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Density-Driven Flow Simulation in Anisotropic Porous Media: Application to CO₂ Geological Sequestration

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Abstract

Carbon dioxide (CO₂) sequestration in saline aquifers is considered as one of the most viable and promising ways to reduce CO₂ concentration in the atmosphere. CO₂ is injected into deep saline formations at supercritical state where its density is smaller than the hosting brine. This motivates an upward motion and eventually CO₂ is trapped beneath the cap rock. The trapped CO₂ slowly dissolves into the brine causing the density of the mixture to become larger than the host brine. This causes gravitational instabilities that is propagated and magnified with time. In this kind of density-driven flows, the CO₂-rich brines migrate downward while the brines with low CO₂ concentration move upward. With respect to the properties of the subsurface aquifers, there are instances where saline formations can possess anisotropy with respect to their hydraulic properties. Such anisotropy can have significant effect on the onset and propagation of flow instabilities. Anisotropy is predicted to be more influential in dictating the direction of the convective flow. To account for permeability anisotropy, the method of multipoint flux approximation (MPFA) in the framework of finite differences schemes is used. The MPFA method requires more point stencil than the traditional two-point flux approximation (TPFA). For example, calculation of one flux component requires 6-point stencil and 18-point stencil in 2-D and 3-D cases, respectively. As consequence, the matrix of coefficient for obtaining the pressure fields will be quite complex. Therefore, we combine the MPFA method with the experimenting pressure field technique in which the problem is reduced to solving multitude of local problems and the global matrix of coefficients is constructed automatically, which significantly reduces the complexity. We present several numerical scenarios of density-driven flow simulation in homogeneous, layered, and heterogeneous anisotropic porous media. The numerical results emphasize the significant effects of anisotropy in driving the migration of dissolved CO₂ along the principal direction of anisotropy even if the porous medium is highly heterogeneous. Furthermore, the impacts of the increase of density difference between the brine and the CO₂-saturated brine with respect to the onset time of convection, the CO₂ flux, and the CO₂ total dissolved mass are also discussed in this paper.

Motivation and background

Nowadays, global warming issue has become the world-widely discussed topic due to the change of climate on the Earth. One of the causes of the global warming is the greenhouse gasses emission, i.e., the release of CO₂ into the atmosphere due to the use of fossil fuels in the industry activities such as power plant, refineries, petrochemical industries, oil and gas processing, etc. The amount of CO₂ concentration in the atmosphere has steadily increased particularly in the last century, from 280 ppm (prior to the industrial revolution) to 390 ppm (at the current time) with annual increase of 1 to 2 ppm [Firoozabadi and Cheng, 2010]. If we let the CO₂ concentration increases continuously in the atmosphere then there will be several consequences that mankind may face in the future such as the continuous increase of Earth's temperature, the increase of ocean acidification that perhaps affect the marine life, etc [Firoozabadi and Cheng, 2010]. To tackle this issue, a mechanism has been proposed to mitigate the CO₂ by injecting it into the subsurface geological formations, which is called as CO₂ geological sequestration. This mechanism is considered as one of the most effective ways to reduce the amount of CO₂ concentration in the atmosphere [IPCC, 2005; Ennis-King and Paterson, 2005; Xu et al., 2006; Firoozabadi and Cheng, 2010; Cheng, et al., 2012, Salama et.al, 2013a]. In this scheme, the CO₂ is injected into deep geological formations (e.g., depleting oil and gas reservoirs, deep saline aquifers, and unminable coal beds) in supercritical condition and it is expected that CO₂ will be accumulated and trapped under the impermeable layer of caprock for long period of time, hundreds to thousands of years. Basically, there are four CO₂ storage mechanisms [IPCC, 2005]:

- (1) *Structural and stratigraphic trapping*: the injected CO₂ occupies the pore space and penetrate up through the porous rock and eventually accumulates beneath the very-low-permeability layers (caprocks).
- (2) *residual trapping*: when the CO₂ is injected into a formation, it displaces the formation liquid through the porous rock and continues to migrate as a separate phase because some of the CO₂ will be left behind in the pores and trapped there as residual CO₂.
- (3) *solubility trapping*: the injected CO₂ is dissolved in the formation liquid (e.g. brine) by the molecular diffusion such that it no longer exists as a separate phase (no buoyant forces which can drive it upwards).
- (4) *mineral trapping*: when the CO₂ dissolved in the formation liquid, it forms a weak acid that will make a chemical reaction with the minerals surrounding the rocks. It is believed that the chemical reaction between the dissolved CO₂ with the minerals will take place over days (for carbonate minerals) up to thousands of years (for silicate minerals).

The solubility and mineral trappings belong to geochemical trapping, which both are the most effective storage mechanisms since they can trap CO₂ for longer geological time scales than the other two mechanisms. In this work, however, we only attempt to model the solubility trapping mechanism by investigating the dissolution-diffusion-convection process. In this mechanism, after the CO₂ is being injected into the subsurface formations, it dissolves into the formation water (brine) such that forming a mixture with its density becomes larger than the host formation water and eventually induces the gravitational instability (fingering). The increase of the density of the formation water can be 0.1-1%, depending on its salinity [Pruess and Zhang, 2008; Pau et al., 2010]. When the CO₂ and formation water have been mixed, the CO₂-rich water formation migrates downward and the CO₂-poor water formation moves upwards. The convection process is typically faster than the diffusion process in such a way the overall dissolution process is mainly dominated by the convective mixing [Xu et al., 2006].

