines) away from the well. The
363result shows that in the injection process the speed at which the gas pressure front propagates into the
364coal seam is different for the four cases. After 1 day of injection, there is no clear difference (dotted
365lines in Fig. 6). Thereafter, the pressure in case B with a constant modulus E and variable
366Poisson's ratio ν (green dashed line in Fig. 6) propagates farthest (about 110m). At the later stage
367(after 60 days injection), the pressure in cases with varying ν (green and red solid lines)
368propagates faster and farther into the coal seam than cases with constant ν (purple and blue solid
369lines). The pressure in the case with a softening elastic modulus E (blue and red solid lines) is
370larger near the wellbore, while smaller away from the wellbore.



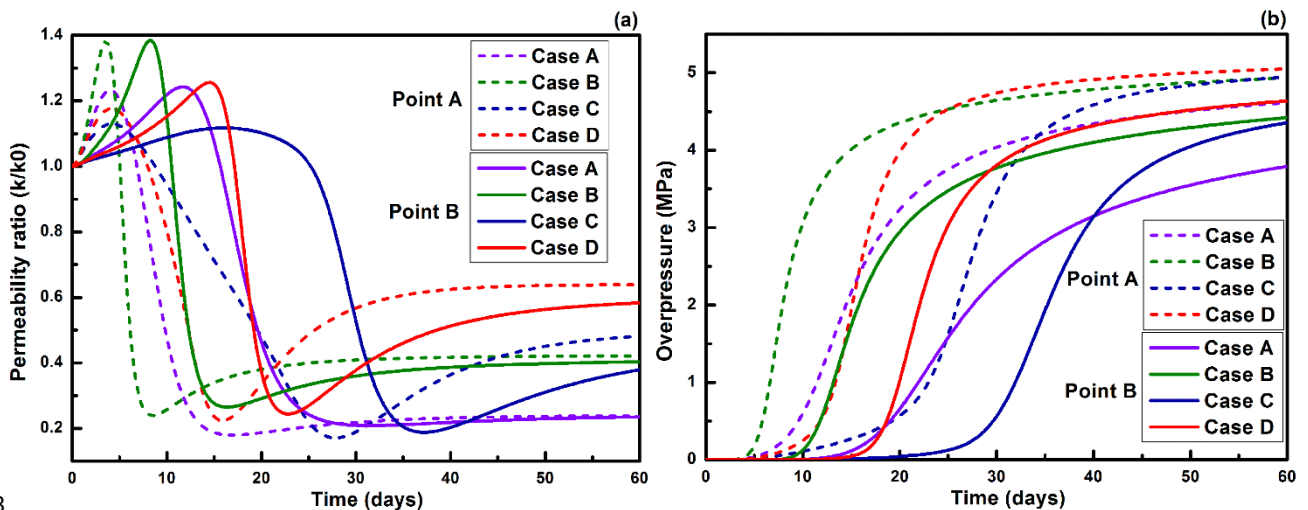
371
 372 **Fig. 6. Distributions of overpressure for four the different cases after 1, 20 and 60 days of injection CO₂**
 373 Fig. 7 shows Young's modulus and the Poisson's ratio along cross-section A in the coal seam after 1,
 374 20 and 60 days of injection for the four different cases. As the overpressure in the coal seam
 375 increases, Young's modulus decreases and Poisson's ratio increases according to the experimentally
 376 fitted exponential relationship in Eqs. (9) and (10). In Fig. 7, the reduction of the modulus E and
 377 enhancement of Poisson's ratio ν of can be observed as far as the overpressure propagates, i.e.
 378 180 and 220 m for E (blue and red solid lines in Fig. 7a) and 220 m for ν (green and red solid
 379 lines in Fig. 7b) from the injection well. The minimum E and ν are approximately 1.00 GPa and
 380 0.415 close to the wellbore.



381
 382 **Fig. 7. Profiles of Young's modulus (a) and Poisson's ratio (b) along cross section A at the mid-elevation of the coal**
 383 **seam after 1, 20 and 60 days.**

384 The time-evolution of permeability ratio (k/k_0 , where k_0 is the initial permeability) and pore
385 pressure at two points (A, B) along the horizontal direction is shown in Fig. 8 for the four different
386 cases. At early stages, before the overpressure reached points A and B the permeability in all the
387 cases (Fig. 8a) increase. This change in permeability ahead of the pressure can be explained by the
388 fact that strain and displacement can propagate ahead of the pressure front in a porous elastic media.
389 The peak permeability is largest in Case B with a varying Poisson's ratio ν (green lines in Fig.
390 8a), whereas the peak permeability increase is much smaller for Case C and D (blue and red lines in
391 Fig. 8a) with a softening elastic modulus E . This demonstrates that an increasing ν promotes
392 the enhancement of permeability and a softening modulus E has an opposite effect. After
393 overpressure reaches points A and B, permeability decreases with increasing overpressure as a result
394 of dominant effect of swelling. Thereafter, the permeability undergoes different rebounds with
395 continued injection as a result of reduced coal swelling effects (Masoudian et al., 2013) and the
396 dominance of pore pressure effects. The pressure propagates fastest in Case B (green lines in Fig. 8b)
397 and slowest in Case A (purple lines in Fig. 8b) that also affect the timing of the permeability rebound.
398 The results in Fig. 8 show that an increase of Poisson's ratio ν and a decrease of Young's modulus
399 E can be beneficial in promoting rebound of permeability. Indeed, with the combination of
400 varying E and ν , Case D displays the largest permeability (rebound) and pore pressure at later
401 time (red lines in Fig. 8a and 8b).

402



403

404 Fig. 8. (a) Permeability (b) pore pressure in the coal seam versus time at different points within the coal seam.

405

406 Fig. 9 shows a comparison of CO₂ injection rate and cumulative CO₂ injection for the four cases of
407 constant or variable elastic properties The CO₂ injection rate Q_d is defined as

