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Modeling and Simulation of Nanoparticle Transport in Multiphase Flows in Porous Media: CO₂ Sequestration

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Abstract

Geological storage of anthropogenic CO₂ emissions in deep saline aquifers has recently received tremendous attention in the scientific literature. Injected CO₂ plume buoyantly accumulates at the top part of the deep aquifer under a sealing cap rock, and some concern that the high-pressure CO₂ could breach the seal rock. However, CO₂ will diffuse into the brine underneath and generate a slightly denser fluid that may induce instability and convective mixing. Onset times of instability and convective mixing performance depend on the physical properties of the rock and fluids, such as permeability and density contrast. The novel idea is to add nanoparticles to the injected CO₂ to increase density contrast between the CO₂-rich brine and the underlying resident brine and, consequently, decrease onset time of instability and increase convective mixing.

As far as it goes, only few works address the issues related to mathematical and numerical modeling aspects of the nanoparticles transport phenomena in CO₂ storages. In the current work, we will present mathematical models to describe the nanoparticles transport carried by injected CO₂ in porous media. Buoyancy and capillary forces as well as Brownian diffusion are important to be considered in the model. Implicit Pressure Explicit Saturation-Concentration (IMPES) scheme is used and a numerical simulator is developed to simulate the nanoparticles transport in CO₂ storages.

Introduction

In the recent years, the applications of nanometer particles (nanoparticles) have been reported in many disciplines. These nanoparticles can modify the rheology, mobility, wettability, and other properties of the fluids and therefore need comprehensive investigations. Using the nanoparticles in oil and gas exploration and production is also a promising field of research. For example, certain types of nanoparticles can be used as tracers for oil and gas exploration. These nanoparticles are designed such that they do not stick to the rock surface or hydrocarbon phases and move faster than the traditional chemical tracers. Moreover, nanoparticles can be used in the oilfields to enhance water injection by virtue of changing the wettability of reservoir rock through their adsorption on porous walls.

The nanometer unit and nanoparticles are often associated with the field of nanotechnology. The nanometer (nm) unit is equal to one billionth of a meter ($\text{nm}=10^{-9} \text{ m}$). On the other hand, particles are classified based on size in terms of diameter. Coarse particles are sized between 10,000 and 2,500 nm. Fine particles have the range between 2,500 and 100 nm. Nanoparticles (ultrafine particles) cover a range between 100 and 1 nm. Nanoclusters have at least one dimension between 10 and 1 nm and a narrow size distribution. Nanopowders are agglomerates of ultrafine particles, nanoparticles, or nanoclusters. One kind of polysilicon nanopowder has the range between 500 and 10 nm and was used in oilfields to enhance water injection by changing wettability of porous media.

In a porous media, the void spaces can be divided into pore throats (the narrowest segments of pores) and pore chambers (the widest segments of pores). For example, the sizes of pore throats in sandstone are in the range of 0.5 - 5.0 μm , and the size of pore chambers are in the range of 5.0 - 50.0 μm [12,13]. The experimental data [Ju] illustrated that the sizes of polysilicon particles are in the range of 10 - 500 nm, while pore radii of a porous medium (sandstone) are from 6 to $6.3 \times 10^4 \text{ nm}$. Therefore, if a particle larger than a pore throat may block at the pore throat during nanoparticles transport with flow in the porous medium. A few numbers of nanoparticles types have sizes slightly less than a pore throat may bridge at the pore throat. However, the nanoparticles can be adhered to the pore walls if the nanoparticles sizes are much less than the pore sizes. The adsorption of polysilicon on pore walls leads to wettability change of pore walls. Ju and Fan [1] have conducted experiments to study the effects of polysilicon nanoparticles on the physical properties of the porous media.

