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# Evaluation of CO<sub>2</sub>-enhanced gas recovery and storage through coupled non-isothermal compositional two-phase flow and geomechanics modelling

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## Abstract

CO<sub>2</sub> injection into unconventional gas reservoir has been recognized as a promising approach to enhance unconventional gas recovery (CO<sub>2</sub>-EUGR) and sequester CO<sub>2</sub> geologically. The CO<sub>2</sub>-EUGR is a complex multi-physics coupling process. To accurately assess the effectiveness of different injection strategies, this paper firstly presents a non-isothermal compositional two-phase flow model coupling with geomechanics, in which a multicomponent adsorption kinetics is incorporated to separate free phase and adsorbed phase. A hybrid numerical approach combining EbFVM and GFEM is used for numerical solutions. The performance of different injection strategies in CO<sub>2</sub>-EUGR is evaluated. The results indicate that CO<sub>2</sub> injection is able to improve CH<sub>4</sub> recovery significantly, over 90% of injected CO<sub>2</sub> can be adsorbed in reservoirs, The performance of CO<sub>2</sub>-EUGR is permeability dependent, the displacement effect occurs earlier when reservoir permeability is higher; Increasing temperature of injected gas and mixed CO<sub>2</sub>/N<sub>2</sub> injection can further improve CH<sub>4</sub> recovery, especially for low permeability gas reservoirs; Mixed gas injection also enables displacement effect to occur earlier; Cyclic injection can hardly increase in CH<sub>4</sub> production, especially when reservoir permeability is higher, while it can cause an increase in amount of adsorbed CO<sub>2</sub> during injection period. Based on these findings, a geothermal-assisted CO<sub>2</sub>-EUGR method is proposed.

**Keywords:** unconventional reservoir, CO<sub>2</sub> sequestration, enhanced gas recovery, numerical modelling, performance evaluation

## 1 Introduction

Carbon capture and storage (CCS) has been considered as a key technology to mitigate the emission of carbon dioxide (CO<sub>2</sub>) resulting from anthropogenic activities into atmosphere [1, 2]. There are a

few of geological sequestration sinks which are available to sequester CO<sub>2</sub>, such as depleted oil and gas reservoirs [3]. In light with the expense of CCS, carbon capture, utilization and storage (CCUS) has been proposed and attracted more attentions in recent years [4, 5]. One of major CO<sub>2</sub> utilization options is using CO<sub>2</sub> injection into unconventional gas reservoirs to enhance unconventional gas recovery (CO<sub>2</sub>-EUGR) like shale gas, coalbed methane (CBM), natural gas hydrate, which can offset the expense for operations of CCUS [6]. Unconventional gas reservoirs have also been considered as target geological sites for CO<sub>2</sub> storage, since a large body of pore volume of gas reservoirs that provides available adsorption sites for gases holds a potential to a huge amount of CO<sub>2</sub> reserve, and meanwhile, their ability to long-term storage of hydrocarbons inside the sealed reservoir with impermeable cap rocks suggests that these reservoirs are safer formations than saline aquifers or other geological sites [7, 8].

Performance of CO<sub>2</sub>-EUGR significantly depends on material properties, geological conditions and operational conditions. Seto et al.[9] reported that the displacement behavior of CO<sub>2</sub> was greatly impacted by relative adsorption strength of CO<sub>2</sub> and CH<sub>4</sub>, the adsorption CO<sub>2</sub> reduced the flow velocity, delaying breakthrough and allowing more CO<sub>2</sub> to be sequestered. Sun et al. [10] believed that CO<sub>2</sub>-EUGR consisted of three stages and simulation results for injection pressure of 6 MPa and 7 MPa shown that injection pressure increase could improve gas production rate improved significantly, similar observations were also presented by Mohagheghian et al.[11]. Jiang et al.[12] evaluated influences of different injection strategies, such as huff-n-puff injection, CO<sub>2</sub>/N<sub>2</sub> mixture injection, on potential for improving shale gas extraction, and the results showed that composition of CO<sub>2</sub>/N<sub>2</sub> mixture injection had a minor effect on CH<sub>4</sub> production even though the N<sub>2</sub> fraction reached 50%, this is contrary to the findings presented by Seto et [9] and Lin et al. [13]. A possible explanation for the different findings is that different geological conditions were considered. The simulation results by Liu et al. [14] indicated that there was a non-monotonous correlation between gas production and CO<sub>2</sub> injection rate before CO<sub>2</sub> breakthrough, while well distance has a negative effect on shale gas production. Tang et al. [15] evaluated the efficiency of CO<sub>2</sub>-enhanced shale gas recovery by developing multicomponent gas flow model and results shown that CH<sub>4</sub> recovery is increased by 10%-15% through CO<sub>2</sub> injection.

Most of these studies on performance evaluation of CO<sub>2</sub>-enhanced gas recovery focus on injection strategies, the impacts of reservoir properties like reservoir permeability and temperature are considered. In addition, the contributions of gases in different phase to both CH<sub>4</sub> recovery and CO<sub>2</sub> storage are not separated [16]. For example, the developed model by Tang et al. [15] for performance evaluation was single phase, geomechanics effect and permeability evolution were ignored. However, in-situ CO<sub>2</sub> injection involves temporal evolutions of reservoir properties. For example, Kamali-Asl et al.[17] reported that permeability evolution of shale exposed CO<sub>2</sub> might experience continuous or cycles of increase/decrease, assumption of constant permeability for numerical model development could lead to deviation from real scenarios. Therefore, the study on performance of

CO<sub>2</sub>-EUGR under different geological conditions is necessary.

CO<sub>2</sub>-EUGR typically involves complex thermo-hydro-chemical-mechanical (THCM) coupling processes, a few attempts have been made to understand these coupled processes by modelling approach. A few of the compositional simulators, such as COMSOL, TOUGH2, CMG-GEM and Eclipse, have been developed for simulating multiphase flow and the interactions between CO<sub>2</sub>, natural gas and formations. Oldenburg et al. [18] simulated the process of CO<sub>2</sub> injection into a depleted natural gas reservoir carried out with TOUGH2/EOS7C and confirmed the plausibility of CO<sub>2</sub>-EUGR. Fan et al.[19] used COMSOL to explore the coupled THMC responses of CO<sub>2</sub> enhanced CBM recovery (CO<sub>2</sub>-ECBM) through THMC numerical simulations. These simulators were developed based on various discretization methods and utilization of structured or unstructured grids. The widely used discretization methods include finite difference method (FDM), finite element method (FEM) and finite volumes method (FVM). FVM- and FEM-based simulations of CO<sub>2</sub>-enhanced gas recovery (CO<sub>2</sub>-EGR) are potentially more accurate than FDM-based simulations [20]. Since it is proved that FEM is powerful to predict the deformation and stress fields and FVM is locally mass conservative, combination of FEM and FVM is an efficient approach to simulation of coupled THCM processes occurring during CO<sub>2</sub>-EGR [21-23]. Following the work by e.g. Amiri et al. [24], the element based FVM (EbFVM) is used for numerical solutions in this study instead of single point or multi-point flux approximation based FVM in order to efficiently combine it with FEM.

The objective of this work is development of a numerical model for non-isothermal compositional two-phase flow coupling with geomechanics in order to quantitatively evaluate efficiency of CO<sub>2</sub> storage and EUGR. The developed numerical model in this work incorporates multicomponent kinetics to separate the free phase and adsorbed phase, which are different from equilibrium adsorption model used in previous work. The temperature effects on gas adsorption and transport behavior are considered as well. A hybrid numerical approach with combining the EbFVM and the standard Galerkin FEM (GFEM) is presented for full coupling of the non-isothermal multiphase multicomponent flow and mechanical deformation equations. The developed numerical model is used to analyze the effects of different injection strategies on CO<sub>2</sub> storage and gas recovery under different geological conditions. According to the performance evaluation, a geo-thermal assisted CO<sub>2</sub> enhanced gas recovery is proposed.

The outline of this paper is as follows: the governing equations for coupled thermo-hydro-mechanical behavior is developed in Section 2. In Section 3, the numerical solutions based on combination of EbFVM and GFEM is details. Verification tests for checking model reliability are shown in Section 4. Section 5 presents a model application of proposed numerical model to analysis of hydro-mechanical behaviour of CO<sub>2</sub> injection into heterogeneous unconventional reservoirs. Finally, conclusions are drawn in Section 6.

## 2 Mathematical model

Considering the reservoir as a multiphase multicomponent system (solid, liquid and gas), the gaseous phase consists of CO<sub>2</sub> and CH<sub>4</sub> and liquid phase includes water along with dissolved CO<sub>2</sub> and CH<sub>4</sub>. The following assumptions are made for development of mathematical model: 1) the deformation is linear elastic; 2) flow of mobile gaseous and aqueous phases obey Darcy's law; 3) the voids of the solid skeleton are unsaturated; 4) reservoir is local thermal non-equilibrium. In the subsequent discussion, the gas phase and liquid phase are labelled by subscripts 'g', 'l', respectively. The soil phase is denoted by the subscript 's'.

### 2.1 Multicomponent adsorption kinetics

Gas retention mechanism in unconventional gas reservoirs like shale reservoirs and coalbeds is adsorption. CO<sub>2</sub> injection increases the number of species of reservoirs, and the multicomponent adsorption model should be used to represent the adsorption characteristics of CO<sub>2</sub>-EUGR. Many studies show that extended Langmuir isotherm can be used for capturing the competitive adsorption of multicomponent gas [e.g. 25, 26, 27]. Following Langmuir's theory, a kinetic process occurs between adsorbed gas molecules and free gas molecules. As shown in Fig. 1, the free gas molecules, upon striking the adsorption sites on the pore surfaces of solid materials, can adhere for a specific duration due to surface forces (referred to as adsorption). Upon acquiring sufficient activation energy, the adsorbed molecules can be released and transition into the free phase (referred to as desorption). Extending the Langmuir kinetics for single component gas to multicomponent gas, the change of adsorption amount of  $i^{th}$  component in a multicomponent system with respect to time is expressed as:

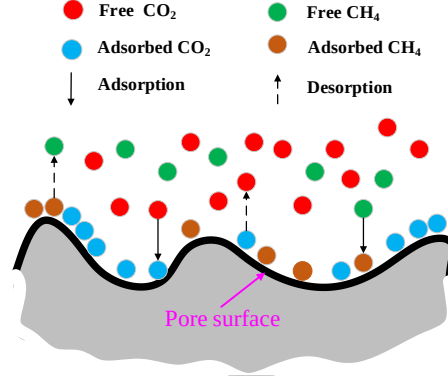
$$\frac{dC_{si}}{dt} = R_{ai} - R_{di} \quad (1)$$

where  $C_{si}$  denotes adsorbed phase concentration of  $i^{th}$  component, mol·kg<sup>-1</sup>,  $t$  is time, s,  $R_{ai}$  and  $R_{di}$  denote adsorption rate and desorption rate of  $i^{th}$  component, mol·kg<sup>-1</sup>·s<sup>-1</sup>. Langmuir theory assumes adsorption rate,  $R_{ai}$ , to be proportional to partial pressure of  $i^{th}$  component,  $p_i$ , and to the number of free sites  $C_{Li}(1 - \sum_{j=1}^n \theta_j)$ ,  $\theta_j = \frac{C_{sj}}{C_{Lj}}$ . The desorption rate,  $R_{di}$ , is associated with the number of occupied adsorption sites [28], written as:

$$R_{ai} = \gamma_{ai} p_i \left( C_{Li} - C_{Li} \sum_{j=1}^n \frac{C_{sj}}{C_{Lj}} \right) \quad (2)$$

$$R_{di} = \gamma_{di} C_{si} \quad (3)$$

where  $\gamma_{ai}$  is rate constants for adsorption,  $\text{Pa}^{-1} \cdot \text{s}^{-1}$ , and  $\gamma_{di}$  is rate constants for desorption,  $\text{s}^{-1}$ ,  $C_{Li}$  is Langmuir volume constant of  $i^{\text{th}}$  component,  $\text{mol} \cdot \text{kg}^{-1}$ ,  $p_i$  is partial pressure of  $i^{\text{th}}$  component, Pa.