$$u dA = 2 * \int u * 1 dl \quad (18)$$

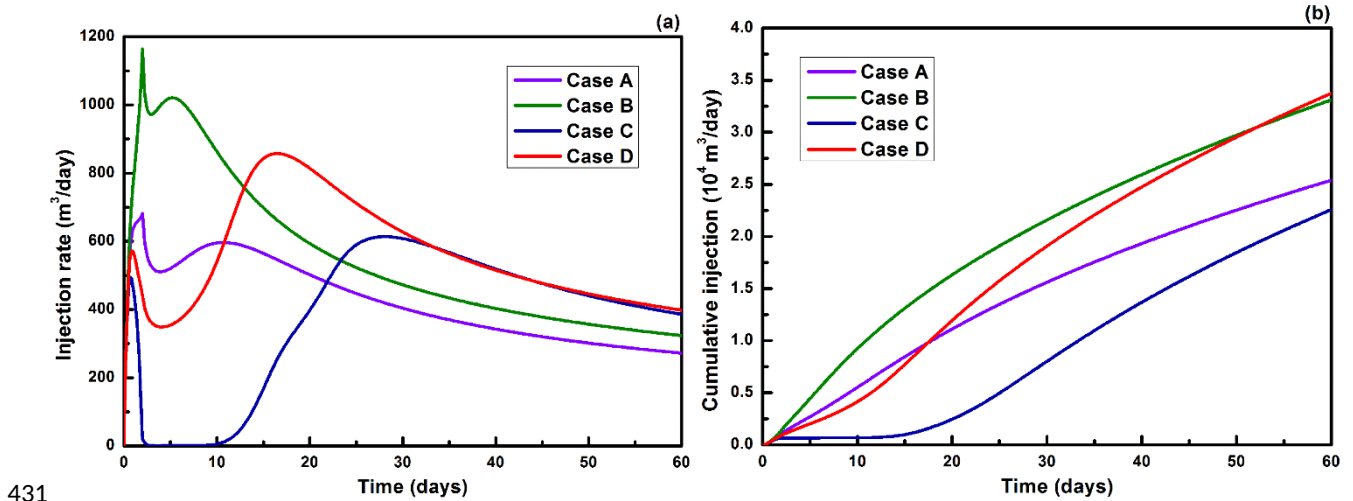
$$Q_d = 2 * \int \dot{v}$$

where u is the CO₂ fluid velocity through the injection boundary, which is directly extracted from simulation results in COMSOL. The cumulative injection Q_t is calculated by

$$Q_t = \int Q_d dt \quad (19)$$

In Eq. (18), A is the injection area representing the horizontal well surface area, where l is the vertical thickness of the injection element ($l=0.1$) and the factor 1 correspond to 1 m of the horizontal well. Thus, the injection rate and cumulative injection in Fig. 9 are per meter well, whereas the total injection rate and cumulative injection volume would be obtained by multiplying with the total length of the horizontal injection rate.

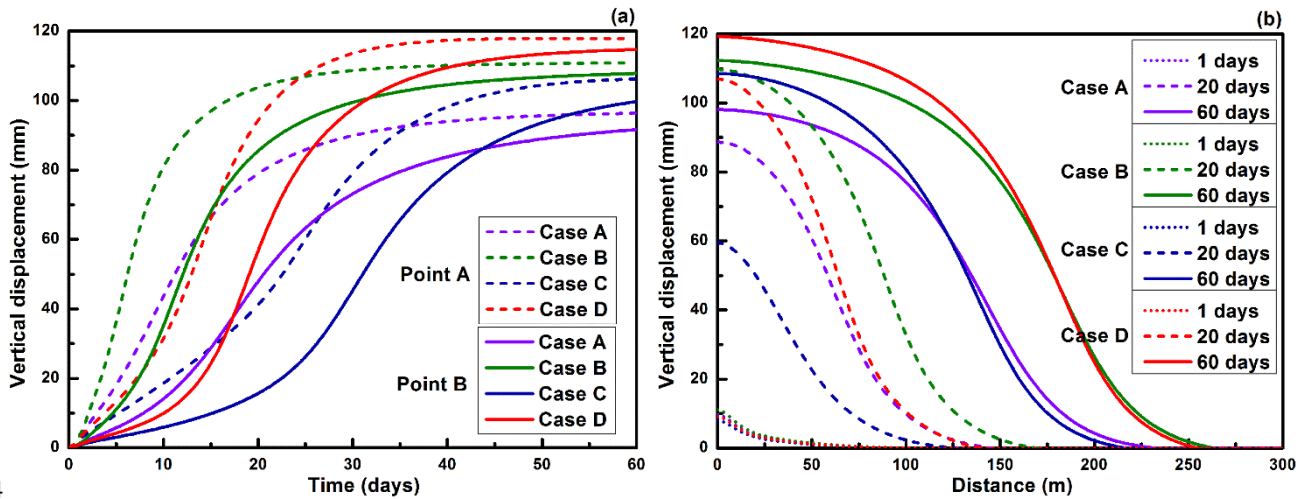
In all four cases an initial peak in the CO₂ injection rate occurs in the first few hours of injection a result of a large pressure contrast between injection pressure and initial pore pressure in the coal seam (Fig. 9a). At early time, the injection rate and cumulative injection in Case B (green lines in Fig. 9a and 9b) are larger than in other cases for its larger enhancement of permeability (green lines in Fig. 8a). With continued CO₂ injecting, the injection rate in Case D exceeds others (red line in Fig. 9a), which tends to decrease the difference of cumulative injection between Case B and D (green and red lines in Fig. 9b). Towards the end of the simulation Case D cumulative injection exceeds that of Case B for its continued high daily injection (red line in Fig. 9). The higher injection rate at later times in the case of a softening modulus and an increasing u are attributed to the stronger permeability rebound in Case D (red lines in Fig. 8a) that accelerates gas pressure and CO₂ propagation into the coal seam. This demonstrates that the CO₂-induced softening of the elastic modulus and rising of Poisson's ratio can enhance CO₂ injectivity and storage capacity for a long-term CO₂ injection into deep coal seams.



431

31
32

432 **Fig. 9. (a) CO₂ injection rate and (b) cumulative CO₂ injection versus time for four different cases.**
 433The injection-induced increase in pore pressure within the coal seam gives rise to vertical
 434displacement in the caprock as shown in Fig. 10. At early stages, the vertical displacements in Case
 435B (green solid lines in Fig. 10a) are larger than for the three other cases, but towards the end of the
 43660 days injection, the displacements magnitudes are the largest for Case D. The evolution and
 437distribution of vertical displacements in Fig. 10 generally follow the pore pressure evolution in Fig.
 4388b and distribution in Fig. 6. This shows that the adsorption induced changed in elastic properties
 439affects coal permeability and pressure diffusion that in turn affect the vertical expansion and uplift.
 440The uplift can be observed far away (150 and 200 m) from the injection boundary, and the maximum
 441uplift in the case of softening elastic modulus E and increasing Poisson's ratio ν is
 442approximately 120 mm (red solid line in Fig. 10b), about 22 mm larger than that in the case of
 443constant E and ν (purple solid line in Fig. 10b).



444
 445**Fig. 10. (a) Vertical displacement versus time at points C and D in the caprock (b) Vertical displacement along**
 446**cross-section B in the caprock 6.7 m above the coal seam after 1, 20 and 60 days of injection.**