A few work papers address the issues related to mathematical and numerical modeling aspects of the nanoparticles transport

phenomena in oilfields. Ju et al. [2] reported that when the suspension of the polysilicon nanoparticles (PN) of one nanosize is injected into an oil reservoir, it could change the wettability of porous surfaces of sandstone and consequently have effects on water and oil flows. Recently, Ju and Dai [1] have used two types of PN in oil fields to improve oil recovery and enhance water injection. They introduced experimental investigations to study both physical properties of the nanoparticles, and pore characteristics of sandstone. Also, they have presented a 1D mathematical model to describe the nanoparticles transport carried by two-phase flow in a porous medium. Ju et al. [2] and Ju and Dai [1] have founded their mathematical model of nanoparticles transport in two-phase flow in porous media based on the formulation of fine particles transport in two-phase flow in porous media provided in Refs. [3-5]. Sbair and Azaroual [6] developed a mathematical model couples the incompressible two-phase fluid flow reservoir equations at the macroscopic level to equations of nanoparticles transport at a smaller, but still macroscopic, secondary scale. Improvements in the recovered volumes by injecting hydrophobic nanoparticles which enhance or reverse the initial reservoir wettability favoring an increase in the relative permeability of the oil phase and the capillary pressure drop between phase pressures [7]. In Ref. [8], we developed a model to represent nanoparticles transport and two-phase flow in porous media including capillarity and Brownian diffusion. A numerical example has been provided of countercurrent imbibition and variation of water saturation, nanoparticles concentration and porosity ratio are studied. In the current work, we extend the introduced modeling and simulation of nanoparticles transport carried by injected CO_2 in porous media. IMplicit Pressure EXplicit Saturation-Concentration (IMPESC) scheme has been used to simulate the problem under consideration.

Mathematical Modeling

In this section, a mathematical model is developed to describe the nanoparticles transport carried by two-phase flow in porous media. Let us consider two-phase immiscible incompressible flow in a heterogeneous porous medium domain governed by the Darcy's law and the equations of mass conservation for each phase as,

Fig. 1:

$$\frac{\partial(\phi \rho_\alpha S_\alpha)}{\partial t} = -\nabla \cdot (\rho_\alpha u_\alpha), \quad \alpha = w, g \quad (1)$$

$$u_\alpha = -\frac{K k_{r\alpha}}{\mu_\alpha} (\nabla p_\alpha - \rho_\alpha g \nabla z), \quad \alpha = w, g \quad (2)$$

where S_α is the saturation, u_α [m/s] is the velocity of phase α . w stands for the wetting phase, and nw stands for the nonwetting phase. ϕ is the porosity of the medium, and $\nabla = (\partial/\partial x, \partial/\partial z)$ is the gradient operator. K [m^2] is the absolute permeability, $k_{r\alpha}$ [dimensionless] is the relative permeability, ρ_α [kg m^{-3}] is the density, and p_α [Pa] is the pressure of the phase α , $g = (0, -g)^T$ is the gravitational acceleration. μ_α is the viscosity and k_α is the effective permeability. The fluid saturations for the two-phase flow of wetting (w) and non-wetting gas (g) are interrelated by,

$$S_w + S_g = 1 \quad (3)$$

The relative permeabilities is considered as a function of the non-wetting saturation as,

$$k_{r\alpha} = k_{r\alpha}(S_g), \quad \alpha = w, g \quad (4)$$

The common formulas for relative permeabilities are of Corey, Naar-Henderson, and van Genuchten (c.f. [9-11]). The most suitable formula for the water-gas system is given by Brook-Corey [12, 13], as follows,

$$k_{rw}(S) = (1 - S_{eg})^{(2+3a)/a}, \quad (5)$$

$$k_{rg}(S) = S_{eg}^2 [1 - (1 - S_{eg})^{(2+a)/a}] \quad (6)$$

Here a is the pore size distribution index, and its value range varies from a small value for heterogeneous material ($a = 0.2$) to ($a = 3.0$) for homogeneous material [9]. S_{eg} is the normalized non-wetting phase saturation defined by,

$$S_{eg} = \frac{S_g - S_{rg}}{1 - S_{rg} - S_{rw}} \quad (7)$$

where S_{rg} is the residual saturation of the non-wetting phase, while S_{rw} is the residual saturation of the wetting phase. The capillary pressure formula that we use in this study refers to Theodoropoulou [11] in terms of the nonwetting phase (CO_2) saturation as:

$$p_c(S_{eg}) = p_g - p_w = p_c^0 (1 - S_{eg} + b_c)^{-m_c} \quad (8)$$

where p_c^0 is the entry capillary pressure, b_c and m_c are constants their values are 10^{-4} and 3 respectively. Since the compressibility of the injected, supercritical CO_2 may be small, it may be possible to consider it as incompressible fluid.