**Fig.1** Dynamic process of adsorption and desorption of gas molecules on a surface

Substituting Eqs. (2) and (3) into Eq. (1) leads to the nonequilibrium mass exchange between adsorbed phase and free phase:

$$\frac{dC_{si}}{dt} = \gamma_{ai} p_i \left( C_{Li} - C_{Li} \sum_{j=1}^n \frac{C_{sj}}{C_{Lj}} \right) - \gamma_{di} C_{si} \quad (4)$$

When multicomponent gas adsorption reaching equilibrium, that is,  $\frac{dC_{si}}{dt} = 0$ , Eq. (4) can be reduced to well-known Extended Langmuir isotherm:

$$C_{si} = \frac{b_{Li} p_i C_{Li}}{1 + \sum_{j=1}^n b_{Lj} p_j} \quad (5)$$

where  $b_{Li} = \gamma_{ai}/\gamma_{di}$  is the Langmuir pressure constant,  $\text{Pa}^{-1}$ .

The adsorption capacity of  $i^{\text{th}}$  component,  $C_{Li}$ , and the Langmuir pressure constant,  $b_{Lj}$  depend on temperature and moisture content, expressed as[29]:

$$C_{Li} = C_{L0i} \exp[-\delta^i (T - T_0) - \xi^i m] \quad (6)$$

$$b_{Li} = b_{L0i} \exp \left[ \frac{E_{in}^i}{R} \left( \frac{1}{T} - \frac{1}{T_0} \right) \right] \quad (7)$$

where  $T$  is temperature, K,  $C_{L0i}$  denotes adsorption capacity for the adsorbent at reference state,  $\text{mol} \cdot \text{kg}^{-1}$ ,  $\delta^i$  and  $\xi^i$  are reduction coefficients associated with temperature and moisture content  $m$ ,  $E_{in}^i$  is the interaction energy, and  $b_{L0i}$  is Langmuir pressure constant at reference temperature  $T_0$ ,

Pa<sup>-1</sup>,  $R$  is the universal gas constant, J·mol<sup>-1</sup>·K<sup>-1</sup>.

## 2.2 Mass balance equation

For a non-isothermal multiphase multicomponent system, the general mass conversation equation for  $i^{th}$  component is expressed as:

$$\frac{\partial(\phi S_{\kappa} \rho_k^i)}{\partial t} = -\nabla \cdot F_k^i + q_k^i \quad \kappa = g, l \quad (8)$$

where  $\rho_k^i$  is density of  $i^{th}$  component,  $i = 1, 2 \dots n$ , kg·m<sup>-3</sup>,  $S_{\kappa}$  is saturation of fluid phase,  $\phi$  is porosity,  $F_k^i$  is mass flux of  $i^{th}$  component, kg·m<sup>-3</sup>·s<sup>-1</sup>, and  $q_k^i$  is source/sink term, kg·m<sup>-3</sup>·s<sup>-1</sup>.

The water density is associated with temperature,  $\rho_l = \rho_l(T)$ , and the density of component  $i$ ,  $\rho_k^i$ , depends on component concentration [30], expressed as:

$$\rho_k^i = c_k^i M^i \quad (9)$$

where  $c_k^i$  is concentration of  $i^{th}$  component, mol·m<sup>-3</sup>, and  $M^i$  is molar mass, kg·mol<sup>-1</sup>.

The water saturation can be calculated based on capillary pressure  $p_c$ , and the following capillary pressure-saturation relationship is used for calculation of water saturation [31]:

$$S_{le} = \frac{S_l - S_{lr}}{S_{lm} - S_{lr}} = \left(1 + \left|\frac{p_c}{p_0}\right|^{\gamma}\right)^{-\psi} \quad (10)$$

where  $S_{le}$ ,  $S_{lm}$  and  $S_{lr}$  are the effective, maximum and residual water saturation, respectively,  $\gamma$  and  $\psi$  ( $\psi = 1 - 1/\gamma$ ) are constants, and  $p_0$  is a characteristic pressure, Pa.

Capillary pressure is defined as:

$$p_c = p_g - p_l \quad (11)$$

where  $p_l$  is liquid pressure, Pa,  $p_g$  is gas pressure, Pa, which is calculated by real gas law, expressed as:

$$p_g = ZRT \sum_{i=1}^{n_c} c_g^i \quad (12)$$

where  $Z$  is the compressibility factor of gas mixture, which is estimated by Peng–Robinson equation of state [32].

The mass flux of each component  $i$  is calculated using Darcy's law, written as:

$$F_k^i = \rho_k^i \mathbf{v}_{\kappa} = \rho_k^i \frac{k_{kr}(S_{\kappa}) \mathbf{k}}{\mu_{\kappa}} \nabla p_{\kappa} \quad (13)$$

where  $\mathbf{v}_\kappa$  is flow velocity of phase  $\kappa$ ,  $\text{m}\cdot\text{s}^{-1}$ ,  $\mathbf{k}$  is permeability tensor,  $\text{m}^2$ ,  $\mu_\kappa$  is the dynamic viscosity,  $\text{Pa}\cdot\text{s}$ ,  $k_{kr}$  is relative permeability, -, which depends on saturation.

The water vapour is neglected in this study. Only source terms for gas component arising from adsorption/desorption and dissolution are considered, expressed as:

$$q_g^i = \rho_s \frac{\partial C_{si}}{\partial t} \quad (14)$$

where  $\rho_s$  is solid density,  $\text{kg}\cdot\text{m}^{-3}$ .

It is assumed that the dissolved species in fluid phases reaches equilibrium instantaneously. Henry's law for solubility is applied to equilibrium of gas dissolution, which is expressed as:

$$c_l^i = H_i x_g^i p_g \quad (15)$$

where  $H_i$  is Henry's constant,  $\text{Pa}^{-1}$ , and  $x_g^i$  is molar fraction of  $i^{\text{th}}$  component, -.

### 2.3 Energy balance equation

Due to local thermal equilibrium assumption, temperature between solid skeleton and fluid in the pore space can reach thermal equilibrium state quickly. Therefore, a single energy balance equation is able to capture the heat transfer in the multiphase system, expressed as:

$$(\rho C_p)_e \frac{\partial T}{\partial t} = \nabla \cdot (\lambda_e \nabla T) - (S_l \rho_l C_{pl} \mathbf{v}_l + S_g \rho_g C_{pg} \mathbf{v}_g) \cdot \nabla T + q_T \quad (16)$$

where  $(\rho C_p)_e$  is effective specific heat capacity,  $\text{J}\cdot\text{K}^{-1}\cdot\text{kg}^{-1}$ ,  $\lambda_e$  is thermal conductivity,  $\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ ,  $q_T$  is heat sink/source term,  $\text{J}\cdot\text{kg}^{-1}\cdot\text{s}^{-1}$ .

The effective specific heat capacity is [33]:

$$(\rho C_p)_e = (1 - \varphi) \rho_s C_{ps} + \varphi S_l \rho_l C_{pl} + \varphi S_g \rho_g C_{pg} \quad (17)$$

where  $C_{ps}$  is specified heat capacity of solid phase,  $\text{J}\cdot\text{K}^{-1}\cdot\text{kg}^{-1}$ ,  $\rho_g$  is density of gas mixture,  $\text{kg}\cdot\text{m}^{-3}$  and  $C_{pg}$  is specific heat capacity of gas mixture,  $\text{J}\cdot\text{K}^{-1}\cdot\text{kg}^{-1}$ , which can be calculated by means of an arithmetic mean averaging technique:

$$\rho_g = \sum_{i=1}^n c_g^i M^i \quad (18)$$

$$C_{pg} = \sum_{i=1}^n X_g^i C_{pg}^i \quad (19)$$

where  $X_g^i$  is mass fraction of  $i^{\text{th}}$  gas component, -, given as:

$$X_g^i = \frac{x_g^i M^i}{\sum_{i=1}^n x_g^i M^i} \quad (20)$$

The effective thermal conductivity can be expressed in terms of the geometric mean of the thermal conductivities of all phases [34]:

$$\lambda_e = \lambda_s^{(1-\varphi)} \lambda_l^{\varphi S_l} \lambda_g^{\varphi(1-S_l)} \quad (21)$$

where  $\lambda_s$ ,  $\lambda_l$  and  $\lambda_g$  are the thermal conductivity of solid, water and gas phases,  $\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ , respectively. The thermal conductivity of gas mixture can be obtained through equation (22):

$$\lambda_g = \sum_{i=1}^n X_g^i \lambda_g^i \quad (22)$$

## 2.4 Deformation

For the solid phase, it is defined that the tensile stress is assumed to be positive, while fluid pressure is positive in compression. The stress equilibrium equation for solid phase is expressed as:

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{F} = 0 \quad (23)$$

where  $\boldsymbol{\sigma}$  is the total stress tensor, Pa,  $\mathbf{F}$  is body force,  $\text{N}\cdot\text{m}^{-3}$ .

According to Biot's theory [35], when a porous medium is filled with fluids, the deformation only occurs as a result of part of total stress supported by solid skeleton. This part of total stress is known as effective stress,  $\boldsymbol{\sigma}'$ , given as:

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} + \alpha p \mathbf{I} \quad (24)$$

where  $\mathbf{I}$  is a vector,  $\mathbf{I}^T = (1,1,1,0,0,0)$  and  $(1,1,0)$  in 2D and 3D problems, and  $\alpha = 1 - K/K_s$  is Biot coefficient,  $K = E/3(1 - 2\nu)$  is bulk modulus, Pa and  $K_s$  are the modulus of solid skeleton, Pa,  $E$  is Young's modulus, Pa,  $\nu$  is Poisson's ratio,  $p$  is effective pore-pressure, Pa.