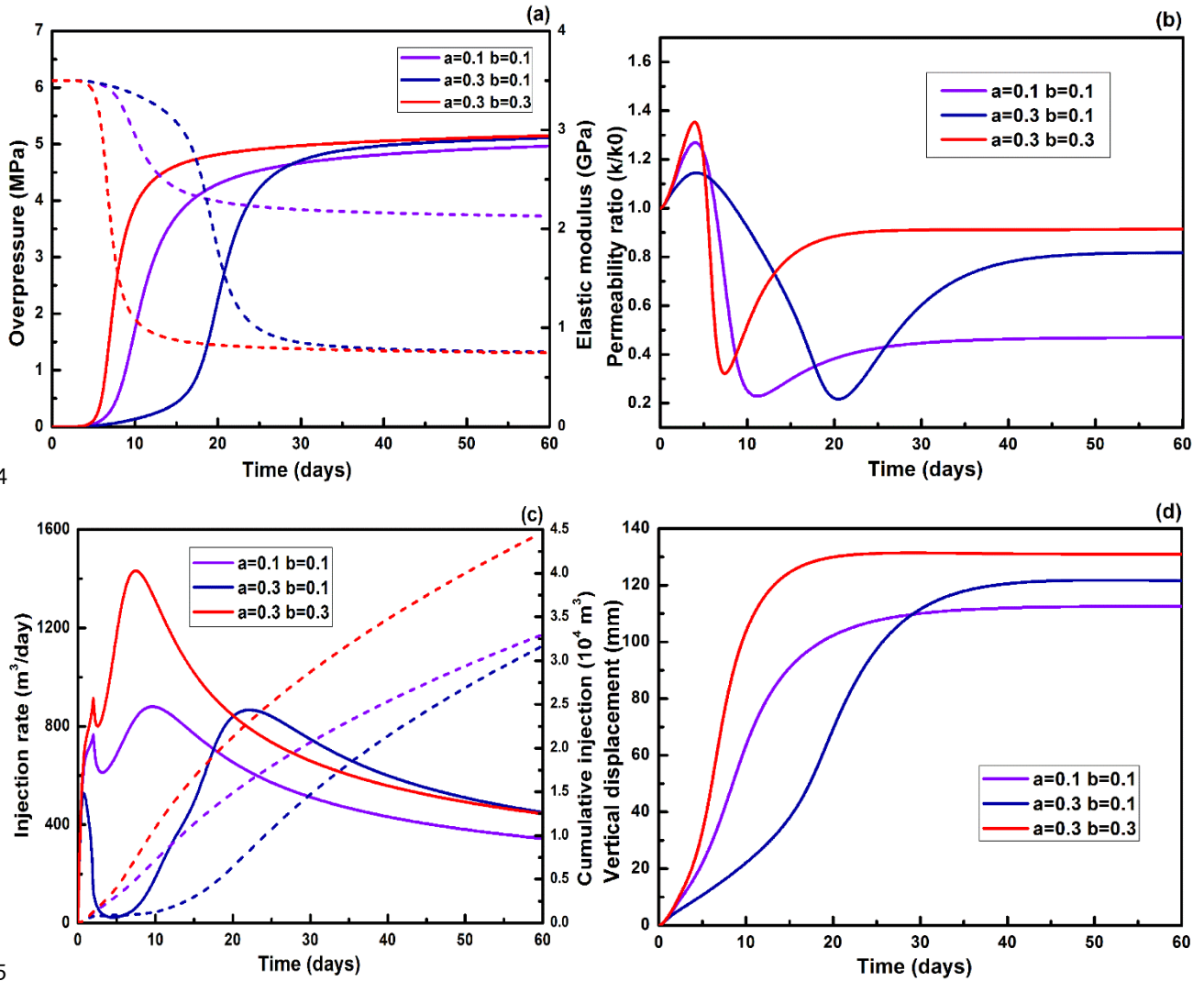
447
 448**5.2 Sensitivity analysis**

449The following subsections (5.2.1-5.2.4) present a sensitivity analysis to study how the CO₂ injection
 450performance depends on coefficients a and b related to CO₂-adsorption-induced changes in
 451elastic properties, hydraulic properties (porosity and permeability) and initial elastic properties
 452(Young's modulus and Poisson's ratio) of coal seams, as well as how the injection pressure affects
 453the performance of the CO₂ injection. In particular, we study the injection rate, cumulative injection
 454and the evolution of parameters at two control points in the model domain. We present the evolution
 455of pore pressure, elastic modulus and permeability at point A, which is located at a distance of 30 m
 456away from the injection wellbore and at the mid-elevation of the coal seam. We also present vertical
 457displacement at point C, located in the caprock 6.7 m above the coal seam.

458 5.2.1 Effect of coefficients a and b

459 Fig. 11 shows the effect of coefficients a (0.1 and 0.3) and b (0.1 and 0.3) on
460 hydromechanical parameters; the time-evolutions of overpressure, elastic modulus, permeability
461 ratio, injection rate, cumulative injection and vertical displacement. The elastic properties of different
462 coal seams may be more or less sensitivity to CO₂ adsorption, which in our model correspond to
463 different values of coefficients a and b . The value of a and b are may be related to the
464 *in-situ* stress state (uniaxial or triaxial compression), mechanical properties (elastic modulus and
465 Poisson's ratio) and components (clay, sand or other mineralogy) of coal ([Levine, 1996](#); [Viète and
466 Ranjith, 2006](#); [Hol et al., 2011](#); Masoudian et al., 2014; Mishra and Dlamini, 2012; [Masoudian et al.,
467 2014](#)). The equation for the softening of the elastic modulus as a function of overpressure implies
468 that a larger value of a induces more elastic modulus softening. The Young's modulus is reduced
469 to 21.3% of its initial value when $a=0.3$, but only to 68.9% when $a=0.1$ (dashed lines in Fig.
470 11a).

471
472 At early stages, the coal with a smaller a and same $b=0.1$ result in a larger overpressure,
473 permeability, injection rate and deformation (purple vs blue line in Fig.11). At later stages, more CO₂
474 is injected into the coal seam for higher values of a (blue solid line in Fig. 11c) and the final
475 cumulative injection at 60 days are close in the two cases with different a (purple vs blue dashed
476 line in Fig. 11c). Among the three cases, the pressure propagates fastest for a coal with larger a
477 and b that results in the highest injection rate, permeability peak and rebound, cumulative
478 injection and deformation (red lines in Fig. 11). As noted previously in this paper, an increase of
479 Poisson's ratio can promote the enhancement of permeability, whereas a decrease of Young's
480 modulus has the opposite effect at the early stages. Compared this conclusion with permeability
481 variations in Fig. 11b, it infers that coefficient a is more influential than coefficient b at early
482 time. Later, under the combination of a smaller modulus and larger Poisson's ratio, the permeability
483 can rebound earlier (red line in Fig. 11b).