Now, let's define the total velocity as,

$$u_t = u_g + u_w, \quad (9)$$

and by summing the saturation equation for non-wetting phase to the other of the wetting phase, one obtains,

$$\nabla \cdot u_t = 0 \quad (10)$$

Adding the constitutive equations for each phase in Eq. (2) then substitute into Eq. (8), we end up,

$$u_t = -K(\lambda_g + \lambda_w) \nabla p_g + K(\lambda_g \rho_g + \lambda_w \rho_w) g \nabla z + \lambda_w K \nabla p_c \quad (11)$$

Now, let's introduce the fractional flow as, $f_\alpha = \lambda_\alpha / \lambda_t$, and the mobility, $\lambda_\alpha = k_{r\alpha} / \mu_\alpha$. In order to derive the pressure equation, substitute Eq. (11) into Eq. (10), we obtain,

$$\nabla \cdot (-\lambda_t K \nabla p_g + (\lambda_g \rho_g + \lambda_w \rho_w) K g \nabla z + \lambda_w K \nabla p_c) = 0 \quad (12)$$

or,

$$\nabla \cdot (K \lambda_t [-\nabla p_g + (f_g \rho_g + f_w \rho_w) g \nabla z] + f_w K \nabla p_c) = 0 \quad (13)$$

where $\lambda_t = \lambda_g + \lambda_w$. However, in this study, we assume that this volume strain time rate is negligibly small. Therefore, the last term of Eq. (13) vanishes. Substituting the constitutive equation for non-wetting phase in Eq. (2) into Eq. (1) gives,

$$\phi \frac{\partial S_g}{\partial t} + \nabla \cdot u_g = 0 \quad (14)$$

where the non-wetting (gas) velocity is given by:

$$u_g = f_g u_t - f_g \lambda_w (\rho_w - \rho_g) K g \nabla z - f_g \lambda_w K \nabla p_c \quad (15)$$

The boundary $\partial\Omega$ is subjected to both Dirichlet and Neumann conditions such that $\partial\Omega = \Gamma_D \cup \Gamma_N$ where Γ_D is the Dirichlet boundary and Γ_N is the Neumann boundary. Here, the Neumann boundary condition is used only to describe the normal

velocity on the inlet as well as the no flow boundaries, otherwise the boundaries are Dirichlet. The boundary conditions considered in this study are summarized as follows,

$$p_n = p^D \text{ on } \Gamma_D \quad (16)$$

$$\mathbf{u}_t \cdot \mathbf{n} = \mathbf{u}^N \text{ at injection} \quad (17)$$

$$\mathbf{u}_t \cdot \mathbf{n} = 0 \text{ on base and top boundaries}$$

$$S_n = \begin{cases} 1, & \text{on } \Gamma_N \\ 0, & \text{on } \Gamma_D \end{cases} \quad (18)$$

Ju and Fan [1] reported that there are two types of polysilicon nanoparticles (PN) can be used in oil fields to improve oil recovery and enhance water injection, respectively. The polysilicon nanoparticles are classified based on wettability of the surface of the PN. The first type is called lipophobic and hydrophilic polysilicon nanoparticles (LHPN) and exists in water phase only, while the second type is called hydrophobic and lipophilic polysilicon nanoparticles (HLPN) and exists in the oil phase only. The sizes of PN are in the range of 10 to 500 nm, therefore, Brownian diffusion is considered. Assuming that we have a number m of size interval of the nanoparticles in water phase, the transport equation for each size interval i of the nanoparticles in the water/oil phase can be written as,

$$\frac{\partial(\phi S_\alpha C_{i,\alpha})}{\partial t} + \mathbf{u}_\alpha \cdot \nabla C_{i,\alpha} = \nabla \cdot (\phi S_\alpha D_{i,\alpha} \nabla C_{i,\alpha}) + R_{i,\alpha} + Q_{i,\alpha} \quad (19)$$

where $i=1,2,\dots,m$. $C_{i,\alpha}$ is the volume concentrations of nanoparticles in size interval i in the phase α . $D_{i,\alpha}$ is the dispersion coefficients of nanoparticles in size interval i in the phase α . $Q_{i,\alpha}$ is the rate of change of particle volume belonging to a source/sink term. $R_{i,\alpha}$ is the net rate of loss of nanoparticles in size interval i in the phase α . The net rate of loss of nanoparticles may be written as [1-5],