With respect to the subsurface formations, the geological structures are geometrically complex due to the geological processes over millions of years. In many cases, the geological formations are anisotropic, with the permeability in one direction is dominant than the others. The anisotropy property emerges during the sedimentation processes that usually produce flow conduits parallel to the bedding plane, which are different from the normal orientation to this plane [Bear and Cheng, 2010]. In anisotropic porous medium, the rock permeability is varying in all directions. In other words, the permeability is dependent on the direction. In this case, the migration of the formation fluid will be mainly driven by the principal direction of anisotropy. Describing such phenomena through the numerical model, we need to treat the permeability as a full tensor (second rank tensor) rather than the diagonal tensor (first rank tensor) or scalar (zeroth rank tensor). In the full tensor case, the off-diagonal element are nonzero and these elements induce the cross flow that makes the flow direction to be different from the linear potential gradient.

A number of literatures that investigate the solubility of CO₂ by considering anisotropy in the permeability fields are available, e.g. Farajzadeh et al. [2008], Rapaka et al. [2009] and Cheng et al. [2012]. However, none of them are considering the permeability field as a full tensor in their model. Mostly the anisotropy permeability is defined as a first rank tensor with different values in the diagonal components, i.e., the horizontal permeability is several times greater than vertical one. Farajzadeh et al. [2008] and Rapaka et al. [2009] have investigated the effect of anisotropy and layering in the permeability fields. Farajzadeh et al. [2008] studied the natural convection effects in dual layered and anisotropic porous media experimentally and numerically. From the simulation results, they reached the conclusion that the decrease of vertical permeability reduces the convection effects and increase the critical time for the onset of convection. Rapaka et al. [2009] discuss the theoretical model to predict the growth of perturbations in anisotropic and layered porous media. The study has shown that the theoretical model works as long as the gradients of permeability in the vertical direction are much larger than the ones in the horizontal direction. Cheng et al. [2012] have studied the effect of anisotropy permeability on the onset with the vertical permeability is fixed while the horizontal permeability increases. They have shown that the enhanced dissolution from convection will be significantly earlier in anisotropic porous media.

Based on the CO₂ sequestration literatures above (and many others), which the consideration of full permeability tensor has not been yet implemented in the density-driven flow simulation, in this paper we are trying to simulate the dissolution-diffusion-convection processes by taking into account the off-diagonal elements in the permeability tensor. We apply a numerical method so-called multipoint flux approximation (MPFA) method that has been introduced that can handle the full tensor of permeability field [Aavatsmark et al., 1998; Aavatsmark, 2002; Edwards and Rogers, 1998]. The MPFA method requires more point stencils than the convectional two-point flux approximation (TPFA) for example in 2-D case, each flux component involves 6 pressure values associated with the neighboring 6 cells and in 3-D case, it involves 18 pressure values in the surrounding 18 cells. Numerical discretization that is dealing with such point stencils will not be easy and much more involved in the construction of the matrix of coefficient. To simplify that, we apply the experimenting pressure field approach, which generates the coefficients of matrix of the pressure equation automatically within the solver routine [Sun et al. 2012]. This technique facilitates the solution of the global problem divided into the solution of multitude of local problems without losing the accuracy of the solution. This significantly reduces the complexity of constructing the matrix of coefficient.

In the following sections, we discuss the governing equations for the density-driven flow in porous media. We then present the numerical method of MPFA. In the results and discussion section, we demonstrate three numerical examples of density-driven flow simulation in homogenous, layered, and heterogeneous anisotropic porous media including the sensitivity analysis of the onset time of convection, the CO₂ dissolution rate and the CO₂ total dissolved mass. Finally, we end up with the last section that contains the summary and conclusions of the work.

Governing equations

This section presents the governing equations of density-driven flow in porous media that consist of the transport (convection-dispersion-diffusion) equation, pressure equation, and Darcy's law. These equations describe the relationship between macroscopic variable based on the continuum hypothesis as applied to porous media, Salama and Van Geel (2008a-b).

Transport (convection-dispersion-diffusion) equation. The transport equation describes the mass balance of a dissolved chemical species due to the physical processes of convection, dispersion, diffusion, and chemical reactions. According to Wexler [1992], convection is defined as the movement of the solute particles along the direction of the fluid flow at the average fluid velocity. Meanwhile, (mechanical) dispersion describes the spreading of the solute particles along the direction of the flow and transverse to it as a result of the local variations of the fluid velocities with respect to Darcy velocity. Molecular diffusion, on the other hand, accounts for the spreading resulting from the difference between molecular velocities and the average fluid velocity. The transport equation is mathematically expressed by a partial differential equation as follows

$$\phi \frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{u}C) - \nabla \cdot (\phi \mathbf{D}_h \nabla C) = q + R \quad (1)$$