The effective pore-pressure is evaluated as:

$$p = S_l p_l + S_g p_g \quad (25)$$

The stress-strain constitutive relation is:

$$\boldsymbol{\sigma}' = 2G\boldsymbol{\varepsilon}^e + \lambda\varepsilon_v^e \mathbf{I} \quad (26)$$

where  $G = E/2(1 + \nu)$  is shear modulus, Pa,  $\lambda = E\nu/(1 + \nu)(1 - 2\nu)$  is the Lamé constant, Pa,  $\boldsymbol{\varepsilon}^e$  is elastic strain tensor due to mechanical stress,  $\varepsilon_v^e$  is the elastic volumetric strain, -.

Generally, the total strain of reservoir can be decomposed into three components: elastic strain,  $\boldsymbol{\varepsilon}^e$ , adsorption/desorption induced swelling/shrinkage,  $\boldsymbol{\varepsilon}^s$ , and thermal expansion/contraction,  $\boldsymbol{\varepsilon}^T$ .

Therefore, total strain can be expressed as:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^e + \frac{\varepsilon^s}{3} \mathbf{I} + \frac{\varepsilon^T}{3} \mathbf{I} \quad (27)$$

where  $\boldsymbol{\varepsilon}$  is the total strain tensor, -.

The relationship between the amount of adsorbed gas,  $C_{si}$ , and the adsorption-induced volumetric strain is approximately linear [36, 37], expressed as:

$$\varepsilon^s = \sum_{i=1}^n \omega_i C_{si} \quad (28)$$

where  $\omega_i$  is coefficient of adsorption-induced volumetric strain,  $\text{m}^3 \cdot \text{mol}^{-1}$ .

And the thermal strain is given by:

$$\varepsilon^T = \alpha_T T \quad (29)$$

Where  $\alpha_T$  is the thermal expansion coefficient,  $\text{K}^{-1}$ .

The strain-displacement relation is expressed as:

$$\varepsilon = \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \quad (30)$$

where  $\mathbf{u}$  is solid displacement vector, m.

## 2.5 Dynamic evolution of porosity and permeability

The porosity is defined as:

$$\varphi = \frac{V_p}{V} \quad (31)$$

where  $V_p$  and  $V$  are pore volume and bulk volume, respectively,  $\text{m}^3$ .

The porosity change of deforming porous media can be represented using pore-volume strain increment  $\frac{dV_p}{V}$  and bulk volumetric strain increment,  $\frac{dV}{V}$ , written as [38]:

$$d\varphi = d\left(\frac{V_p}{V}\right) = \varphi \left( \frac{dV_p}{V} - \frac{dV}{V} \right) \quad (32)$$

The bulk volumetric strain increment is:

$$\frac{dV}{V} = -\frac{d(\bar{\sigma} + \alpha p)}{K} + d\varepsilon^s + d\varepsilon^T \quad (33)$$

where  $\bar{\sigma} = \sigma_{ii}/3$  is the mean stress, Pa.

Similarly, the pore-volume strain increment can be written as:

$$\frac{dV_p}{V} = -\frac{d(\bar{\sigma} + \beta p)}{K_p} + d\varepsilon^s + d\varepsilon^T \quad (34)$$

where  $\beta = 1 - K_p/K_s$ ,  $K_p$  is the modulus of pores, Pa.

Where there is no adsorption induced deformation or thermal deformation, the volumetric variation

obeys the Betti–Maxwell reciprocal theorem  $\left(\frac{\partial V}{\partial p}\right)_{\bar{\sigma}} = \left(\frac{\partial V_p}{\partial \bar{\sigma}}\right)_p$ , given as:

$$K_p = \frac{\varphi}{\alpha} K \quad (35)$$

Substituting equations (33-35) into equation (32) yields:

$$d\varphi = \varphi \left( \frac{1}{K_p} - \frac{1}{K} \right) d(\bar{\sigma} + p) \quad (36)$$

The permeability varies with porosity, which can be described by the widely used cubic relationship between permeability and porosity, given as:

$$\frac{k}{k_0} = \left( \frac{\varphi}{\varphi_0} \right)^3 \quad (37)$$

where  $k_0$  and  $\varphi_0$  are initial permeability,  $\text{m}^2$ , and porosity, -.

Integrating equation (36) yields:

$$\frac{\varphi}{\varphi_0} = \exp \left\{ \left( \frac{1}{K_p} - \frac{1}{K} \right) [(\bar{\sigma} + p) - (\bar{\sigma}_0 + p_0)] \right\} \quad (38)$$

where  $\bar{\sigma}_0, p_0$  are initial mean stress and pore pressure, Pa.

It is well recognized that that  $K_p$  is generally a few orders of magnitude lower than the bulk modulus

$K$ , i.e.  $\frac{1}{K_p} \gg \frac{1}{K}$ . After replacement of  $\frac{1}{K_p}$  with  $C_p$ , the permeability model can be written as the

following form:

$$k = k_0 \exp \{ -3C_p [(\bar{\sigma} + p) - (\bar{\sigma}_0 + p_0)] \} \quad (39)$$

where  $C_p$  is compressibility factor of reservoir pores,  $\text{Pa}^{-1}$ .

### 3 Numerical solutions

In this study, the numerical solutions are obtained by combining the element-based finite volume method (EbFVM) and standard Galerkin finite element method (GFEM) [22, 24]. Temporal discretization is achieved by an implicit mid-interval backward-difference time-stepping algorithm [39]. The spatial discretization of mass balance equation and energy balance equation is achieved using EbFVM, while the GFEM is applied to spatially discretize the linear momentum balance equation. The selected primary variables in this work are capillary pressure  $p_c$ , chemical concentration  $c_{\kappa}^i$ , temperature  $T$  and displacement  $\mathbf{u}$ . These variables are approximated based on their respective nodal values at the element level, expressed as:

$$p_c(\xi, \eta, \zeta) = \sum_{j=1}^N N_j(\xi, \eta, \zeta) p_{lj} = \mathbf{N} \hat{\mathbf{p}}_c \quad (40a)$$

$$c_{\kappa}^i(\xi, \eta, \zeta) = \sum_{j=1}^N N_j(\xi, \eta, \zeta) c_{\kappa j}^i = \mathbf{N} \hat{\mathbf{c}}_{\kappa}^i \quad (40b)$$

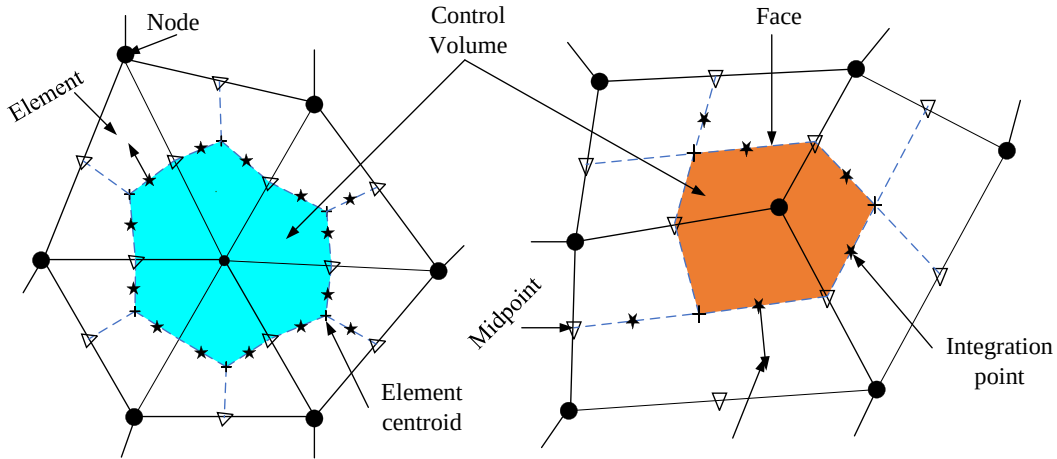
$$T(\xi, \eta, \zeta) = \sum_{j=1}^N N_j(\xi, \eta, \zeta) c_{\kappa j}^i = \mathbf{N} \hat{\mathbf{T}} \quad (40c)$$

$$\mathbf{u}(\xi, \eta, \zeta) = \sum_{j=1}^N N_j(\xi, \eta, \zeta) \mathbf{u}_j = \mathbf{N} \hat{\mathbf{u}} \quad (40d)$$

where  $N$  is number of nodes,  $N_j$  is shape function. Shape function built for EbFVM is the same as that for GFEM.  $\xi, \eta, \zeta$  are local coordinate inside each element.

The discretization of the mass balance equation above is expressed at the level of control volumes. A control volume around each node is constructed by connecting the center of the element containing this node to the centers of the element's faces that pass through the node. Fig. 2 shows the control volume for triangular and quadrilateral grids. Each control volume around a node is divided into sub-control volumes. To make discretized balance equations expressed in the element-wise formulation, the following weighting function  $W$  is necessary, which is unit for the sub-control volume belonging to the node  $j$  and zero elsewhere in a given element [40], given by:

$$W_j = \begin{cases} 1 & \text{sub-control volume sharing node } j \\ 0 & \text{otherwise} \end{cases} \quad (41)$$



**Fig. 2** Control volume constructed around a shared node of triangular and quadrilateral elements.

To solve numerically the set of nonlinear partial differential equations, appropriate boundary conditions are required (Fig.3), including Dirichlet conditions and Neumann conditions, expressed as:

$$p_c = \tilde{p}_c(t) \quad \text{in } \Gamma_{p_c} \quad (41a)$$

$$c_k^i = \tilde{c}_k^i(t) \quad \text{in } \Gamma_{c_k^i} \quad (41b)$$

$$T = \tilde{T}(t) \quad \text{in } \Gamma_T \quad (41c)$$

$$\mathbf{u} = \tilde{\mathbf{u}}(t) \quad \text{in } \Gamma_u \quad (41d)$$

and

$$\mathbf{v}_l \rho_l \cdot \mathbf{n} = \tilde{q}_l(t) \quad \text{on } \Gamma_{q_l} \quad (42a)$$

$$\mathbf{v}_k c_k^i \cdot \mathbf{n} = \tilde{q}_k^i(t) \quad \text{on } \Gamma_{q_k^i} \quad (42b)$$

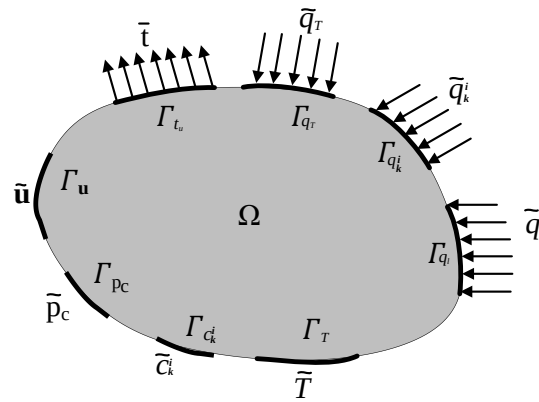
$$\lambda \nabla T \cdot \mathbf{n} = \tilde{q}_T(t) \quad \text{on } \Gamma_{q_T} \quad (42c)$$

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \tilde{\mathbf{t}}_u \quad \text{on } \Gamma_{t_u} \quad (42d)$$

where  $\tilde{p}_c$ ,  $\tilde{c}_k^i$ ,  $\tilde{T}$  and  $\tilde{\mathbf{u}}$  are pressure, concentration, temperature and displacement boundary

condition,  $\tilde{q}_l$ ,  $\tilde{q}_k^i$ ,  $\tilde{q}_T$  and  $\tilde{\mathbf{t}}$  are water flux, component flux, thermal flux, traction boundary condition, respectively,  $\mathbf{n}$  is normal vector of boundary.