$$R_{i,\alpha} = \frac{\partial(\delta\phi)_{i,\alpha}}{\partial t}, \quad (20)$$

where $(\delta\phi)_{i,\alpha} = v_{i,\alpha} + v_{i,\alpha}^*$ is the porosity change due to release or retention of nanoparticles of interval i in the phase α . $v_{i,\alpha}$ is the volume of the nanoparticles of interval size i in contact with the phase α available on the pore surfaces per unit bulk volume of the porous medium. $v_{i,\alpha}^*$ is the volume of the nanoparticles of interval size i entrapped in pore throats from the phase α per unit bulk volume of porous medium due to plugging and bridging. Also, $v_{i,\alpha}$ and $v_{i,\alpha}^*$ may be defined in terms of the mass of particles per unit fluid volume deposited at the pore bodies $\sigma_{i,\alpha}$ and pore throats $\sigma_{i,\alpha}^*$ of the porous medium, as,

$$v_{i,\alpha} = \sigma_{i,\alpha} / \rho_b, \quad v_{i,\alpha}^* = \sigma_{i,\alpha}^* / \rho_b$$

where ρ_b is the density of particulate suspensions.

At the critical velocity of the surface deposition only particle retention occurs while above it retention and entrainment of the nanoparticles take place simultaneously (Gruesbeck and Collins [14]). A modified Gruesbeck and Collins's model for the surface deposition is expressed by [1],

$$\frac{\partial v_{i,\alpha}}{\partial t} = \begin{cases} \gamma_{d,i,\alpha} \|\mathbf{u}_\alpha\| C_{i,\alpha} & \text{when } \mathbf{u}_\alpha \leq \mathbf{u}_{\alpha c} \\ \gamma_{d,i,\alpha} \|\mathbf{u}_\alpha\| C_{i,\alpha} - \gamma_{e,i,\alpha} v_{i,\alpha} \|\mathbf{u}_\alpha - \mathbf{u}_{\alpha c}\| & \text{when } \mathbf{u}_\alpha > \mathbf{u}_{\alpha c} \end{cases}, \quad (21)$$

where $\gamma_{d,i,\alpha}$ is the rate coefficients for surface retention of the nanoparticles in interval i in the phase α . $\gamma_{e,i,\alpha}$ is the rate coefficients for entrainment of the nanoparticles in interval i in the phase α . $\mathbf{u}_{\alpha c}$ is the critical velocity for the phase α .

Similarly, the rate of entrapment of the nanoparticles in interval i in the phase α is,

$$\frac{\partial v_{i,\alpha}^*}{\partial t} = \gamma_{pt,i,\alpha} \|\mathbf{u}_\alpha\| C_{i,\alpha}, \quad (22)$$

where $\gamma_{pt,i,\alpha}$ is the pore throat blocking constants.

Porosity may be changed because nanoparticles deposition on the pore surfaces or blocking of pore throats. The porosity variation may be by [1, 3],

$$\varphi = \varphi_0 - \sum_{i,\alpha} (\delta\varphi)_{i,\alpha} \quad (23)$$

where φ_0 is the initial porosity. Also, the permeability variation due to nanoparticles deposition on the pore surfaces or blocking of pore throats may be expressed as [2],

$$K = K_0 \left[(1-f) k_f + f\varphi / \varphi_0 \right]^l \quad (24)$$

where K_0 is the initial permeability, k_f is a constant for fluid seepage allowed by the plugged pores. The flow efficiency factor expressing the fraction of unplugged pores available for flow is given by,

$$f = 1 - \sum_i \gamma_{f,i} \left(\sum_\alpha v_{i,\alpha}^* \right) \quad (25)$$

$\gamma_{f,i}$ is the coefficient of flow efficiency for particles i . The value of the exponent l has range from 2.5 to 3.5. For the nanoparticles transport carried by fluid stream in the porous media, deposition on pore surfaces and blockage in pore throats may occur. The retained particles on pore surfaces may desorb for hydrodynamic forces, and then possibly adsorb on other sites of the pore bodies or get entrapped at other pore throats.