where C is the solute concentration, ϕ is the porosity, $\mathbf{u}$ is the Darcy velocity, $\mathbf{D}_h$ is the hydrodynamic dispersion tensor (m^2/s), q is the sources/sinks (1/s), and R is the chemical reactions. Any sources/sinks and chemical reactions are ignored in this model. In this work, we evaluate the transport equation by the implicit scheme. The third term of the left-hand side of (1) describes the hydrodynamic dispersion tensor, $\mathbf{D}_h$, which accounts for both mechanical dispersion, $\mathbf{D}$, and molecular diffusion, $\mathcal{D}$,

$$\mathbf{D}_h = \mathbf{D}(\mathbf{u}) + \mathcal{D} \quad (2)$$

According to Lichtner et al. [2002], the mechanical dispersion is a function of Darcy velocity with the main and off-diagonal elements are given by (in 2-D space),

$$D_{ii} = \left[\alpha_L \frac{u_i^2}{u^2} + \alpha_T \frac{u_j^2}{u_i^2 + u_j^2} \right] u, \quad i = j = 1, 2 \quad (3)$$

$$D_{ij} = \left[\alpha_L \frac{u_i u_j}{u^2} + \alpha_T \frac{u_i u_j}{u_i^2 + u_j^2} \right] u, \quad i = j = 1, 2 \quad (4)$$

where α_L and α_T are the longitudinal and transverse dispersivities of the porous medium, respectively. These three coefficients are defined as

$$\begin{aligned} \alpha_L &= \alpha_1 + \alpha_2 - \alpha_3 \cos^2 \beta \\ \alpha_T &= \alpha_1 \end{aligned} \quad (5)$$

The α_1 , α_2 , and α_3 are the three material coefficients while β is the angle between the material axis and the flow direction. In density driven flows, the induced velocity is usually small and hence there is a great deal of motivation to only consider diffusion. In this case the whole dispersion tensor reduces to a scalar quantity. The types of boundary conditions that we use in the model are Dirichlet and Neumann, which are defined as

$$C(\mathbf{x}, t) = C_B(\mathbf{x}, t) \quad \text{on } \Gamma_D \quad (6)$$

$$\mathbf{D} \nabla C \cdot \mathbf{n} = f_B(\mathbf{x}, t) \quad \text{on inflow } \Gamma_N \quad (7)$$

Here, C_B is the concentration at the Dirichlet boundary and f_B is the mass flux normal to the Neumann boundary. Meanwhile, the initial concentration in the domain is given by

$$C(\mathbf{x}, 0) = C_0(\mathbf{x}) \quad \mathbf{x} \in \Omega \quad (8)$$

C_0 is the initial concentration in the domain at time $t = 0$.

Pressures and fluxes. The governing equations for the flow model are the mass conservation equation and Darcy's law. The mass conservation equation describes the balance principle of inflow and outflow of mass in a specified region whereas Darcy's law expresses the relationship between the velocity with the potential (pressure) gradient, the porous medium and the fluid properties. The mass conservation equation is written in mathematical form as the following

$$\frac{\partial(\phi \rho)}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = q \quad (9)$$

where ϕ is the porosity of the porous medium, $\mathbf{u}$ is the Darcy velocity (or flux) (m/s) and q is the sources/sinks (1/s). If we consider the incompressible flow case and ignoring any sources/sinks then we obtain

$$\nabla \cdot \mathbf{u} = 0 \quad (10)$$

Darcy's law is given by

$$\mathbf{u} = -\frac{\mathbf{K}}{\mu}(\nabla p - \rho \mathbf{g}) \quad (11)$$

Here, $\mathbf{K}$ is the rock permeability tensor (m^2), μ is the fluid viscosity (Pa.s), p is the fluid pressure (Pa), and $\mathbf{g}$ is the gravitational force (m/s^2). The permeability in this model is defined as a full tensor, which means its off-diagonal elements are no longer zero. For 2-D case, the form of permeability tensor is

$$\mathbf{K} = \begin{bmatrix} K_{xx} & K_{xy} \\ K_{yx} & K_{yy} \end{bmatrix} \quad (12)$$

The permeability tensor is assumed symmetric ($K_{xy} = K_{yx}$) and positive definite ($K_{xx}K_{yy} - K_{xy}^2 \geq 0$), implying that there are only three independent components exist. We can calculate all the components of the full tensor by

$$\mathbf{K} = \begin{bmatrix} K_1 \cos^2 \theta + K_2 \sin^2 \theta & (K_1 - K_2) \sin \theta \cos \theta \\ (K_1 - K_2) \sin \theta \cos \theta & K_1 \sin^2 \theta + K_2 \cos^2 \theta \end{bmatrix} \quad (13)$$

where θ is the degree of anisotropy as depicted in Figure 1, K_1 and K_2 are the permeability values along the principle direction of anisotropy.

Figure 1. The anisotropy orientation in porous medium.

Furthermore, in this model, the fluid density is defined as a function of concentration, implying that the density is changing with respect to the change of concentration in space and time. The density of the formation water increases about 0.1 to 1%, depending on its salinity, when CO_2 is dissolved [Pruess and Zhang, 2008; Pau et al., 2010]. There are many expressions available in the literatures to compute the change of the density [Ennis-King, 2005; Yang and Gu, 2006; Farajzadeh et al., 2007; Hassanzadeh et al., 2007; Allen and Sun, 2012; Ranganathan et al., 2012]. In this work, we refer to Allen and Sun [2012] for the density change formulation

$$\rho = \rho_0 + \Delta \rho \frac{C}{C_{\text{sat}}} \quad (14)$$

where ρ is the mixture density between the formation water and the dissolved CO_2 , ρ_0 is the pure density of the unsaturated formation water, $\Delta \rho$ is the density difference between the formation water and the CO_2 -saturated formation water. The mixture density could also be calculated from basic thermodynamics as discussed in Cheng et al. [2012].