The numerical model developed in this study was implemented into in-house hybrid finite volume-finite element code developed by Chen et al. [29, 41] based on the work by Thomas and co-workers from Geoenvironmental Research Centre of Cardiff University [e.g. 42, 43, 44]. A variable timestep is employed to enhance the solution efficiency. If the number of iterations surpasses a certain threshold, the timestep is decreased by a factor. Conversely, if the iterations required for convergence are fewer than the specified limit, the timestep is increased by a factor. The maximum number of iterations is 10 used in this work. A flowchart of numerical solution of coupled model is presented in Fig. 4. All the coding work and simulation running are completed through Microsoft Visual Studio 2013 on Windows 10.



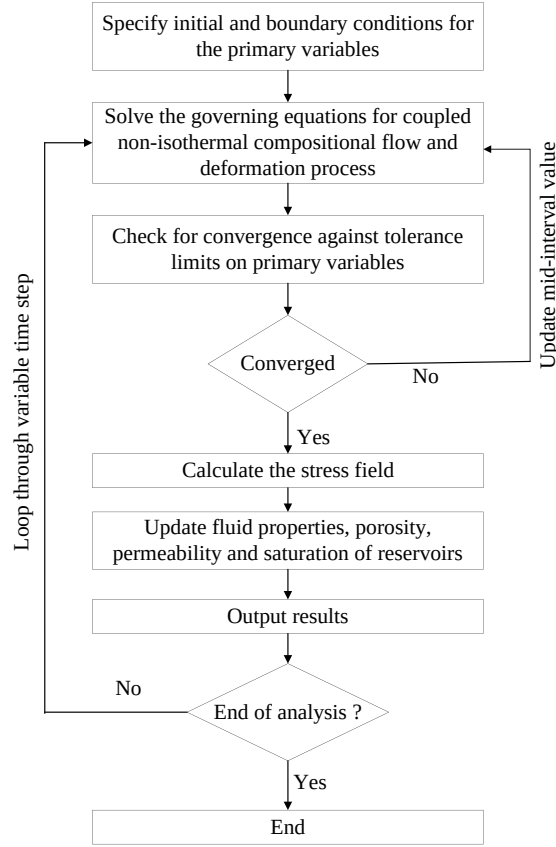
**Fig. 3** Numerical implementation procedure of coupled model

## 4 Model Verification and Validation

Model verification and validation are required for the developed models that can be used to make engineering predictions with quantified confidence. The aim of verification test is to ensure the accurate implementation of the solution algorithm. Similarly, validation exercise aims to confirm the reliability of the developed model to correctly capture the various chemo-physical mechanisms.

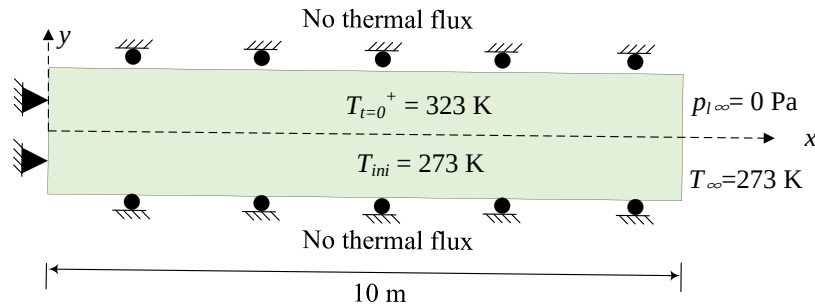
### 4.1 Model verification

This section presents a verification exercise to show the accurate implementation of developed numerical model. This test considers a 1D poroelastic column as a simulation domain, as shown in Fig. 5. The boundary conditions for deformation are: the bottom surface is fixed and the lateral movement in  $x$  direction is restrained. Fixed pressure and temperature are prescribed at top surface. No mass flux and thermal flux are assigned at on other sides. The temperature of column is instantaneously increased to 323 K at  $t=0$  s. Table 1 lists the material properties for this verification, which are from Selvadurai and Suvorov[45]. The analytical solutions for coupled THM model derived by Selvadurai and Suvorov [45] are used as a benchmark for this verification test.



**Fig. 4** Numerical implementation procedure of coupled model.

Figs. 6 shows temporal evolutions of temperature, pressure at bottom surface and displacement at top surface as time goes. The numerical solutions agree well with the analytical solutions, which indicates that an accurate implementation of numerical model developed in this study has been achieved.

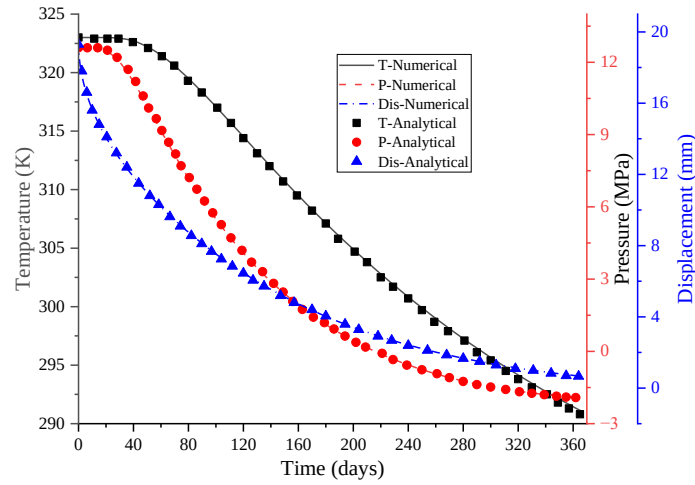


**Fig. 5** Schematic of the domain and simulation conditions.

**Table 1** Parameters used for verification test.

| Parameters                 | Value |
|----------------------------|-------|
| Bulk modulus, $K$ (GPa)    | 5     |
| Poisson's ratio, $\nu$ (-) | 0.3   |

|                                                                         |                       |
|-------------------------------------------------------------------------|-----------------------|
| Permeability, $k$ (m <sup>2</sup> )                                     | $6.0 \times 10^{-19}$ |
| Porosity, $\phi$ (-)                                                    | 0.25                  |
| Fluid viscosity, $\mu$ (Pa·s)                                           | $1.0 \times 10^{-3}$  |
| Biot coefficient, $\alpha$ (-)                                          | 0.75                  |
| Modulus of solid constituent, $K_s$ (GPa)                               | 20                    |
| Fluid compressibility, $c_f$ (GPa <sup>-1</sup> )                       | 0.4545                |
| Effective thermal conductivity, $\lambda_e$ (W/m/K)                     | 1.62                  |
| Effective specific heat capacity, $(\rho C_p)_e$ (J/K/ m <sup>3</sup> ) | $1.0 \times 10^6$     |
| Thermal expansion coefficient of solid, $\alpha_T$ (1/K)                | $8.3 \times 10^{-6}$  |
| Thermal expansion coefficient of water, $\alpha_T$ (1/K)                | $6.9 \times 10^{-5}$  |



**Fig. 6** Comparison of analytical and numerical solutions for temperature (T) and pressure (p) at bottom surface and displacement (Dis) at top surface.

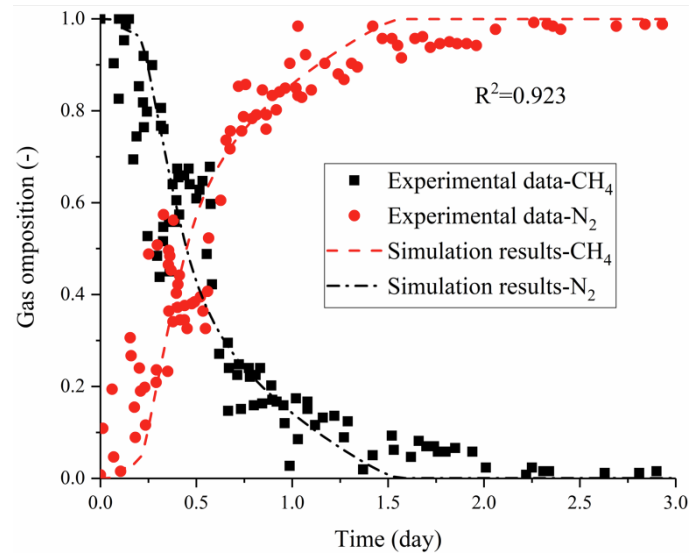
#### 4.2 Model validation

The reliability of developed model for representing the coupled processes during CO<sub>2</sub>-EUGR is examined by comparing the numerical results against the experimental result presented in Zhou et al. [46]. Zhou et al. [46] carried out an experimental measurement on N<sub>2</sub> long-core flooding and displacing CH<sub>4</sub> at temperature of 25 °C. The sample of 3.8 cm in diameter and 7.7 cm in length was taken from coal reservoir in the Qinshui Basin of China. The main operations include: 1) apply confining pressure of 9.7 MPa and core sample was filled with CH<sub>4</sub> at 3.6 MPa; 2) pure N<sub>2</sub> was injected to displace CH<sub>4</sub>, injection pressure at inlet and mole composition of CH<sub>4</sub> and N<sub>2</sub> were recorded, which were presented in [46]. For matching the experimental results, [46] presented numerical study using compositional simulator GEM<sup>TM</sup>. Details on simulation setup and model parameters except for pore compressibility factor were included as well, which were used in this validation test, as listed in Table 2. The pore compressibility factor was obtained by matching experimental data, while its value falls within the range of 0.006-0.6 MPa<sup>-1</sup> reported by Tan et al. [47]. The time dependent injection pressure and constant production pressure were used as boundary conditions.

Fig. 7 shows the comparison of gas composition between experimental observations and numerical results. It can be seen that simulation results agree the experimental results well. The root mean square error (RMSE) is 0.14, and the R-square is 0.923. This validation test demonstrates the reliability of developed model for predicting the coupled processes during CO<sub>2</sub>-EUGR.