The relative permeability may be changed due to nanoparticles retention in a porous media. In order to define the variation of relative permeabilities caused by the nanoparticles let us firstly define the following quantities. A specific area of a sand core can be calculated by the following empirical equation [15],

$$a_{sp} = 7000\varphi \sqrt{\frac{\varphi}{K}} \quad (26)$$

On the other hand, it is important to define the total surface area in contact with fluids for all the size intervals of the nanoparticles per unit bulk volume as follows [1, 2],

$$a_{tot} = 6\beta \sum_{i,\alpha} (\delta\varphi)_{i,\alpha} / d_i \quad (27)$$

d_i is the diameter of particle interval size i . When $a_{tot} \geq a_{sp}$ the total surfaces per unit bulk volume of the porous medium are completely covered by the nanoparticles adsorbed on the pore surfaces or entrapped in pore throats, while if $a_{tot} < a_{sp}$ the surfaces per unit bulk volume of the porous medium are partially covered by the nanoparticles. Therefore, the relative permeabilities of the water and gas phases can be expressed as a linear function of the surface covered by the nanoparticles, i.e. $0 < a_{tot} < a_{sp}$, thus,

$$k_{r\alpha,p} = k_{r\alpha} + \frac{a_{tot}}{a_{sp}} (k_{r\alpha,c} - k_{r\alpha}) \quad (28)$$

where $k_{r\alpha,c}$ is the relative permeabilities of water/gas phase when the surfaces per unit bulk volume of the porous media is

completely occupied by the nanoparticles. Ju and Fan [1] reported that the effective permeability $k_{ew} = Kk_{rw,c}$ of water after nanoparticles treating is improved 1.627 - 2.136 times the effective permeability before nanoparticles treating. However, the absolute permeability decreases about 10%. So, one may write $k_{rw,c} = \theta_w k_{rw}$, such that θ_w is a constant of relative permeability change due to nanoparticles suspension in the water phase. Therefore, one may write Eq. (28) as follows,

$$k_{rw,p} = [1 + r_a(\theta_w - 1)]k_{rw} \quad (29)$$

where $r_a = a_{tot} / a_{sp}$. Similarly, for gas phase, one may write,

$$k_{rg,p} = [1 + r_a(\theta_g - 1)]k_{rg} \quad (30)$$

where θ_g is a constant of relative permeability change due to nanoparticles suspension in the gas phase.

Numerical Scheme

The cell-centered finite difference is a finite volume type of method that is very useful in solving petroleum reservoir simulation problems. There are two types of grid systems commonly employed in reservoir simulation: cell-centered and point-distributed. The problem under consideration is discretized numerically using cell-centered finite difference (CCFD) method with the IMplicit Pressure Explicit Saturation-Concentration (IMPESc) scheme. The scheme of cell-centered finite difference is depicted in Fig. 2. As the figure indicates, the pressure is calculated at the center of the cells, while the the mobility is calculated at the edges.

The computational rectangular domains Ω , were considered in this study. The domain of (20, 30) m is discretized into non-uniform mesh. The graded meshes around the inlet source of injection are finer than the rest of the domain. In other words, the interval size of axis either x or z increases gradually. Let specify Δx_1 is the width of the first mesh and Δx_M is the width of the last mesh, then we can define the ratio, $r_x = \Delta x_M / \Delta x_1$, which is related to the expansion coefficient of the element size γ by, $r_x = \gamma_x^{M-1}$, therefore, $\Delta x_m = \gamma_x^{m-1} \Delta x_1$, $m = 1, 2, \dots, M$, and $L = (1 - \gamma_x^M) \Delta x_1 / (1 - \gamma_x)$. Similarly, we can generate the mesh on the z axis. If Δz_1 is the width of the first mesh and Δz_N is the width of the last mesh, the ratio, $r_z = \Delta z_N / \Delta z_1$, which is related to the expansion coefficient of the element size γ_z by, $r_z = \gamma_z^{N-1}$, therefore, $\Delta z_m = \gamma_z^{m-1} \Delta z_1$, $m = 1, 2, \dots, N$, and $L = (1 - \gamma_z^N) \Delta z_1 / (1 - \gamma_z)$.

Fig. 2: Cell-centered finite difference scheme diagram.