Substituting Darcy's law (11) into the mass conservation equation (10), one obtains the pressure equation,

$$\nabla \cdot (-\mathbf{K} \nabla p) = 0 \quad (15)$$

From (15), we have the system of linear equation

$$\mathbf{A} \mathbf{p} = \mathbf{b} \quad (16)$$

with $\mathbf{A}$ is the matrix of coefficient, $\mathbf{p}$ is the unknown of pressures, and $\mathbf{b}$ contains information about the boundary conditions. As mentioned earlier, we constructed the matrix of coefficient using the experimenting pressure field approach. This technique was introduced by Sun et al. [2012] with the aim to simplifying the construction of the matrix of coefficient, which involves large expressions of algebraic equations after the pressure equation being discretized numerically. In this technique, the matrix of coefficient is constructed automatically within the solver routine. The experimenting pressure field technique is significantly useful when dealing with complex multipoint stencils such as multipoint flux approximation (MPFA) method. A

more comprehensive discussion on this technique as applied to multipoint flux approximation method can be found in Salama et al. [2014] and will not be repeated here. This technique provides a coding-friendly framework in which the local problems are solved using predefined pressure fields and through this the matrix of coefficients are obtained automatically. The simplicity of this technique is that local problems are usually easy to solve than to track each element of the global system.

Multipoint flux approximation and its numerical discretization

Multipoint flux approximation (MPFA) is a numerical method that has shown a number of desirable features including faster convergence rates. Furthermore, it can handle full permeability tensor, which is not possible using traditional two-point flux approximation. This method is an extension of the two-point flux approximation (TPFA) and has been derived based on finite volume method. Multipoint flux approximation (MPFA) has been introduced in the late nineties by Edwards and Rogers [1998], Aavatsmark et al. [1998], and Aavatsmark [2002]. There are several types of MPFA such as O, L, U, and Z-methods, which the details of them could be found in Aavatsmark et al. [1998] and Lee et al. [2002] for MPFA O-method, Aavatsmark et al. [2008] and Cao et al. [2009] for MPFA L-method, Aavatsmark and Eigestad [2006] for MPFA U-method, and Nordbotten and Eigestad for MPFA Z-method [2005]. In this work, we only implement the MPFA O-method. MPFA O-method (later simply called MPFA) has been widely implemented for simulating the fluid flow behavior in anisotropic porous media, either single-phase or multiphase flow [Keilegavlen et al., 2012; Wolff et al., 2012; Osman et al., 2012; Negara et al. 2013], as well as to the problem of conduction heat transfer in anisotropic porous media [Salama et al. 2013b]. MPFA method provides advantage in particular when the discretizations are not aligned with the principal directions of permeability in the model. The method, however, is limited only for the quadrilateral grids.

Figure 2. The cell stencil of (a) TPFA and (b) MPFA.

MPFA involves more point stencils than the TPFA as shown in Figure 2. Looking at Figure 2a, one flux requires 2-point stencil, i.e., cells 1 and 2. Meanwhile, in MPFA, one flux requires 6-point stencil, which is not only affected by the pressures in cells 1 and 2 but also the others, i.e., cells 3, 4, 5, and 6 (Figure 2b). In MPFA method, each flux is approximated by

$$u_i \approx \sum_{j \in \pi} T_{ij} \Phi_j \quad (17)$$

with T_{ij} , Φ_j , and π are the transmissibility coefficients, the pressure gradient, and the cells which influences the velocity, respectively. In 2-D problems, π comprises of 6 cells while in 3-D case it contains 18 cells. MPFA introduces so-called interaction volume, i.e., a region that is connecting the four surrounding cells with the midpoint of the edges of the cells (see Figure 3). These midpoints (p_x^+ , p_x^- , p_y^+ , p_y^-) are to ensure the continuity of the pressure gradient and fluxes. The interaction region is defined in each node in the domain such that the numbers of interaction regions are equal to the numbers of nodes in the domain. Thus, if we have $m \times n$ cells in the domain then there are $(m+1) \times (n+1)$ interaction regions.

Figure 3. An interaction region in MPFA method for 2-D problem.