**Table 2** Parameters for numerical simulations

| Material parameters                                                                | Values |
|------------------------------------------------------------------------------------|--------|
| Reservoir density, $\rho_s$ (kg/ m <sup>3</sup> )                                  | 1470   |
| Reservoir porosity, $\phi$ (-)                                                     | 0.066  |
| Young's modulus, $E$ (GPa)                                                         | 2.6    |
| Poisson's ratio, $\nu$ (-)                                                         | 0.35   |
| Initial permeability, $k_0$ (md)                                                   | 0.03   |
| Pore compressibility factor, $C_p$ (MPa <sup>-1</sup> )                            | 3.8e-2 |
| Langmuir volume constant for CH <sub>4</sub> , $C_L$ (mol/kg)                      | 1.36   |
| Langmuir pressure constant for CH <sub>4</sub> , $b_L$ (MPa <sup>-1</sup> )        | 1.3.   |
| Volumetric strain coefficient for CH <sub>4</sub> , $\omega$ (m <sup>3</sup> /mol) | 6.5e-6 |
| Langmuir volume constant for N <sub>2</sub> , $C_L$ (mol/kg)                       | 0.848  |
| Langmuir pressure constant for N <sub>2</sub> , $b_L$ (MPa <sup>-1</sup> )         | 0.58   |
| Volumetric strain coefficient for N <sub>2</sub> , $\omega$ (m <sup>3</sup> /mol)  | 6.1e-6 |



**Fig. 7** Comparison of experimental data on N<sub>2</sub>-enhanced CH<sub>4</sub> recovery by Zhou et al. (2013) and numerical solutions.

## 5 Performance analysis of CO<sub>2</sub>-enhanced gas recovery

Different injection strategies have been developed for CO<sub>2</sub>-enhanced gas recovery. In this section, performance of injection strategies in CO<sub>2</sub> storage and improvement of gas recovery is

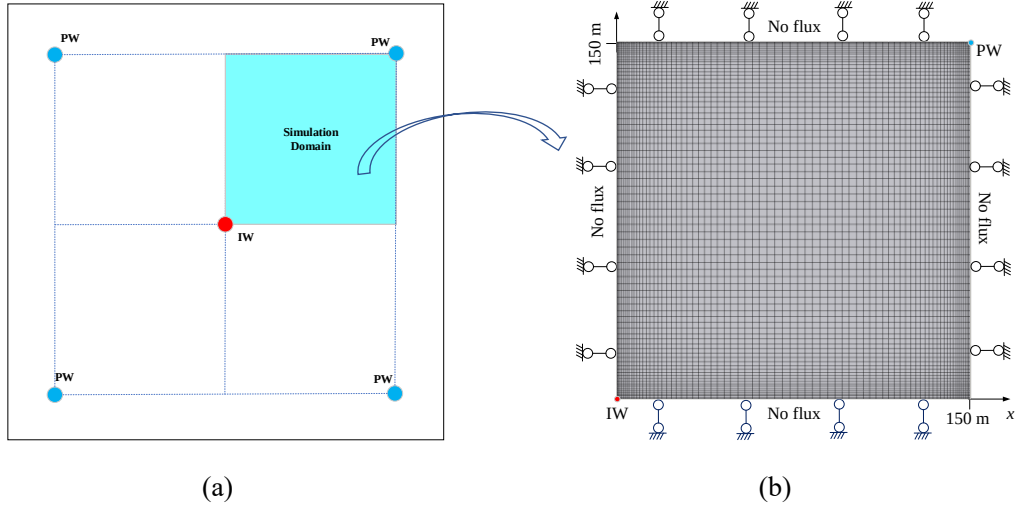
quantitatively evaluated through developed numerical model. As shown in Fig. 8, a five-spot injection-production system is often designed for CO<sub>2</sub>-enhanced gas recovery, that is, CO<sub>2</sub> injection well (IW) is drilled at the center of reservoir domain, its diameter is 0.12m. And four production wells (PW) are drilled around IW. Because of symmetry, a quarter of five-spot domain of 150 m × 150 m area is used for simulations. The reservoir thickness is 10 m. The domain is discretized with 5827 unstructured quadrilateral grids.

For water and gas flow, the fixed capillary pressure and gas concentrations are assigned to PW, there is no mass flux at other boundaries. A fixed temperature is prescribed at IW. Constant volume condition is used as boundary condition for deformation, as given in Fig.8(b). It is assumed that water drainage has been carried out before CO<sub>2</sub> injection. Initial reservoir pressure and temperature are 4 MPa and 303 K, respectively. It is assumed that there is no initial CO<sub>2</sub> in the reservoir, and the water saturation is 0.3 before CO<sub>2</sub> injection. The initial horizontal vertical stress (perpendicular to x-y plane) and horizontal stress are 9 MPa and 6.3 MPa [39]. Considering the pilot test of Nagaoka in Japan as a reference [48], the CO<sub>2</sub> injection rate is set 20 tons/day. Table 3 lists the parameters for this simulation, most of which are chosen from previous work [30, 38, 49, 50]. All simulations run for 3 years.

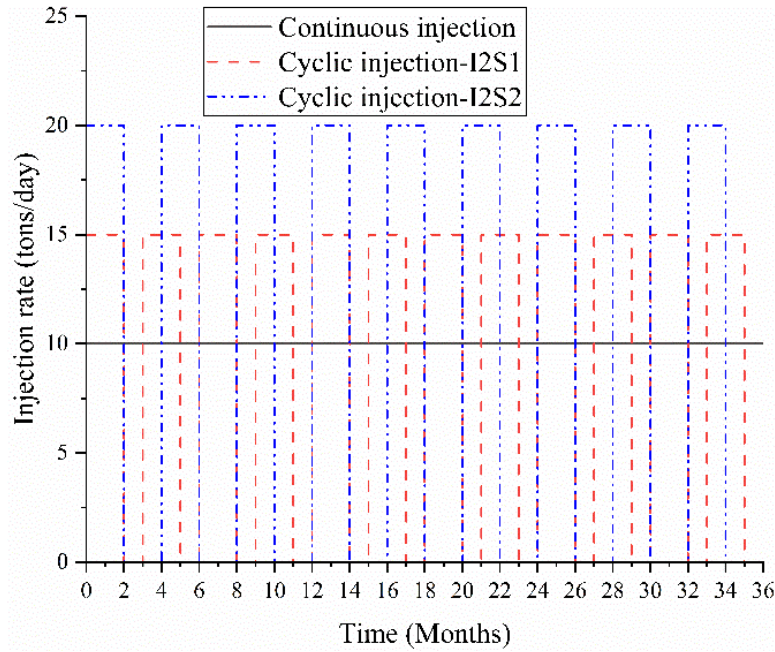
To investigate temperature effect on performance of CO<sub>2</sub>-enhanced gas recovery, different temperatures of injected CO<sub>2</sub> are considered: 303K, 343 K and 383 K, which are assigned at injection well. Performance of injection of CO<sub>2</sub>/N<sub>2</sub> mixture is also evaluated with a gas composition of 50%CO<sub>2</sub>/50%N<sub>2</sub> and 75%CO<sub>2</sub>/25%N<sub>2</sub>. In addition to, continuous injection and alternating injection strategy has also been used in field pilot, the performance of cyclic and continuous CO<sub>2</sub> injection is analyzed. The injection rate for continuous and cyclic injection are shown in Fig. 9. Two injection periods are designed, one is injection for two months and stop for one month (I2S1), the interval is one month, and the other is injection for two months and stop for two months (I2S2), the interval is two months. As a benchmark, the pure CH<sub>4</sub> extraction without CO<sub>2</sub> injection is also simulated. Reservoir permeability is an important parameter for both CH<sub>4</sub> exploitation and CO<sub>2</sub> storage, therefore, different reservoir permeabilities ranging from 0.5 md to 3.0 md are also considered in numerical simulations.

## 5.1 Results and Discussions

The performance of different injection strategies (injected gas temperature, CO<sub>2</sub>/N<sub>2</sub> gas mixture and cyclic gas injection) is evaluated in this section. The cumulative CH<sub>4</sub> production and total adsorbed CO<sub>2</sub> are plotted for quantitative performance.



**Fig. 8** (a) Typical five-spot pattern for CO<sub>2</sub>-enhanced gas recovery and (b) Simulation domain, mesh and boundary conditions.



**Fig. 9** Injection rate for continuous and cyclic injection scenarios.

**Table 3** Parameters for numerical simulations

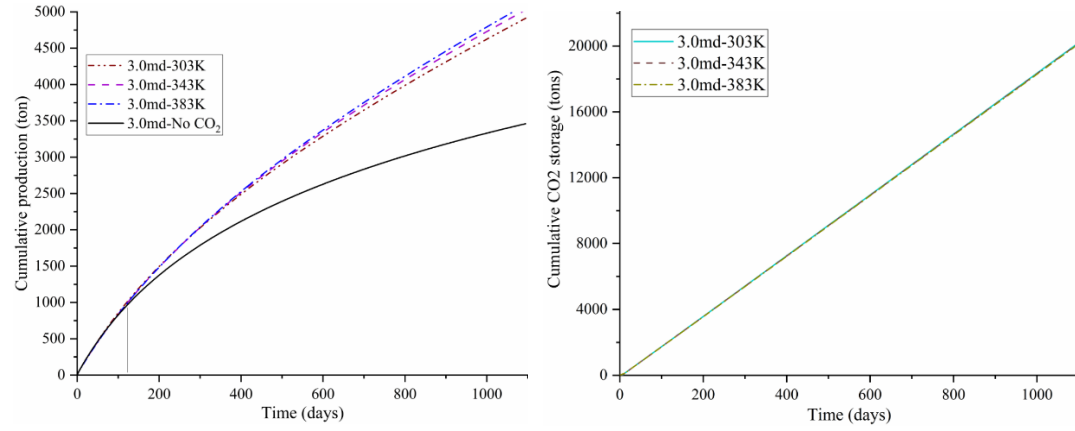
| Material parameters                                           | Values |
|---------------------------------------------------------------|--------|
| Reservoir density, $\rho_s$ (kg/ m <sup>3</sup> )             | 1470   |
| Reservoir porosity, $\phi$ (-)                                | 0.063  |
| Young's modulus, $E$ (GPa)                                    | 3.02   |
| Poisson's ratio, $\nu$ (-)                                    | 0.32   |
| Pore compressibility factor, $C_p$ (MPa <sup>-1</sup> )       | 0.135  |
| Maximum water saturation, $S_{lmax}$ (-)                      | 0.99   |
| Langmuir volume constant for CO <sub>2</sub> , $C_L$ (mol/kg) | 1.5    |