The pressure distribution for each cell along the entire domain is given by the following implicit difference equation which is corresponding to the pressure equation,

$$\nabla \cdot K[-\lambda_t(S_g^n) \nabla p_g^{n+1} + (f_g(S_g^n) \rho_n + f_w(S_g^n) \rho_w) g \nabla z + f_w(S_g^n) \nabla p_c(S_g^n)] = 0 \quad (31)$$

The pressure at the current step $n + 1$ is evaluated based on the above equation with considering λ_t , f_{nw} , f_w and p_c as

functions of the non-wetting phase saturation S_{nw}^n at the previous time step n , $\lambda_t(S_g^n)$, $f_g(S_g^n)$, $f_w(S_g^n)$ and $p_c(S_{eg}^n)$. If the permeability field is defined as a given continuous function of space, its value at the location of the mid-edge points of each cell may be determined directly. In this work, however, we consider the permeability as a piecewise constant function over each cell. In this case, the permeability at cell edges is the weighted harmonic mean of the permeability of the neighboring cells. Therefore, we have,

$$K = \begin{cases} K_{xx}(i, j) = \frac{\frac{\Delta x(i) + \Delta x(i-1)}{K_{xx}(i, j)} + \frac{\Delta x(i-1)}{K_{xx}(i-1, j)}}{\frac{\Delta x(i) + \Delta x(i-1)}{K_{xx}(i, j)} + \frac{\Delta x(i-1)}{K_{xx}(i-1, j)}} \\ K_{zz}(i, j) = \frac{\frac{\Delta z(j) + \Delta z(j-1)}{K_{zz}(i, j)} + \frac{\Delta z(j-1)}{K_{zz}(i, j-1)}}{\frac{\Delta z(j) + \Delta z(j-1)}{K_{zz}(i, j)} + \frac{\Delta z(j-1)}{K_{zz}(i, j-1)}} \end{cases}$$

The left hand side permeability corresponds to that at the face-centers while those at the left hand side are those at cell centers.

Using the obtained pressure, the total velocity u_t^{n+1} which has been evaluated explicitly on edges of the cell, is given by the following equation,

$$u_t^{n+1} = K \left[-(\lambda_g(S_g^n) + \lambda_w(S_g^n)) p_g^{n+1} + (\lambda_g(S_g^n) \rho_g + \lambda_w(S_g^n) \rho_w) g \nabla z + \lambda_w(S_g^n) \nabla p_c(S_g^n) \right] \quad (32)$$

Therefore, the non-wetting phase saturation can be obtained explicitly as follows,

$$\phi \frac{S_g^{n+1} - S_g^n}{\Delta t^n} + \nabla \cdot (f_g(S_g^n) u_t^{n+1}) = \nabla \cdot \{ K f_g(S_g^n) \lambda_w(S_g^n) [\Delta \rho g \nabla z + \nabla p_c(S_g^n)] \} \quad (33)$$

where $\Delta \rho = \rho_w - \rho_g$, and $\Delta t^n = t^{n+1} - t^n$, is the time step length. The second term of the left hand side of Eq. (33) may be spatially discretized using the upwind scheme such that,

$$\nabla \cdot (f_g(S_g^n) u_t^{n+1}) = \frac{u_{t,x}^n(i+1, j+\frac{1}{2}) f_g(S_g^{n*}(i+1, j+\frac{1}{2})) - u_{t,x}^n(i, j+\frac{1}{2}) f_g(S_g^{n*}(i, j+\frac{1}{2}))}{x_{i+1} - x_i} + \frac{u_{t,z}^n(i+\frac{1}{2}, j+1) f_g(S_g^{n*}(i+\frac{1}{2}, j+1)) - u_{t,z}^n(i+\frac{1}{2}, j) f_g(S_g^{n*}(i+\frac{1}{2}, j))}{z_{j+1} - z_j} \quad (34)$$

where

$$S_g^{n*}(i, j+\frac{1}{2}) = \begin{cases} S_g^n(i-\frac{1}{2}, j+\frac{1}{2}) & \text{if } u_{t,x}^n(i, j+\frac{1}{2}) > 0 \text{ and } i \geq 1 \\ S_g^n(i+\frac{1}{2}, j+\frac{1}{2}) & \text{if } u_{t,x}^n(i, j+\frac{1}{2}) < 0 \text{ and } i \leq M-1 \\ S_g^n(1, j+\frac{1}{2}) & \text{if } u_{t,x}^n(1, j+\frac{1}{2}) > 0 \text{ and } i = 1 \\ S_g^n(N, j+\frac{1}{2}) & \text{if } u_{t,x}^n(N, j+\frac{1}{2}) < 0 \text{ and } i = M \end{cases} \quad (35a)$$