Referring to Figure 3, we have

$$\begin{aligned} u_x^- &\approx -T_{11}^x(p_x^- - p_{11}) - T_{11}^x(p_y^- - p_{11}) \\ &\approx -T_{21}^x(p_{21} - p_x^-) - T_{21}^x(p_y^+ - p_{21}) \end{aligned} \quad (18)$$

$$\begin{aligned} u_x^+ &\approx -T_{12}^x(p_x^+ - p_{12}) - T_{12}^x(p_{12} - p_y^-) \\ &\approx -T_{22}^x(p_{22} - p_x^+) - T_{22}^x(p_{22} - p_y^+) \end{aligned} \quad (19)$$

$$\begin{aligned} u_y^- &\approx -T_{11}^y(p_y^- - p_{11}) - T_{11}^y(p_x^- - p_{11}) \\ &\approx -T_{21}^y(p_{12} - p_y^-) - T_{21}^y(p_x^+ - p_{12}) \end{aligned} \quad (20)$$

$$\begin{aligned} u_y^+ &\approx -T_{21}^y(p_y^+ - p_{21}) - T_{21}^y(p_{21} - p_x^-) \\ &\approx -T_{22}^y(p_{22} - p_y^+) - T_{22}^y(p_{22} - p_x^+) \end{aligned} \quad (21)$$

The transmissibility coefficients above contain information about the permeability, the grids, and the fluid viscosity. Expressions of (18)-(21) can be written more details as follows

u_x^- :

$$\begin{aligned} u_x^- &= -K_{11}^{xx} \frac{p_x^- - p_{11}}{\frac{1}{2} \Delta x_{11}} - K_{11}^{xy} \frac{p_y^- - p_{11}}{\frac{1}{2} \Delta y_{11}} + K_{11}^{xy} \rho g \\ u_x^- &= -K_{21}^{xx} \frac{p_{21} - p_x^-}{\frac{1}{2} \Delta x_{21}} - K_{21}^{xy} \frac{p_y^+ - p_{21}}{\frac{1}{2} \Delta y_{21}} + K_{21}^{xy} \rho g \end{aligned} \quad (22)$$

u_x^+ :

$$\begin{aligned} u_x^+ &= -K_{12}^{xx} \frac{p_x^+ - p_{12}}{\frac{1}{2} \Delta x_{12}} - K_{12}^{xy} \frac{p_{12} - p_y^-}{\frac{1}{2} \Delta y_{12}} + K_{12}^{xy} \rho g \\ u_x^+ &= -K_{22}^{xx} \frac{p_{22} - p_x^+}{\frac{1}{2} \Delta x_{22}} - K_{22}^{xy} \frac{p_{22} - p_y^+}{\frac{1}{2} \Delta y_{22}} + K_{22}^{xy} \rho g \end{aligned} \quad (23)$$

u_y^- :

$$\begin{aligned} u_y^- &= -K_{11}^{yy} \frac{p_y^- - p_{11}}{\frac{1}{2} \Delta y_{11}} - K_{11}^{yx} \frac{p_x^- - p_{11}}{\frac{1}{2} \Delta x_{11}} + K_{11}^{yy} \rho g \\ u_y^- &= -K_{12}^{yy} \frac{p_{12} - p_y^-}{\frac{1}{2} \Delta y_{12}} - K_{12}^{yx} \frac{p_x^+ - p_{12}}{\frac{1}{2} \Delta x_{12}} + K_{12}^{yy} \rho g \end{aligned} \quad (24)$$

u_y^+ :

$$\begin{aligned} u_y^+ &= -K_{21}^{yy} \frac{p_y^+ - p_{21}}{\frac{1}{2} \Delta y_{21}} - K_{21}^{yx} \frac{p_{21} - p_x^-}{\frac{1}{2} \Delta x_{21}} + K_{21}^{yy} \rho g \\ u_y^+ &= -K_{22}^{yy} \frac{p_{22} - p_y^+}{\frac{1}{2} \Delta y_{22}} - K_{22}^{yx} \frac{p_{22} - p_x^+}{\frac{1}{2} \Delta x_{22}} + K_{22}^{yy} \rho g \end{aligned} \quad (25)$$

The unknowns from the equations above are the cell-centered pressures, the interface pressures, and the fluxes. From (22) to (25) above we eliminate the interface pressures through mathematical manipulation so that the remaining unknowns are the cell-centered pressures and the fluxes. In each interaction region, we have system of equations which consist of four equations and written in the matrix form as the following

$$\mathbf{R} \mathbf{u} = \mathbf{C} \mathbf{p} + \mathbf{G} \quad (26)$$

where $\mathbf{R}$ is constructed based on the permeability, the grids, and the fluid viscosity. The matrix of $\mathbf{R}$ is expressed in the matrix form as:

$$\mathbf{R} = \frac{1}{2} \begin{bmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{bmatrix} \quad (27)$$

where

$$R_{11} = \begin{bmatrix} (R_{11}^{xx}\Delta x_1 + R_{21}^{xx}\Delta x_2) & 0 \\ 0 & (R_{12}^{xx}\Delta x_1 + R_{22}^{xx}\Delta x_2) \end{bmatrix} \quad (28)$$

$$R_{22} = \begin{bmatrix} (R_{11}^{yy}\Delta y_1 + R_{12}^{yy}\Delta y_2) & 0 \\ 0 & (R_{21}^{yy}\Delta y_1 + R_{22}^{yy}\Delta y_2) \end{bmatrix} \quad (29)$$

$$R_{21} = \begin{bmatrix} R_{11}^{yx}\Delta y_1 & R_{12}^{yx}\Delta y_2 \\ R_{21}^{yx}\Delta y_1 & R_{22}^{yx}\Delta y_2 \end{bmatrix} \quad (30)$$

$$R_{12} = \begin{bmatrix} R_{11}^{xy}\Delta x_1 & R_{21}^{xy}\Delta x_2 \\ R_{12}^{xy}\Delta x_1 & R_{22}^{xy}\Delta x_2 \end{bmatrix} \quad (31)$$