|                                                                                    |         |
|------------------------------------------------------------------------------------|---------|
| Langmuir pressure constant for CO <sub>2</sub> , $b_L$ (MPa <sup>-1</sup> )        | 0.73    |
| Volumetric strain coefficient for CO <sub>2</sub> , $\omega$ (m <sup>3</sup> /mol) | 1.53e-5 |
| Langmuir volume constant for CH <sub>4</sub> , $C_L$ (mol/kg)                      | 0.63    |
| Langmuir pressure constant for CH <sub>4</sub> , $b_L$ (MPa <sup>-1</sup> )        | 0.5     |
| Volumetric strain coefficient for CH <sub>4</sub> , $\omega$ (m <sup>3</sup> /mol) | 1.0e-5  |
| Langmuir volume constant for N <sub>2</sub> , $C_L$ (mol/kg)                       | 0.38    |
| Langmuir pressure constant for N <sub>2</sub> , $b_L$ (MPa <sup>-1</sup> )         | 0.29    |
| Volumetric strain coefficient for N <sub>2</sub> , $\omega$ (m <sup>3</sup> /mol)  | 0.3e-5  |
| Initial saturation, $S_i$ (-)                                                      | 0.3     |
| Residual water saturation, $S_{lr}$ (-)                                            | 0.01    |
| Saturation constant, $\gamma$ (-)                                                  | 1.54    |
| Saturation constant, $p_0$ (Pa)                                                    | 2.0e4   |
| Water viscosity, $\mu_l$ (Pa · s)                                                  | 1.0e-3  |
| Reservoir temperature, $T$ (K)                                                     | 303     |
| Initial permeability, $k_0$ (md)                                                   | 0.5-3.0 |
| Interaction energy of CO <sub>2</sub> , $E_{in}$ (J/mol)                           | 5266    |
| Reduction coefficient of CO <sub>2</sub> , $\delta$ (K <sup>-1</sup> )             | 0.023   |
| Interaction energy of CH <sub>4</sub> , $E_{in}$ (J/mol)                           | 9238    |
| Reduction coefficient of CH <sub>4</sub> , $\delta$ (K <sup>-1</sup> )             | 0.0083  |
| Decay coefficient with moisture content for CO <sub>2</sub> , $\xi$ (-)            | 0.172   |
| Decay coefficient with moisture content for CH <sub>4</sub> , $\xi$ (-)            | 0.145   |
| Thermal expansion coefficient, $\alpha_T$ (K <sup>-1</sup> )                       | 9.0e-5  |
| Thermal conductivity of CO <sub>2</sub> , $\lambda_g$ (W/m/K)                      | 0.0246  |
| Thermal conductivity of CH <sub>4</sub> , $\lambda_g$ (W/m/K)                      | 0.0371  |
| Thermal conductivity of solid skeleton, $\lambda_s$ (W/m/K)                        | 0.33    |
| Specific heat capacity of solid skeleton, $C_{ps}$ (J/K/kg)                        | 1250    |
| Specific heat capacity of water, $C_{pl}$ (J/K/kg)                                 | 4200    |

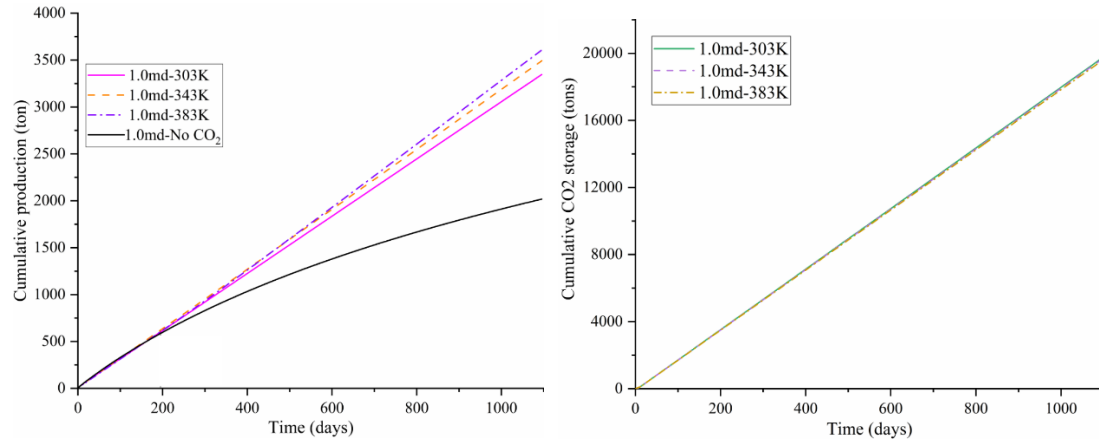
### 5.1.1 Injection gas temperature

The thermal effects on cumulative CH<sub>4</sub> production and total adsorbed CO<sub>2</sub> are presented in Fig. 10. The cumulative CH<sub>4</sub> production through pure CH<sub>4</sub> drainage is included as well. It is shown that the reservoir permeability plays a significant role in CH<sub>4</sub> production. When the reservoir permeability is 0.5 md, the cumulative CH<sub>4</sub> production arrives at about 560 tons for pure CH<sub>4</sub> extraction after one year, and it increases to about 970 tons and 2010 tons for 1.0 md and 3.0 md. After 3 years, the cumulative CH<sub>4</sub> production through pure CH<sub>4</sub> extraction reaches about 1300 tons, 2000 tons and 3500 for 0.5 md, 1.0 md and 3.0 md, respectively. It can be concluded that the correlation between CH<sub>4</sub> production and reservoir permeability is nonlinear. Since the curve shows the cumulative CH<sub>4</sub>

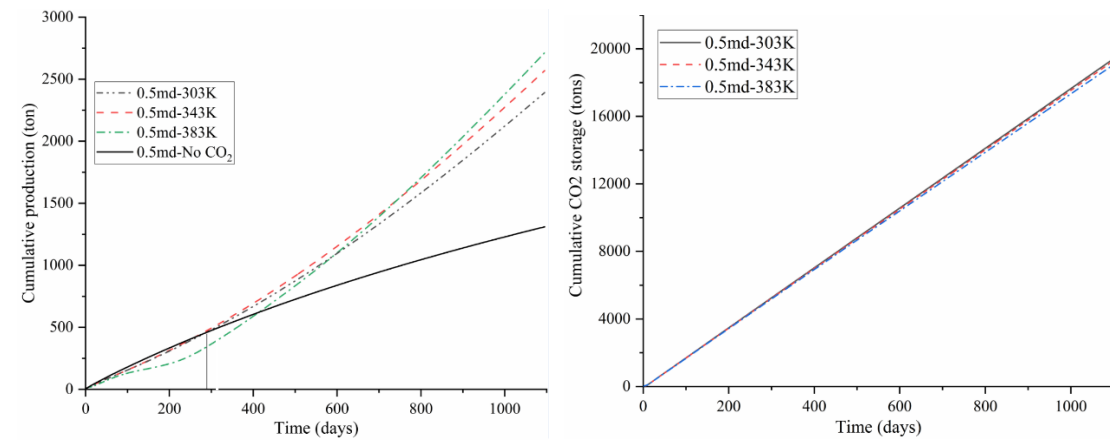
production, the slope of the curve is the CH<sub>4</sub> production rate. All curves of cumulative CH<sub>4</sub> production without CO<sub>2</sub> injection is convex, therefore, the production rate is highest at early stage and then experiences a gradual drop.



(a) 3.0 md



(b) 1.0 md



(c) 0.5 md

**Fig. 10** Cumulative CH<sub>4</sub> production (left column) and total adsorbed CO<sub>2</sub> (right column) at different injection gas temperature of 303 K, 343K and 383K.

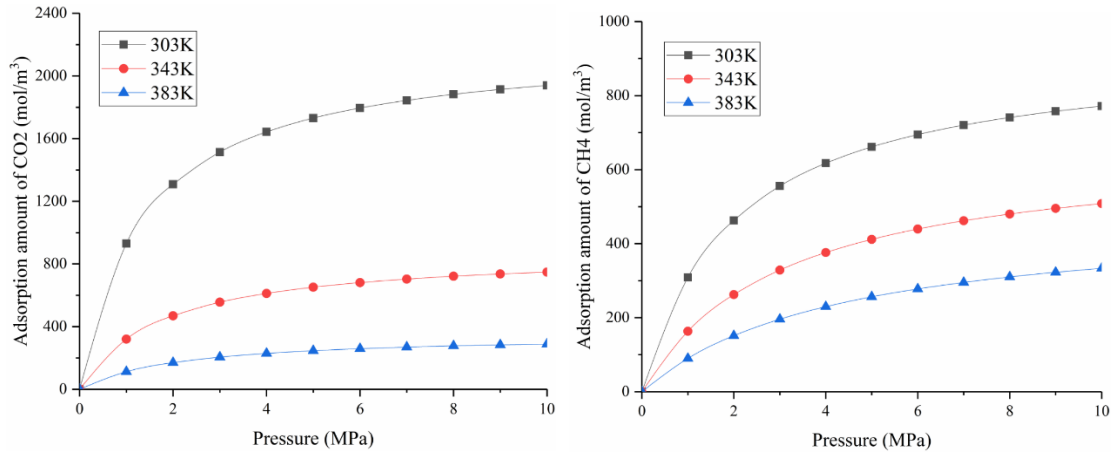
Compared to pure CH<sub>4</sub> extraction, the displacement efficiency of CO<sub>2</sub> is obvious. However, the

improvement of CH<sub>4</sub> production could not occur immediately, this is because the displaced CH<sub>4</sub> will accumulate near the CO<sub>2</sub> front and could not reach the production well [29]. The higher the permeability, the shorter it takes to make displacement of CH<sub>4</sub> by CO<sub>2</sub> to work. For example, when reservoir permeability is 1.0 md and 3.0 md, about 100 and 200 days are required for cumulative CH<sub>4</sub> production with CO<sub>2</sub> injection surpassing that without CO<sub>2</sub> injection, as shown in Fig. 10(a) and Fig. 10(b). It is worth pointing out that the temperature increase could not lead to occurring of displacement effect of CO<sub>2</sub> ahead of time when reservoir permeability is higher than 1.0 md. Particularly, the higher the permeability is, the later the distinction of displacement effect under different temperatures emerges. For example, when considering reservoir permeability of 3.0 md, it takes about 400 days to show the difference of cumulative CH<sub>4</sub> production due to temperature difference of injected gas. Compared to the required time for 3.0 md, it occurs earlier when the permeability is 1.0 md (about 100 days earlier). This is because adsorption is an exothermal, increasing temperature will lead to drop in CO<sub>2</sub> adsorption capacity [51], as shown in Fig. 11, which leads to more free phase CO<sub>2</sub>. More free phase CO<sub>2</sub> in reservoir can cause a buildup of higher gas pressure, which further facilitates the release of more adsorbed CH<sub>4</sub> and speeds up gas transport toward production well.