484

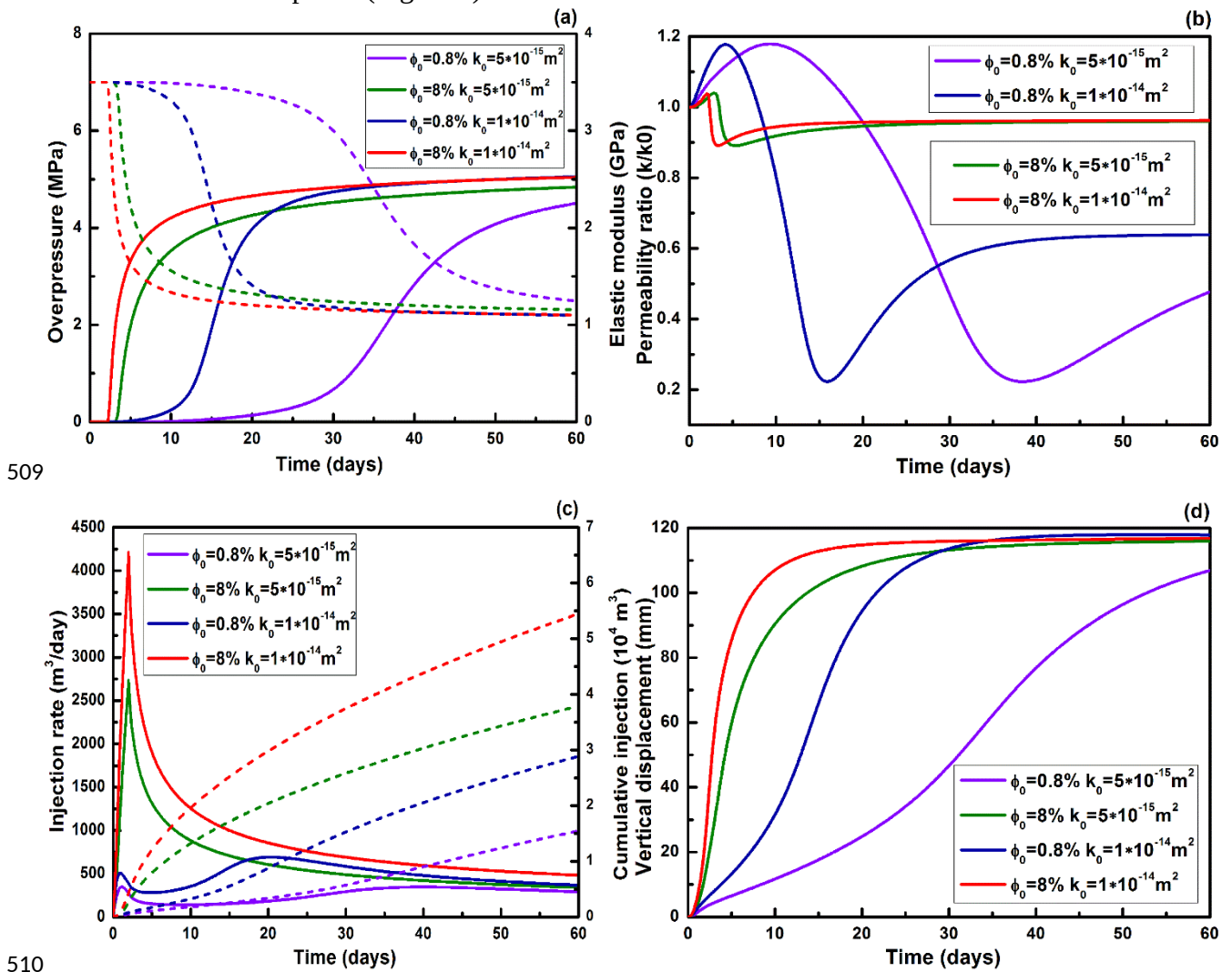
485

486 Fig. 11. Effect of coefficient a and b on (a) pore pressure and elastic modulus, (b) permeability, (c)
 487 injection rate and cumulative injection, and (d) vertical displacement. An initial reference porosity of 0.8%,
 488 permeability of $1 \times 10^{-14} \text{ m}^2$, injection pressure of 6 MPa and an initial coal-seam pressure of 0.5 MPa are
 489 applied in all simulations.

490 5.2.2 Effect of hydraulic properties (permeability and porosity)

491 Permeability of the cleat system is recognized as one of the most important parameters for the
 492 injectivity into coal seams (Wei and Zhang, 2010). Varying permeability and related porosity result in
 493 large changes in overpressure, which then in turn affects elastic modulus, Poisson's ratio,
 494 permeability changes, injection rate, cumulative injection and vertical displacement (Fig. 12). In a
 495 coal-seam with a higher permeability and same porosity, the gas overpressure front and CO_2 reaches
 496 the same distance away from the wellbore in a shorter time. For example, in the case of a relatively
 497 high initial permeability $k_0 = 1 \times 10^{-14} \text{ m}^2$, the gas pressure front reaches point A after about 2
 498 days of injection, while it takes approximately 4 days with a smaller permeability of $5 \times 10^{-15} \text{ m}^2$

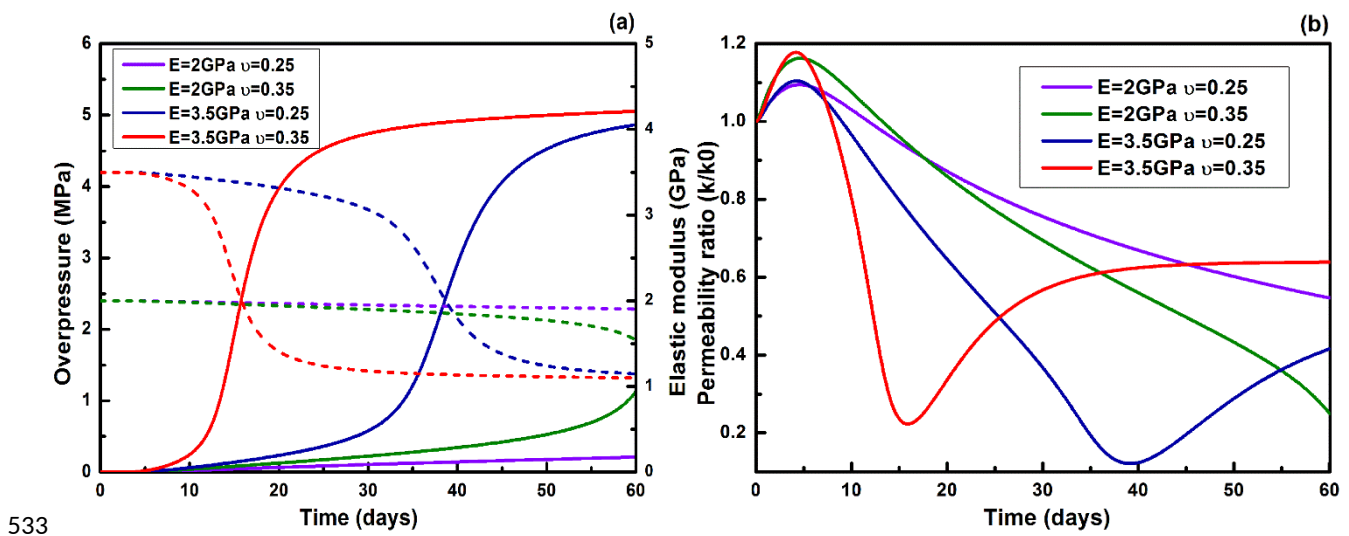
499(red vs green solid line in Fig. 12a). In other words, in the case of higher permeability more CO₂ can
500be injected and adsorbed inside a coal seam over the same injection time period. The permeability
501decreases to 90% of its original value for the case with a high porosity ($\phi_0=8$) (red and green
502lines in Fig. 12b) and as low as 20% of initial permeability (blue and purple lines in Fig. 10b) for a
503case with a small porosity ($\phi_0=0.8$). This also contributes to improve CO₂ daily and cumulative
504injection efficiency (dashed and solid lines in Fig. 12c). In other words, the initial porosity is more
505influential than initial permeability on the change of permeability and CO₂ injection. Higher initial
506porosity and permeability are preferable for the improvement of CO₂ injection efficiency into coal
507seams. The higher overpressure and corresponding softening of elastic modulus also cause a larger
508deformation in the caprock (Fig. 12d).