$\mathbf{C}$ is the matrix of coefficient,

$$\mathbf{C} = \begin{bmatrix} -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix} \quad (32)$$

$\mathbf{u}$ is the vector of unknowns velocities,

$$\mathbf{u} = [u_x^- \quad u_x^+ \quad u_y^- \quad u_y^+]^T \quad (33)$$

$\mathbf{p}$ is the vector of unknown pressures,

$$\mathbf{p} = [p_{11} \quad p_{21} \quad p_{12} \quad p_{22}]^T \quad (34)$$

$\mathbf{G}$ is the vector containing the gravity term and some other parameters,

$$\mathbf{G} = \frac{1}{2} \begin{bmatrix} 0 \\ 0 \\ -\Delta y_{11}\rho g - \Delta y_{12}\rho g \\ -\Delta y_{21}\rho g - \Delta y_{22}\rho g \end{bmatrix} \quad (35)$$

From (35), it is clear that the gravity term exists only in the y -component. Solving (26), we obtain the solution for the fluxes in each node. After obtaining the fluxes in each node, we are averaging the two neighboring fluxes in the same edge in order to get the flux at the midpoint of the edge. In other words, we return back to the framework of TPFA. This section is only demonstrating the derivation for 2-D problem but implementation in 3-D problem is straightforward. In 3-D case, the interaction region consists of 8 adjacent cells and the size of matrices $\mathbf{R}$, $\mathbf{u}$, $\mathbf{C}$, $\mathbf{p}$, and $\mathbf{G}$ are 12×12 , 12×1 , 12×8 , 8×1 , and 12×1 , respectively.

Results and Discussion

This section presents three numerical examples of density-driven flow in homogeneous, layered, and heterogeneous anisotropic porous media. For all numerical examples, we consider no-flow boundary conditions in the flow model. Meanwhile, in the transport model we impose saturated dissolved CO_2 on the top boundary of the domain and no-mass flux for the rest of the boundaries. The porous medium and fluid properties for the three numerical examples are summarized in Table 1 except the permeability tensor, which will be presented separately in each numerical example. The numerical simulations were carried out by our own simulator, which is written in MATLAB. In this work, we solve the transport equation implicitly and subsequently the formation water density is updated as a function of concentration. Then, we solve the pressure equation to obtain the Darcy velocity, which is used in the convection term of transport equation. Both the transport and flow models are time dependent and simulated with the given initial condition (concentration).

Table 1. Reservoir and fluid properties for all numerical examples.

Reservoir and Fluid properties	Example 1	Example 2	Example 3
Width (W)	1 m	1 m	1 m
Height (H)	1 m	1 m	1 m
Grids (m $\times$ n)	50 $\times$ 50	50 $\times$ 50	50 $\times$ 50
Porosity (ϕ)	0.1	0.18	0.14
Water density (ρ_w)	1000 kg/m ³	1000 kg/m ³	996.54 kg/m ³
Viscosity (μ)	0.595 cP	0.595 cP	0.595 cP
CO ₂ concentration at the top of boundary	1000 mol/m ³	900 mol/m ³	1100 mol/m ³
Density difference	10 kg/m ³	20 kg/m ³	11.4 kg/m ³
Effective diffusion coefficient	2×10^{-9} m ² /s	2×10^{-9} m ² /s	2×10^{-9} m ² /s

Case 1: Homogeneous anisotropic porous medium. For the first numerical example, we consider a porous medium with the anisotropy property exist in the whole domain. The anisotropy orientation is set to be $\theta = 60^\circ$ as illustrated in Figure 4. The size of the domain is $1 \text{ m} \times 1 \text{ m}$ and it is discretized into 50×50 meshes. In the flow model, we consider the following full tensor of permeability field

$$\mathbf{K} = \begin{bmatrix} 2.541 & 4.231 \\ 4.231 & 7.427 \end{bmatrix} \times 10^{-12} \text{ m}^2 \quad (36)$$

We impose constant saturated CO_2 equal to 1000 mol/m^3 on the top of the boundary and the domain is initially saturated with the formation water. We run the example for $6.912 \times 10^6 \text{ s}$ simulation time. Figures 5a-d demonstrate the snapshots of the concentration profiles of dissolved CO_2 at different times. From Figure 5a, we can see that at $t = 1.728 \times 10^6 \text{ s}$, the movement of CO_2 is mainly driven by the pure diffusion. After sometime later particularly at $t = 3.456 \times 10^6 \text{ s}$, more CO_2 dissolves in the formation water such that instabilities starts to emerge, particularly at the top right corner (Figure 5b). As more CO_2 dissolves over time, the convection dominates the migration of dissolved CO_2 and causing the density-driven flow (fingering) phenomena. The formation water density is increasing as the change of dissolved CO_2 concentration in the domain. The more CO_2 dissolves in the formation water, the more fingers will be appearing. From Figures 5c-d, we can see that the direction of the movement of dissolved CO_2 is strongly influenced by the principal direction of anisotropy.

Figure 4. Problem setup for homogeneous anisotropic porous medium.