When gas reservoirs whose permeability is less than 1md are low permeable, the temperature effect is significant. During the early period, the cumulative CH<sub>4</sub> production with CO<sub>2</sub> injection is less than that by pure CH<sub>4</sub> extraction, especially at 383 K temperature of injected gas. As shown in Fig. 9(c), when reservoir permeability is lower, increasing temperature of injected CO<sub>2</sub> can extended the required time for displacement effect occurring. It takes about 400 days to make the cumulative CH<sub>4</sub> production through CO<sub>2</sub> injection to exceed that produced by only CH<sub>4</sub> drainage when temperature of injected gas is 383 K, which is over 100 days longer than that at 303 K and 343 K. Also, the cumulative CH<sub>4</sub> production at 383 K temperature of injected CO<sub>2</sub> is less than that at 303 K and 343 K during the first half of injection period.

As time goes, the temperature effect is shown. It can be observed from Fig. 10 that increase in temperature can lead to rise of CH<sub>4</sub> production, and this rise is permeability dependent. The lower the reservoir permeability, the more significant the effect of temperature rise is. For example, when the reservoir permeability is 3.0 md, increasing temperature of injected CO<sub>2</sub> from 303 K to 383 K can cause an increase of the cumulative CH<sub>4</sub> production by 4.1% after 3 years, which increases to 5100 tons from 4900 tons. However, the cumulative CH<sub>4</sub> production increases to about 2700 tons from 2400 tons and to about 3600 tons from 3350 when the reservoir permeability is 0.5 md and 1.0 md, it increases by 12.5% and by 6.9%. Compared to pure CH<sub>4</sub> exploitation, the cumulative CH<sub>4</sub> production doubles for permeability of 0.5 md. Although increasing temperature of injected CO<sub>2</sub> enable CH<sub>4</sub> production to be improved, but the efficiency is not positively correlated with temperature rise. After 3 years, when temperature increases from 303 K to 343 K and from 343 K to 383 K, the cumulative CH<sub>4</sub> production from gas reservoirs with a permeability of 0.5 md increases

by about 180 tons and by 120 tons, respectively. This is because the when temperature is lower, increasing temperature can lead to desorption of more adsorbed CH<sub>4</sub>. Similarly, permeability increases to 1.0 md, the cumulative CH<sub>4</sub> production increases by about 145 tons and by 115 tons, respectively. For gas reservoir with a permeability of 3.0 md, temperature rises from 303 K to 343 K and from 343 K to 383 K cause an increase in cumulative CH<sub>4</sub> production by 115 tons and by 70 tons, respectively. It can be concluded that the increase in temperature is more suitable for low permeability gas reservoir.



**Fig. 11** Effects of pressure and temperature on gas adsorption.

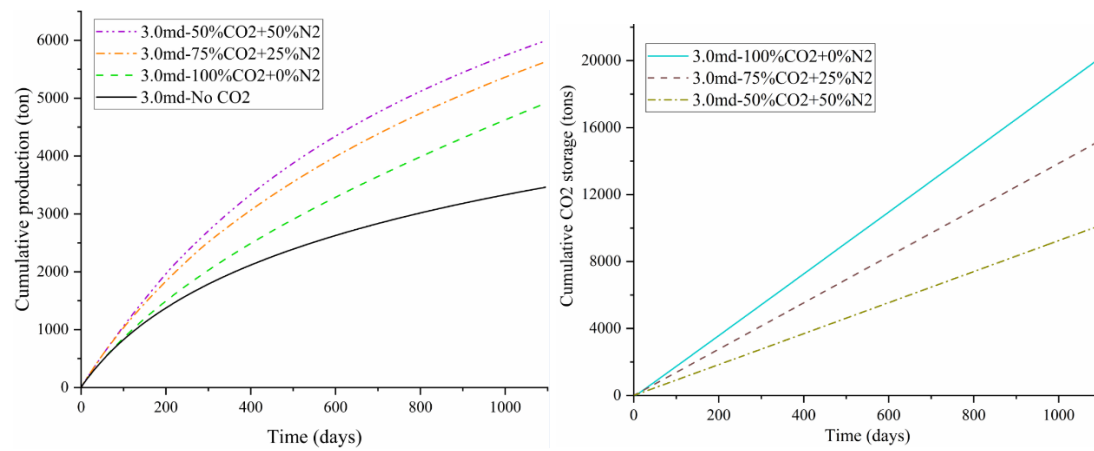
CO<sub>2</sub> injection can cause a significant change in CH<sub>4</sub> production rate (slope of cumulative production curve). Interestingly, CO<sub>2</sub> injection induced change in the CH<sub>4</sub> production rate is associated with reservoir permeability. When the permeability is 3.0 md, the cumulative CH<sub>4</sub> production curve is convex, indicating the CH<sub>4</sub> production rate experiences gradual drop as time goes. However, the nearly linear increase in cumulative CH<sub>4</sub> production implies that the CH<sub>4</sub> production rate is almost the same. Increasing the temperature can cause a bit increase in production rate when permeability is higher. Lower permeability gas reservoir (0.5 md) shows a little complex cumulative CH<sub>4</sub> production curve. the cumulative CH<sub>4</sub> production curve is concave. This indicates that the production rate is nonlinear, which undergoes a gradual increase when temperature of injected CO<sub>2</sub> is 303 K and 343 K. For higher temperature of 383 K, the production rate firstly experiences a drop, and then it increases more significantly than those at temperature of 303 K and 343 K. This is because higher temperature can reduce the CO<sub>2</sub> adsorption capacity significantly, and more adsorbed CH<sub>4</sub> where CO<sub>2</sub> reaches will be displaced, however, the released CH<sub>4</sub> could not arrive at the production well, and will accumulate in which no CO<sub>2</sub> reaches, leading to pressure increase and adsorption of more CH<sub>4</sub>. This will reduce the free phase CH<sub>4</sub> flowing toward production well.

In addition to improvement of CH<sub>4</sub> recovery via CO<sub>2</sub> injection, the injected CO<sub>2</sub> can also be sequestered in gas reservoirs. In unconventional gas reservoir, such as coal seams, shales, most gas is adsorbed in reservoirs. The total CO<sub>2</sub> adsorbed in reservoirs is computed and plotted, as shown in left column of Fig. 10. There is totally 21900 tons of CO<sub>2</sub> injected into gas reservoir, over 90%

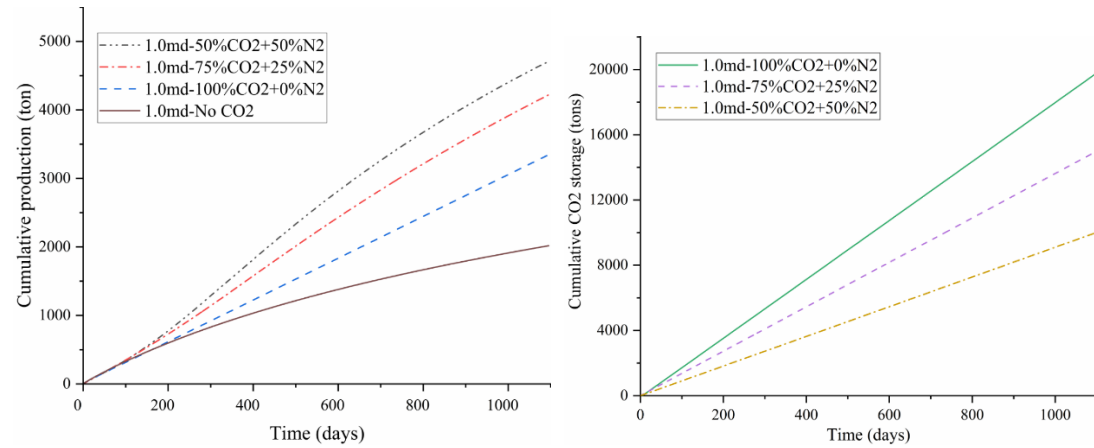
of injected gas is adsorbed in reservoirs, reaching about 20000 tons. The cumulative adsorbed CO<sub>2</sub> increases linearly as time goes. The effect of temperature on CO<sub>2</sub> adsorption is less significant, especially for highly permeable reservoir.

### 5.1.2 Gas mixture injection

N<sub>2</sub> has a lower adsorption capacity, the CO<sub>2</sub>/N<sub>2</sub> mixture injection is usually considered to be one of injection strategies to enhance CH<sub>4</sub> production [52, 53]. The performance of CO<sub>2</sub>/N<sub>2</sub> mixture injection in improvement of CH<sub>4</sub> recovery is shown in Fig. 12. The reservoir permeabilities of 1.0 md and 3.0 md are considered. It can be observed that mixed gas injection enables the displacement effect of CO<sub>2</sub> to occur early than pure CO<sub>2</sub> injection. It takes about 30 days and 100 days to show the displacement effect.



(a) 3.0 md



(b) 1.0 md

**Fig. 12** Cumulative CH<sub>4</sub> production (left column) and total adsorbed CO<sub>2</sub> (right column) at different gas compositions

The higher molar fraction of N<sub>2</sub> in mixed gas is, the better the displacement efficiency is, while the adsorption amount of CO<sub>2</sub> is reduced. As fraction of N<sub>2</sub> increases, the increase in cumulative CH<sub>4</sub> production slows down, especially for gas reservoir with a higher permeability. When the reservoir

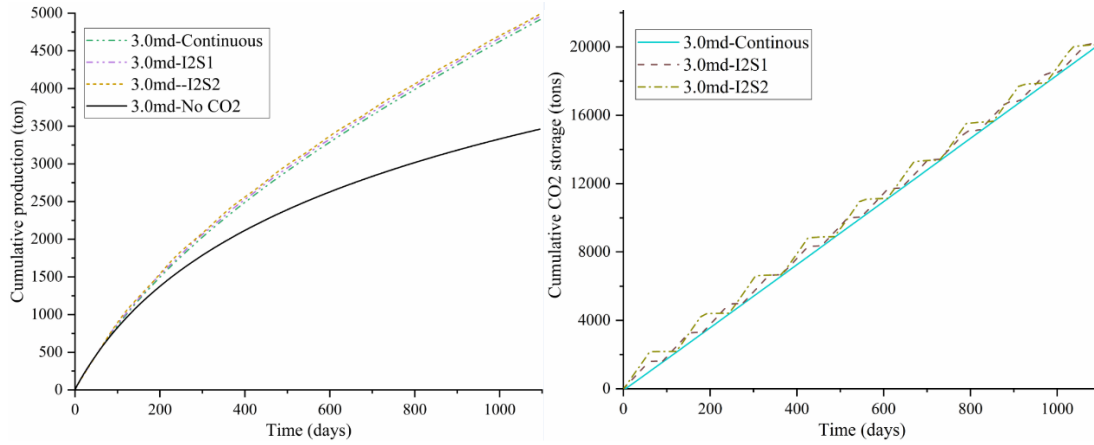
permeability is 3.0 md, the cumulative CH<sub>4</sub> production increases from 4900 tons to 5600 tons as a result of drop in fraction of CO<sub>2</sub> from 100% to 75% after three years. The injection of 50%CO<sub>2</sub>/50%N<sub>2</sub> only renders cumulative CH<sub>4</sub> production to increase by about 400 tons, arriving at 6000 tons. For gas reservoir with a permeability of 1.0 md, cumulative CH<sub>4</sub> production increases from about 3350 tons to 4200 tons and to 4700 tons when N<sub>2</sub> fraction in gas mixture reaches to 25% and 50%. From the slope of cumulative CH<sub>4</sub> production, it can be found that mixed gas injection can improve the CH<sub>4</sub> production rate, especially for reservoirs with lower permeability. When reservoir permeability is 1.0 md, the cumulative CH<sub>4</sub> production curve exhibits an approximately S-shaped pattern for mixed gas injection with higher fraction of N<sub>2</sub>, this implies that the CH<sub>4</sub> production rate experiences an increase during early injection period, followed by a gradual drop.