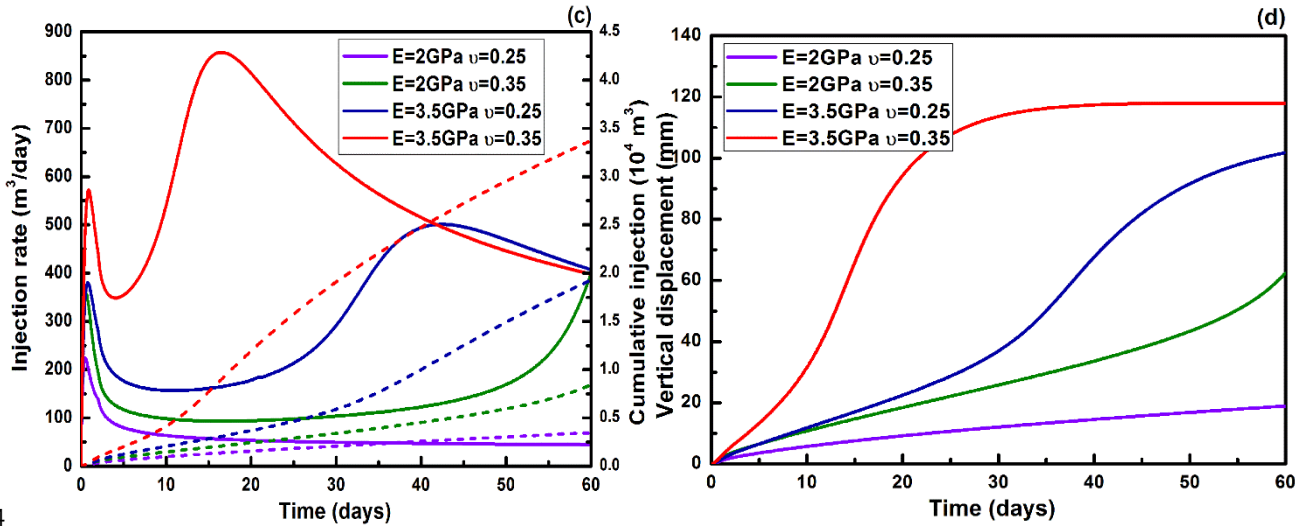
511Fig. 12. Effect of hydraulic properties on (a) pore pressure and elastic modulus (b) permeability (c) injection rate
512and cumulative injection (d) vertical displacement. The coal seam has an initial reference cleat system porosity of
5130.8% or 8% and an initial reference permeability of 1×10^{-14} or $5 \times 10^{-15} \text{ m}^2$. A softening coefficient of
5140.2291, an injection pressure of 6 MPa and initial coal-seam pressure of 0.5 MPa are applied in all simulations.

515.2.3 Effect of elastic properties (Young's modulus and Poisson's ratio)

516 The coal mechanical properties (Young's modulus E and Poisson's ratio ν) control the
 517 variation of permeability (Bustin and Bustin, 2012) that affects the CO₂ injection efficiency. Fig. 13
 518 presents hydromechanical parameters versus time for various Young's modulus E and Poisson's
 519 ratio ν . For a coal with a larger Poisson's ratio ($\nu=0.35$) and same E , the injection
 520 efficiency of CO₂, permeability peak and caprock deformation are larger than a coal with a small ν
 521 (green vs purple and red vs blue lines in Fig.11). For a coal with a larger Young's modulus (
 522 $E=3.5\text{GPa}$), the pore pressure is obviously higher (red and blue solid lines in Fig.11a) that
 523 causes larger changes of modulus (red and blue dashed lines in Fig.11a) and Poisson's ratio with
 524 continued injecting. The permeability in the four cases displays similar trends with an increase
 525 during the first few days and then a decrease. The permeability undergoes a significant rebound from
 526 around 15 and 40 days of injection (red and blue lines in Fig.11b). At the later time, no recovery of
 527 permeability (green and purple lines in Fig.11b) occurs for the smaller pore pressure and the higher
 528 rebound pressure in a stiffer coal with larger Young's modulus (green and purple dashed lines in
 529 Fig.11a). Consequently, less CO₂ injection rate and caprock deformation are predicted for a coal with
 530 smaller E (blue and purple lines in Fig.13c and 13d). Overall, initial Poisson's ratio is less
 531 influential than initial Young's modulus on permeability rebound. The larger pore pressure and more
 532 soft coal with a smaller E cause larger deformation in the caprock (Fig.13d).