Figure 5. Snapshots of dissolved CO₂ in homogenous anisotropic porous media at (a) 1.728×10^6 s, (b) 3.456×10^6 s, (c) 5.184×10^6 s, and (d) 6.912×10^6 s.

Case 2: Layered anisotropic porous medium. The second numerical example considers the porous medium that consists of three different layers (Figure 6). The first two top layers are anisotropic with different orientation and the bottom layer is isotropic. The first anisotropic layer (top layer) has anisotropy orientation of $\theta = 70^\circ$ whereas in the second anisotropic layer it is oriented as $\theta = -70^\circ$. We apply the same boundary conditions as in the previous example. The saturated CO₂, which is imposed on the top of the boundary, is given by 900 mol/m³. The first anisotropic layer has the full permeability tensor as follows

$$\mathbf{K} = \begin{bmatrix} 1.242 & 3.140 \\ 3.140 & 8.726 \end{bmatrix} \times 10^{-12} \text{ m}^2 \quad (37)$$

Meanwhile, the permeability field in the second anisotropic layer is

$$\mathbf{K} = \begin{bmatrix} 1.242 & -3.140 \\ -3.140 & 8.726 \end{bmatrix} \times 10^{-12} \text{ m}^2 \quad (38)$$

and the permeability field in the isotropic layer is a diagonal tensor with same values in its diagonal components (isotropic)

$$\mathbf{K} = \begin{bmatrix} 9.869 & 0 \\ 0 & 9.869 \end{bmatrix} \times 10^{-12} \text{ m}^2 \quad (39)$$

Figure 6. Problem setup for layered anisotropic porous medium.

Figure 7. Snapshots of dissolved CO₂ in layered anisotropic porous media after (a) 1.296×10^6 s, (b) 2.592×10^6 s, (c) 3.888×10^6 s, and (d) 5.184×10^6 s.

We run the example for 5.184×10^6 s simulation time. Similar with the previous example, in this second example we present the snapshots of dissolved CO₂ concentration profiles at different time scales. At $t = 1.296 \times 10^6$ s (Figure 7a), the fingers has not arises yet, which means only the molecular diffusion drives the transport of CO₂. The rate of transport of CO₂ depends on the effective diffusion coefficient, $\mathcal{D}$, in this example is given by 2×10^{-9} m²/s. We observe the convection starts at $t = 2.592 \times 10^6$ s that arises near to the top right of the domain, which indicates the CO₂ begins to dissolve into the formation water. Since then, we observe more fingers are formed mainly in the first top anisotropic layer as depicted by Figure 7c. In Figure 7d, we can see obviously the fingers in the two different anisotropic layers, according to the principal directions of anisotropy in each anisotropic layer.

Case 3: Heterogeneous anisotropic porous medium. In the last example, we present the heterogeneous anisotropic porous media where the permeability in the domain is randomly distributed as depicted in Figure 8b. The randomly permeability is generated by the MATLAB Reservoir Simulation Toolbox (MRST), an open-source MATLAB toolkit that contains a collections of routines and data structures that can be used for (new) discretization and solutions methods in reservoir simulation [Lie et al., 2012]. From this randomly permeability, we calculate the full tensor permeability using equation (13), given K_1 is a hundred times greater than K_2 and anisotropy orientation is $\theta = 75^\circ$. The concentration of CO₂-saturated fluid that is imposed on the top boundary is 1100 kg/m³. We run the case for 6.048×10^6 s simulation time. Figures 9a-d display the dissolved CO₂ concentration profiles. These figures demonstrate that the migration of dissolved CO₂ is still following the principal directions of anisotropy even though the permeability field is highly heterogeneous in the porous medium.

Figure 8. (a) Problem setup and (b) the permeability distribution in the heterogeneous porous medium.

Figure 9. Snapshots of dissolved CO_2 in layered anisotropic porous media after (a) $1.512 \times 10^6 \text{ s}$, (b) $3.024 \times 10^6 \text{ s}$, (c) $4.536 \times 10^6 \text{ s}$, and (d) $6.048 \times 10^6 \text{ s}$.

Onset of natural convection. In addition to the simulation of fluid flow behavior of dissolved CO₂ in anisotropic porous media, we are also investigating the onset of natural convection, i.e., the time at which the CO₂ starts to dissolve in the formation water (brine) and causing gravitational instability due to the increase of the density of formation water. The onset time of convection denotes the transition from pure diffusion to convection-dominated mechanism. There are numbers of literatures that have studied the linear stability analysis to predict the onset of convection [Ennis-King and Paterson, 2005; Hassanzadeh et al., 2007; Pruess and Zhang, 2008; Pau et al., 2010]. In this work, the calculation of the onset time of convection is referred to Pruess and Zhang [2008],