However, the mixed gas injection reduces the amount of adsorbed CO<sub>2</sub>. When gas mixtures of 75%CO<sub>2</sub>/25%N<sub>2</sub> and 50%CO<sub>2</sub>/50%N<sub>2</sub> are injected into reservoirs, there are total 16425 tons and 10950 tons of CO<sub>2</sub> injected after three years. After three years, the cumulative adsorbed CO<sub>2</sub> reaches about 15000 tons and 10000 tons, which takes up over 90% of total injected CO<sub>2</sub>. It can be concluded that the percentage of adsorbed CO<sub>2</sub> can still be remaining for injection of CO<sub>2</sub>/N<sub>2</sub> mixed gas.

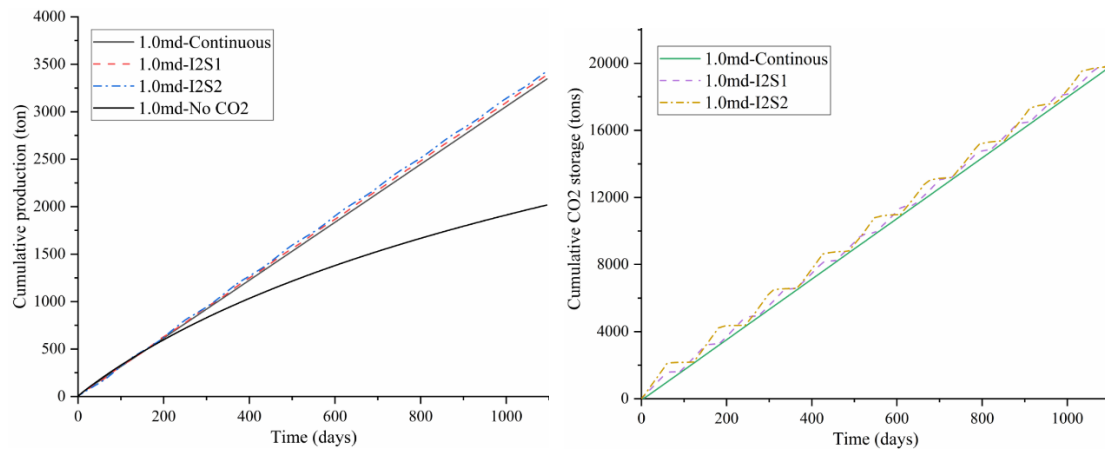
### **5.1.3 Alternating gas injection**

Cyclic CO<sub>2</sub> injection was usually used to improve oil recovery [e.g. 54], and its efficiency for improvement of gas recovery has also been investigated in recent years [e.g. 55, 56]. This study designed two alternating gas injection scenarios (I2S1 and I2S2). The performance of alternating gas injection approach is shown in Fig. 13. It can be observed that the time it takes to show the displacement effect is almost the same as that for continuous injection. Also, the alternating CO<sub>2</sub> injection only causes only a little increase in cumulative CH<sub>4</sub> production, alternating CO<sub>2</sub> injection cannot efficiently enhance the CH<sub>4</sub> production, especially when the reservoir permeability is higher, similar results were also presented by Mansi et al. Mansi, Almobarak [55]. In comparison, the performance of injection scenario I2S2 is better than that of I2S1 since the injection period for I2S2 is short than that for I2S1 and the injection rate of CO<sub>2</sub> is higher. This implies that increase in injection rate is useful for that CH<sub>4</sub> production.

In contrast, cyclic CO<sub>2</sub> injection can improve the CO<sub>2</sub> adsorption during injection period, especially when using I2S2, as shown in left column of Fig. 13, this is because higher injection rate can cause buildup of higher gas pressure, leading to occurring of more CO<sub>2</sub> adsorption. The work Thomas and Chen [57] indicates that increase in adsorbed CO<sub>2</sub> can contribute to long-term storage of CO<sub>2</sub> after injection ceasing, therefore, alternating gas injection is useful for CO<sub>2</sub> sequestration.



(a) 3.0 md



(b) 1.0 md

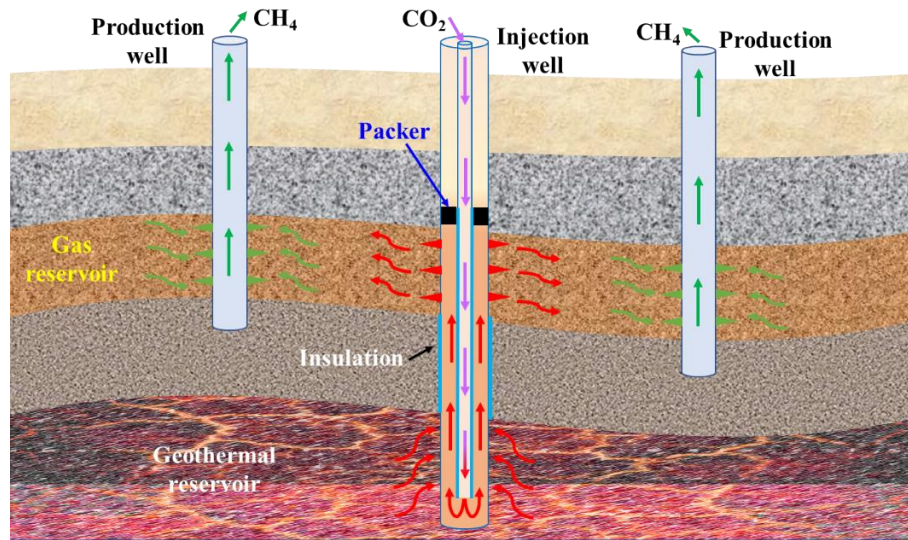
**Fig. 13** Cumulative CH<sub>4</sub> production (left column) and total adsorbed CO<sub>2</sub> (right column) for continuous and alternating injection strategies.

## 5.2 Implications for CO<sub>2</sub>-enhanced gas recovery

Performance of different injection strategies in CO<sub>2</sub>-enhanced gas recovery with simultaneous sequestration is evaluated by non-isothermal compositional two-phase modelling approach, as shown above. Analysis results indicate that the injection strategy should be determined according to reservoir permeability and properties of injected gases. The numerical results show that CO<sub>2</sub> injection can more efficiently improve CH<sub>4</sub> recovery from low permeability gas reservoirs. Since the reservoir permeability generally drops as the depth of reservoirs increases[58], CO<sub>2</sub> enhanced gas recovery should be considered for exploitation of deep gas reservoirs, another advantage is the mitigation of leak risk of injected CO<sub>2</sub>. In addition, mixed CO<sub>2</sub>/N<sub>2</sub> gas can enhance CH<sub>4</sub> production significantly, therefore, mixtures of CO<sub>2</sub>/N<sub>2</sub> with higher fraction of N<sub>2</sub> can be injected during early injection period. After the CH<sub>4</sub> production rare reaches the maximum, the fraction of CO<sub>2</sub> should be increased, this will be useful to achieve both enhanced CH<sub>4</sub> recovery and CO<sub>2</sub> geological storage.

The temperature effects show that increasing the temperature of injected gas can improve the CH<sub>4</sub>

production, especially for low permeability reservoirs. Geothermal energy can be used for gas heating. A geothermal-assisted CO<sub>2</sub>-enhanced gas recovery is proposed (Fig. 14). The IW is drilled into the geothermal reservoir for injected gas heating, a packer is installed in injection well above the gas reservoirs. The injected gas flows downward through the geothermal reservoir and will be heated, and then heated gas flow upward into gas reservoirs to improve CH<sub>4</sub> production, which achieves a combination of CO<sub>2</sub> and geothermal stimulation.



**Fig. 14** Schematics of wellbore layout for geothermal-assisted CO<sub>2</sub>-enhanced gas recovery.

It is worth pointing out that this work evaluates the performance of CO<sub>2</sub>-enhanced gas recovery and storage by considering a 2D problem. The effects of overburden and gravity have not been investigated in this work. Hence, extension of model application to three dimensional problems combining high performance computing technique is suggested for future research with inclusion of the effects of overburden, gravity and reservoir heterogeneity.

## 6 Conclusions

CO<sub>2</sub>-EUGR is a complex THCM coupling processes. In order to accurately assess the efficiency of CO<sub>2</sub>-EUGR, this paper presents a numerical model for capturing the coupled non-isothermal compositional two-phase flow and geomechanics behavior of CO<sub>2</sub>-EUGR. The developed model incorporates multicomponent kinetics to separate the free phase and adsorbed phase instead of equilibrium adsorption model used in previous work. The non-isothermal effects on gas adsorption and transport behavior are included. A hybrid numerical approach combining EbFVM and GFEM is employed to obtain numerical solutions. The accuracy of developed model is examined through a verification test. The developed model is then used to evaluate the performance of CO<sub>2</sub>-EUGR with various injection strategies, including temperature rise of injected gas, mixed gas injection and alternating gas injection.

The results demonstrate that CO<sub>2</sub> injection is capable of enhancing CH<sub>4</sub> recovery significantly, and

the efficiency is associated with reservoir permeability. Higher permeability can render the displacement effect to occur earlier. Increasing temperature can improve CH<sub>4</sub> recovery, especially for low permeability gas reservoir. Based on this finding, a geothermal-assisted CO<sub>2</sub>-enhanced gas recovery is proposed for combination of CO<sub>2</sub> and geothermal stimulation. The improving performance of mixed CO<sub>2</sub>/N<sub>2</sub> injection is greatest amount these injection strategies. Mixed CO<sub>2</sub>/N<sub>2</sub> injection not only enable displacement effect to earlier, but also enhance the CH<sub>4</sub> production rate, especially for low permeability reservoir. Cyclic injection causes only a little increase in CH<sub>4</sub> production, while it can increase the amount of adsorbed CO<sub>2</sub> during injection period. More than 90% of injected CO<sub>2</sub> can be adsorbed for all injection strategies.

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