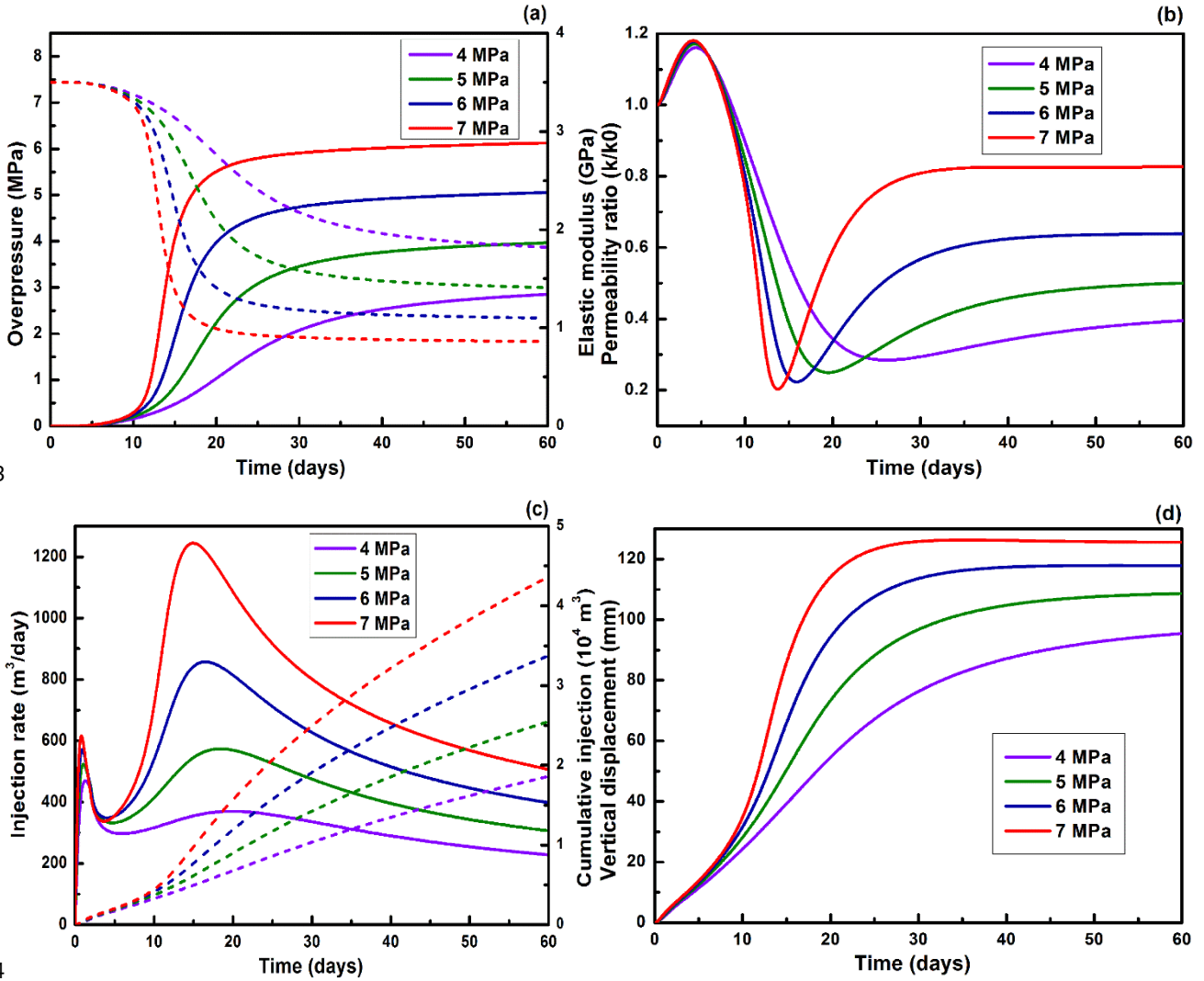
533



534
 535 Fig. 13. Effect of initial Young's modulus and Poisson's ratio property on (a) pore pressure and elastic modulus,
 536 (b) permeability ratio, (c) injection rate and cumulative injection, and (d) vertical displacement. An initial
 537 reference porosity of 0.8%, an initial reference permeability of $1 \times 10^{-14} \text{ m}^2$, softening coefficient of 0.2291 and
 538 an injection pressure of 6 MPa are applied in all simulations.
 539

540 5.2.4 Effect of injection pressure

541 The evolution of overpressure, elastic modulus, permeability ratio and vertical displacement for
 542 different injection pressures is shown in Fig. 14. The injection pressure governs the total amount of
 543 CO_2 that can be injection into a coal seam (Cui and Bustin, 2005); CO_2 can be injected at a higher
 544 rate and more CO_2 can be adsorbed with a high injection pressure. For coal seams with same initial
 545 gas pressure, a higher injection pressure results in a higher coal-seam overpressure and injection rate
 546 peak (solid line in Fig. 14a and 14c). The higher overpressure, in turn, results in a greater elastic
 547 modulus softening (dashed lines in Fig. 12a) and Poisson's ratio rising, higher permeability increase,
 548 injectivity, and storage efficiency. Larger injection pressure advance the pore pressure to reach the
 549 rebound pressure that causes an earlier and larger rebound of permeability. The permeability
 550 undergoes a more significant rebound for the case with a higher injection pressure (Fig. 11b). The
 551 peak of injection rate and cumulative injection is correspondingly higher for the cases with a larger
 552 injection pressure (Fig. 11c).



553

554

555 Fig. 14. Effect of injection pressure on (a) pore pressure and elastic modulus, (b) permeability, (c) injection rate
 556 and cumulative injection and (d) vertical displacement. An initial reference porosity of 0.8%, an initial reference
 557 permeability of $1 \times 10^{-14} \text{ m}^2$, softening coefficient of 0.2291 and an initial coal-seam pressure of 0.5 MPa are
 558 applied in all simulations.

559 A high injection pressure helps improve the injectivity and storage efficiency, but it also leads to a
 560 larger rock deformation in the caprock. The vertical displacement (uplift) increases from
 561 approximately 95 to 125 mm when injection pressure increases from 4 to 7 MPa (Fig. 14d). Thus, it
 562 is necessary to consider potential impact of such uplift on the overburden integrity and surface
 563 structures when designing an injection operation for an efficient injection and acceptable uplift.

5646. Conclusions

565 In this study, CO₂ injection into coal seams was studied using a coupled flow-deformation model
566 with a new stress-dependent porosity and permeability model that considers CO₂-induced elastic
567 property variation. This model incorporates free and adsorbed CO₂, coal deformation, and changes
568 in elastic properties (Young's modulus and Poisson's ratio) with CO₂-content. Coefficients that
569 govern changes in Young's modulus and Poisson's ratio with CO₂ pressure were determined from
570 triaxial compression tests of coal samples extracted from the site of the first CO₂-ECBM recovery
571 pilot tests in China. The triaxial compression tests shows that the elastic modulus softens and
572 Poisson's ratio increases significantly with increasing CO₂ content when the CO₂-pressure increases
573 from atmospheric to 4.52 MPa. The objective of this study is to investigate the effects of varying
574 elastic properties on the performance of CO₂ sequestration into coal seams, including injectivity,
575 stored mass (cumulative injection) and caprock deformation, and how such performance is affected
576 by the evolution of parameters such as permeability, porosity, modulus and Poisson's ratio.

577
578 Simulation results showed that the injectivity, stored mass, and caprock deformation are significantly
579 affected by the CO₂-induced changes in Young's modulus and Poisson's ratio.. At early stages of
580 injection, an increase of Poisson's ratio promotes an increase of permeability that in increases the
581 injection efficiency while the elastic modulus softening has an opposite effect of decreasing injection
582 efficiency. With continued injecting, a decrease of elastic modulus has a dominated impact on
583 reducing the rebound pressure required to rebound permeability, which significantly improves the
584 longer term CO₂ injectivity and storage efficiency. However, a smaller elastic modulus and higher
585 overpressure also lead to larger deformations in the caprock and overburden. A sensitivity study
586 showed that hydromechanical characteristics including larger changes in elastic properties through
587 coefficients a and b , high initial permeability and porosity, large initial Young's modulus and
588 Poisson ratio and injection pressure all contribute synergistically to increase CO₂ injectivity and
589 adsorption in coal seams, but also result in larger caprock deformations and uplift. Overall, the study
590 shows the importance of considering the CO₂-induced elastic property variations when analyzing the
591 performance and environmental impact of a CO₂-sequestration operation in unminable coal seams.

592
593 **Appendix A**
594 With consideration of the CO₂-sorption induced volumetric strain, the strain and stress relationship
595 for a deforming coal seam is ([Shi and Durucan, 2004](#))

$$596 \quad \sigma'_{ij} = 2G \varepsilon_{ij} + \lambda \varepsilon_t \delta_{ij} - \left(\lambda + \frac{2}{3}G \right) \varepsilon_s \delta_{ij} \quad (A.1)$$

597 where ε_t is the bulk volumetric strain, δ_{ij} is the Kronecker symbol; ε_s is sorption-induced
598 volumetric strain, G and λ are the Lamé constants, described in terms of Young's modulus, E
599 and Poisson's ratio, ν as

$$600 \quad G = \frac{E}{2(1+\nu)}, \lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}$$

601 In this paper, the adopted sign convention is that tensile strain and stress are positive and
602 compressive are negative. The effective stress σ' is calculated as

$$603 \quad \sigma'_{ij} = \sigma_{ij} + \alpha p \delta_{ij} \quad (A.2)$$

604 where σ is the total stress. The Biot coefficient α is defined as

$$605 \quad \alpha = 1 - \frac{K}{K_s} = 1 - \frac{E}{E_s} \quad (A.3)$$

606 where K and E is the bulk modulus and K_s is the modulus of the coal grains.