$$t_{onset} = C_0 \frac{\mu^2 \phi^2 D}{(\Delta\rho)^2 g^2 K^2} \quad (40)$$

where C_0 is the constant, μ is the fluid viscosity (cP), ϕ is the porosity of the porous medium, $\Delta\rho$ is the increase of density due to CO₂ dissolution (kg/m³), g is the gravitational acceleration (m/s²), and K is the permeability (m²). The values of C_0 are varying in literatures for example it is reported to be 75-78 [Ennis-King and Paterson, 2005; Ennis et al., 2005], 500 [Riaz et al., 2006], 96.23 [Xu et al., 2006], 1155.6 and 1411.5 [Pruess and Zhang, 2008], 1796 and 3670 [Pau et al., 2011]. The discrepancies for the values of C_0 can be caused by the different definition and criteria of onset time in each study [Pau et al., 2010]. The onset time of convection is mainly affected by the magnitudes of the permeability, porosity, effective diffusivity, and the grids (resolution). The resolution plays significant role in fluctuating the onset time of convection as discussed by Pau et al. [2010]. In all the presented numerical examples above, we use very fine mesh with the resolution of $\Delta x = \Delta y = 2$ cm. We can predict the onset time from the simulated results by plotting the maximum absolute velocity against simulation time as depicted by Figures 10-12. We also study the sensitivity analysis of the onset time with respect to the change of $\Delta\rho$. From these three figures, we can see the trend, i.e., initially there is no fluid velocity and after some time the velocity becomes nonzero. The zero fluid velocity implies that the on-going physical process is pure diffusion. When the fluid velocity becomes nonzero, it indicates the convection process begins. Therefore, we may predict the onset time of convection as a point where the transition from zero velocity to nonzero velocity for example in Figure 10, we can see that the onset time for the case of for $\Delta\rho = 10$ kg/m³ is about 3.35×10^6 s. Observing the pattern of the graphs in Figures 10-12, we may conclude that the smaller the value of $\Delta\rho$, the shorter the onset time of convection (with the same grid resolution).

CO₂ dissolution rate and total dissolved mass. In this work, we are also interested to calculate the CO₂ flux (dissolution rate) and total dissolved mass. The CO₂ flux is the rate of CO₂ which is passing the dissolution boundary, per unit cross-sectional area [Pruess and Zhang, 2008],

$$J(y = 0, t) = \phi C_0 \sqrt{\frac{D}{\pi t}} \quad (41)$$

Substituting (40) into (41), we have the CO₂ flux at the onset time of convection,

$$J(y = 0, t_{onset}) = \frac{C_0 \Delta\rho g k}{\mu \sqrt{\pi C_0}} \quad (42)$$

Integrating (41) over time, one obtains the total dissolved CO₂,

$$M = 2\phi C_0 \sqrt{\frac{Dt}{\pi}} \quad (43)$$

Figures 13-15 show the results of the CO₂ flux at the top of the boundary and total mass dissolved of CO₂ over time in the domain for homogeneous, layered, and heterogeneous cases, respectively. From these figures, we can see that initially the simulated results fit very well with the analytically computed diffusive flux and mass. At first, the diffusion process governs the CO₂ from the top boundary to the layer slightly below it. In this process, CO₂ dissolves into the brine with its propagation rate depends on the molecular diffusion and the density of brine set to increase such that causing instability (fingering). At this state, the convection dominates the transport of dissolved CO₂, which makes the simulated results start to deviate from the analytical one. The point where the simulated results start to deviate implies the onset of convection. We do the sensitivity analysis to investigate the impact of $\Delta\rho$ with respect to the CO₂ flux and total dissolved mass. For all the considered examples, the trend is the same, i.e., the CO₂ flux and total dissolved mass have linear relationship with the increase of $\Delta\rho$.

Figure 10. Maximum absolute velocity for x - and y -directions against time: case 1.

Figure 11. Maximum absolute velocity for x - and y -directions against time: case 2.

Figure 12. Maximum absolute velocity for x - and y -directions against time: case 3.

Figure 13. Simulated CO₂ (a) flux at the top boundary and (b) dissolved mass for different $\Delta\rho$: case 1.

Figure 14. Simulated CO₂ (a) flux at the top boundary and (b) dissolved mass for different $\Delta\rho$: case 2.

Figure 15. Simulated CO₂ (a) flux at the top boundary and (b) dissolved mass for different $\Delta\rho$: case 3.

Summary and conclusions

We have modeled and simulated the solubility trapping mechanism of carbon sequestration by investigating the transport of dissolved CO_2 in anisotropic porous media, which includes the dissolution-diffusion-convection process. In this process, certain amount of CO_2 is dissolved into the formation water such that the density of the formation water increases and eventually causes the gravitational instability (fingering). The increase of the density of formation water is about 1%, depending on its salinity. The CO_2 -rich formation water will migrate downward and the CO_2 -poor water formation moves upwards. Such phenomena can be described mathematically in particular through the transport and phase flow models. In this work, we solve both models implicitly with the density of formation water is updated as a function of concentration. In most of the literatures, anisotropy permeability is defined as a diagonal tensor with different values in the diagonal components. In this work we consider the full permeability tensor, implying that the off-diagonal elements are no longer vanished. We have applied the multipoint flux approximation (MPFA) to handle the full tensor of permeability field. We have presented three numerical examples, including the homogeneous, layered, and heterogeneous anisotropic porous media. Numerical results demonstrate that the migration of dissolved CO_2 is mainly driven by the principal direction of anisotropy. We have studied the sensitivity analysis of the change of density difference (between the brine and the CO_2 -saturated brine) with respect to the onset time of convection, the CO_2 flux and total dissolved mass. The results show the same trend, i.e., the onset of convection, the CO_2 flux and total dissolved mass have linear relationship with the increase of $\Delta\rho$.

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