607 The bulk volumetric strain can be derived from Eq. (A.1) as

$$608 \quad \varepsilon_t = \frac{dV_t}{V_t} = \frac{1}{K} (d\sigma + \alpha dp) + d\varepsilon_s \quad (A.4)$$

609 The pore volumetric strain can also be expressed as

$$610 \quad \varepsilon_p = \frac{dV_p}{V_p} = \frac{1}{K_p} d\sigma + \left(\frac{1}{K_p} - \frac{1}{K_s} \right) dp + d\varepsilon_s \quad (A.5)$$

611 where V_t and V_p are the bulk and pore volumes, respectively; K_p is the pore modulus.

612

613 The fracture-cleat porosity of a coal seam is defined as

$$614 \quad \phi = \frac{V_p}{V_t} \quad (A.6)$$

615 Thus, the porosity change of a deforming coal seam can be described as

$$616 \quad d\phi = d\left(\frac{V_p}{V_t}\right) = \frac{V_p}{V_t} \left(\frac{dV_p}{V_p} - \frac{dV_t}{V_t} \right) \quad (A.7)$$

617 According to the Betti-Maxwell reciprocal theorem ([Detournay and Cheng, 1993](#)), K_p is a

618 function of ϕ , described as

$$619 \quad \frac{1}{K_p} = \frac{\alpha}{\phi} \frac{1}{K} \quad (A.8)$$

620 Substituting Eq. (A.8) into Eq. (A.7), then

$$621 \quad \frac{d\phi}{\phi} = \left(\frac{\alpha}{\phi} \frac{1}{K} - \frac{1}{K} \right) (d\sigma + dp) \quad (A.9)$$

622 Integrating the equation yields

$$623 \quad \phi = \alpha + (\phi_0 - \alpha) \exp\left\{\frac{-1}{K} [(\sigma - \sigma_0) + (p - p_0)]\right\} \quad (A.10)$$

624 Rewriting the Eq. (A.10) as a function of mean effective stress and pore pressure, it's expressed as

$$625 \quad \phi = \alpha + (\phi_0 - \alpha) \exp\left\{\frac{-1}{K} [(\sigma' - \sigma'_0) + (1 - \alpha)(p - p_0)]\right\} \quad (A.11)$$

626 By assuming $\alpha = 1$, $K_p \ll K$ and K_p is a constant and simply approximated to be

627 $K_p = \phi_0 K$, Eq. (A.9) can be integrated yielding

$$628 \quad \phi = \phi_0 \exp\left\{\frac{-1}{K_p} [(\sigma - \sigma_0) + (p - p_0)]\right\} \quad (A.12)$$

629 By assuming $\phi \ll 1$, Eq. (A.9) can be integrated yielding

$$630 \quad \phi = \phi_0 + \frac{\alpha}{K} [(\sigma - \sigma_0) + (p - p_0)] \quad (A.13)$$

631 Without consideration of the Klinkenberg effect, a cubic law is used to describe the relationship
632 between the permeability and porosity of the porous media, which is shown as follows

$$633 \quad \frac{k}{k_0} = \left(\frac{\phi}{\phi_0}\right)^3 = \left\{\frac{\alpha}{\phi_0} + \frac{(\phi_0 - \alpha)}{\phi_0} \exp\left\{\frac{-1}{K} [(\sigma - \sigma_0) + (p - p_0)]\right\}\right\}^3 \quad (A.14)$$

$$634 \quad \frac{k}{k_0} = \left(\frac{\phi}{\phi_0}\right)^3 = \left\{\exp\left\{\frac{-1}{K_p} [(\sigma - \sigma_0) + (p - p_0)]\right\}\right\}^3 \quad (A.15)$$

$$635 \quad \frac{k}{k_0} = \left(\frac{\phi}{\phi_0}\right)^3 = \left\{1 + \frac{\alpha}{K \phi_0} [(\sigma - \sigma_0) + (p - p_0)]\right\}^3 \quad (A.16)$$

636 Eqs. (A.15) and (A.16) are the C&B and P&M models ([Cui and Bustin, 2005](#); [Palmer and Mansoori, 1998](#)), respectively, assuming that the reservoirs are under conditions of uniaxial strain, constant

638 reservoir loading and $\alpha = 1$. The horizontal stress σ_x or σ_y is given from equation (A.1) as

$$639 \quad \sigma_x = \sigma_y = \frac{\nu}{1 - \nu} \sigma_z - \frac{1 - 2\nu}{1 - \nu} p - \frac{1 - 2\nu}{1 - \nu} K \varepsilon_s \quad (A.17)$$

640 Substituting Eq. (A.17) into Eq. (A.14), (A.15) and (A.16) gives

$$641 \quad \frac{k}{k_0} = \left\{\frac{\alpha}{\phi_0} + \frac{(\phi_0 - \alpha)}{\phi_0} \exp\left\{\frac{-1}{K} \left[\frac{(1 + \nu)}{3(1 - \nu)} (p - p_0) - \frac{2E}{9(1 - \nu)} (\varepsilon_s - \varepsilon_{s0})\right]\right\}\right\}^3 \quad (A.18)$$

$$642 \quad \frac{k_{C \wedge B}}{k_0} = \exp \left\{ \frac{3}{K_p} \left[\frac{(1+\nu)}{3(1-\nu)} (p-p_0) - \frac{2E}{9(1-\nu)} (\varepsilon_s - \varepsilon_{s0}) \right] \right\}^3 \quad (A.19)$$

$$643 \quad \frac{k_{P \wedge M}}{k_0} = \left\{ 1 + \frac{1}{K_p} \left[\frac{(1+\nu)}{3(1-\nu)} (p-p_0) - \frac{2E}{9(1-\nu)} (\varepsilon_s - \varepsilon_{s0}) \right] \right\}^3 \quad (A.20)$$

644 Acknowledgments

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650 References

- 651 Ates, Y., Barron, K., 1988. The effect of gas sorption on the strength of coal. *Mining Science and Technology* 6, 291-300.
- 652 Bachu, S., 2008. CO₂ storage in geological media: Role, means, status and barriers to deployment. *Progress in Energy* 653 and *Combustion Science* 34, 254-273.
- 654 Bustin, A.M.M., Bustin, R.M., 2012. Importance of rock properties on the producibility of gas shales. *International* 655 *Journal of Coal Geology* 103, 132-147.
- 656 Cui, X., Bustin, R.M., 2005. Volumetric strain associated with methane desorption and its impact on coalbed gas 657 production from deep coal seams. *AAPG Bulletin* 89, 1181-1202.
- 658 Detournay, E., Cheng, A.H.-D., 1993. *Fundamentals of Poroelasticity* 1.
- 659 Durucan, S., Shi, J.-Q., 2009. Improving the CO₂ well injectivity and enhanced coalbed methane production 660 performance in coal seams. *International Journal of Coal Geology* 77, 214-221.
- 661 Ferronato, M., Gambolati, G., Janna, C., Teatini, P., 2010. Geomechanical issues of anthropogenic CO₂ sequestration in 662 exploited gas fields. *Energy Conversion and Management* 51, 1918-1928.
- 663 Gale, J., 2004. Geological storage of CO₂: What do we know, where are the gaps and what more needs to be done? 664 *Energy* 29, 1329-1338.
- 665 Goodman, A.L., Favors, R.N., Larsen, J.W., 2006. Argonne coal structure rearrangement caused by sorption of CO₂. 666 *Energy & Fuels* 20, 2537-2543.
- 667 Gou, Y., Hou, Z., Liu, H., Zhou, L., Were, P., 2014. Numerical simulation of carbon dioxide injection for enhanced gas 668 recovery (CO₂-EGR) in Altmark natural gas field. *Acta Geotech.* 9, 49-58.
- 669 Gray, I., 1987. Reservoir engineering in coal seams: Part 1-The physical process of gas storage and movement in coal 670 seams. *SPE Reservoir Engineering* 2, 28-34.
- 671 Haszeldine, R.S., 2009. Carbon Capture and Storage: How Green Can Black Be? *Science* 325, 1647-1652.
- 672 Hol, S., Peach, C.J., Spiers, C.J., 2011. Applied stress reduces the CO₂ sorption capacity of coal. *International Journal of* 673 *Coal Geology* 85, 128-142.
- 674 Kumar, H., Elsworth, D., Mathews, J.P., Liu, J., Pone, D., 2014. Effect of CO₂ injection on heterogeneously permeable 675 coalbed reservoirs. *Fuel* 135, 509-521.
- 676 Levine, J.R., 1996. Model study of the influence of matrix shrinkage on absolute permeability of coal bed reservoirs. 677 *Geological Society, London, Special Publications* 109, 197-212.

678Li, X., Fang, Z.-m., 2014. Current status and technical challenges of CO₂ storage in coal seams and enhanced coalbed
679methane recovery: an overview. *Int J Coal Sci Technol* 1, 93-102.

680Liu, H.-H., Rutqvist, J., 2010. A new coal-permeability model: internal swelling stress and fracture–matrix interaction.
681*Transport in Porous Media* 82, 157-171.

682Masoudian, M., Airey, D., El-Zein, A., 2013. A chemo-poro-mechanical model for sequestration of carbon dioxide in
683coalbeds. *Geotechnique* 63, 235-243.

684Masoudian, M.S., Airey, D.W., El-Zein, A., 2014. Experimental investigations on the effect of CO₂ on mechanics of coal.
685*International Journal of Coal Geology* 128–129, 12-23.

686Mishra, B., Dlamini, B., 2012. Investigation of Swelling and Elastic Property Changes Resulting from CO₂ Injection into
687Cuboid Coal Specimens. *Energy & Fuels* 26, 3951-3957.

688Palmer, I., Mansoori, J., 1998. How Permeability Depends on Stress and Pore Pressure in Coalbeds: A New Model.
689Reucroft, P.J., Patel, H., 1986. Gas-Induced Swelling in Coal. *Fuel* 65, 816-820.

690Rubin, E.S., 2005. IPCC Special Report on Carbon Dioxide Capture and Storage.

691Rutqvist, J., Börgesson, L., Chijimatsu, M., Kobayashi, A., Jing, L., Nguyen, T.S., Noorishad, J., Tsang, C.F., 2001.
692Thermohydrromechanics of partially saturated geological media: governing equations and formulation of four finite
693element models. *International Journal of Rock Mechanics and Mining Sciences* 38, 105-127.

694Rutqvist, J., Tsang, C.F., 2002. A study of caprock hydromechanical changes associated with CO₂-injection into a brine
695formation. *Environmental Geology* 42, 296-305.

696Seidle, J.P., Huitt, L., 1995. Experimental measurement of coal matrix shrinkage due to gas desorption and implications
697for cleat permeability increases, *International meeting on petroleum Engineering*, pp. 575-582.

698Shi, J.Q., Durucan, S., 2004. Drawdown Induced Changes in Permeability of Coalbeds: A New Interpretation of the
699Reservoir Response to Primary Recovery. *Transport in Porous Media* 56, 1-16.

700Shukla, R., Ranjith, P., Haque, A., Choi, X., 2010. A review of studies on CO₂ sequestration and caprock integrity. *Fuel*
70189, 2651-2664.

702Siriwardane, H., Haljasmaa, I., McLendon, R., Irdi, G., Soong, Y., Bromhal, G., 2009. Influence of carbon dioxide on
703coal permeability determined by pressure transient methods. *International Journal of Coal Geology* 77, 109-118.

704Van Bergen, F., Gale, J., Damen, K., Wildenborg, A., 2004. Worldwide selection of early opportunities for CO₂-enhanced
705oil recovery and CO₂-enhanced coal bed methane production. *Energy* 29, 1611-1621.

706Viète, D.R., Ranjith, P.G., 2006. The effect of CO₂ on the geomechanical and permeability behaviour of brown coal:
707Implications for coal seam CO₂ sequestration. *International Journal of Coal Geology* 66, 204-216.

708Warren, J.E., Root, P.J., 1963. The Behavior of Naturally Fractured Reservoirs. *Society of Petroleum Engineers Journal*
7093, 245-255.

710Wei, Z., Zhang, D., 2010. Coupled fluid-flow and geomechanics for triple-porosity/dual-permeability modeling of
711coalbed methane recovery. *International Journal of Rock Mechanics and Mining Sciences* 47, 1242-1253.

712White, C.M., Smith, D.H., Jones, K.L., Goodman, A.L., Jikich, S.A., LaCount, R.B., DuBose, S.B., Ozdemir, E., Morsi,
713B.I., Schroeder, K.T., 2005. Sequestration of carbon dioxide in coal with enhanced coalbed methane recovery a review.
714*Energy & Fuels* 19, 659-724.

715Wong, S., Law, D., Deng, X., Robinson, J., Kadatz, B., Gunter, W.D., Jianping, Y., Sanli, F., Zhiqiang, F., 2007.
716Enhanced coalbed methane and CO₂ storage in anthracitic coals—Micro-pilot test at South Qinshui, Shanxi, China.
717*International Journal of Greenhouse Gas Control* 1, 215-222.

718Wong, S., Macdonald, D., Andrei, S., Gunter, W.D., Deng, X., Law, D., Ye, J., Feng, S., Fan, Z., Ho, P., 2010. Conceptual
719economics of full scale enhanced coalbed methane production and CO₂ storage in anthracitic coals at South Qinshui
720basin, Shanxi, China. *International Journal of Coal Geology* 82, 280-286.

721Zakkour, P., Haines, M., 2007. Permitting issues for CO₂ capture, transport and geological storage: A review of europe,

722USA, Canada and Australia. *International Journal of Greenhouse Gas Control* 1, 94-100.

723Zhang, H., Liu, J., Elsworth, D., 2008. How sorption-induced matrix deformation affects gas flow in coal seams: A new

724FE model. *International Journal of Rock Mechanics and Mining Sciences* 45, 1226-1236.

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