and

$$S_g^{n*}(i+\frac{1}{2}, j) = \begin{cases} S_g^n(i+\frac{1}{2}, j-\frac{1}{2}) & \text{if } u_{t,z}^n(i+\frac{1}{2}, j) > 0 \text{ and } j \geq 1 \\ S_g^n(i+\frac{1}{2}, j+\frac{1}{2}) & \text{if } u_{t,z}^n(i+\frac{1}{2}, j) < 0 \text{ and } j \leq N-1 \\ S_g^n(i+\frac{1}{2}, 1) & \text{if } u_{t,z}^n(i+\frac{1}{2}, 1) > 0 \text{ and } j = 1 \\ S_g^n(i+\frac{1}{2}, N) & \text{if } u_{t,z}^n(i+\frac{1}{2}, N) < 0 \text{ and } j = N \end{cases} \quad (35b)$$

Similar with the saturation equation, after applying the CCFD method to the transport equation, it is obtained,

$$\frac{\phi S_\alpha^{n+1}}{t^{n+1} - t^n} (C_{i,\alpha}^{n+1} - C_{i,\alpha}^n) + \nabla \cdot (u_\alpha^{n+1} C_{i,\alpha}^n - \phi S_\alpha^{n+1} \mathbf{D}_{i,\alpha} \nabla C_{i,\alpha}^n) = R_{i,\alpha}(C_{i,\alpha}^n) + Q_{i,\alpha}^n \quad (36)$$

Also, the upwind scheme is applied again in the advection term of the above equation. Moreover, the ordinary differential equations (21)-(22) are solved explicitly.

There are eight different locations of the boundary conditions employed as shown by Fig. 2. There are also eight types of discretization equations for the pressure, velocity, saturation, concentration, and ODEs in areas 1 to 8. The discretization of cells located outside of the domain has special treatment depending on the boundary condition type. We may consider it on the boundary of the domain or consider the closest cell to the boundary. For instance, in the discretization of area 1 (inlet) above, the term in the first derivative of the gas phase pressure along x-direction is substituted by the Neumann boundary that is defined as the velocity. Another slightly different treatment of the boundary condition is in the term of the first derivative of the capillary pressure, either in the pressure or the saturation equations. Since the capillary pressure is considered in the center of the cell, there is no capillary pressure defined in the edge of the cell, particularly in the boundary. In this case, we consider that the capillary pressure in the boundary taken is the same as the one that is located in the closest cell to the boundary. Therefore, the second terms of the capillary pressure, both in x and z-directions, are vanished.

Fig. 2: Eight types of the boundary condition treatments of the domain.

Results

The parameters used in the current calculations are selected from Ref. [29] as, porosity $\varphi = 20\%$; $\mu_g = 5.916 \times 10^{-5} \text{ kg m}^{-1}\text{s}^{-1}$; $\mu_w = 6.922 \times 10^{-4} \text{ kg m}^{-1}\text{s}^{-1}$; $\rho_g = 716.7 \text{ kg m}^{-3}$; $\rho_w = 997.4 \text{ kg m}^{-3}$; $S_{rg} = 0.001$; $S_{rw} = 0.2$; $S_0 = 0.001$; $P_c^0 = 10000 \text{ Pa}$; $\lambda = 2$ and $mc = 2$. The injection rate at the inlet is 0.1 PV/year. The pressure at the right boundary is 2 atm. Fig. 3 shows the saturation contours of the non-wetting phase after one year of injection. Furthermore, Figs. 4 and 5 show, respectively, the x- and z-displacement contours after one year of injection.

In this work, we only consider one size nanoparticles of concentration $C_{in} \text{ cm}^3\text{cm}^{-3}$ dissolved in the water phase at the inlet, with the following parameter as given in Ref. [2], $\gamma_{dg} = 0.16 \text{ cm}^{-1}$, $\gamma_{dg} = 0.3 \text{ cm}^{-1}$, $\gamma_{ptg} = 0.0128 \text{ cm}^{-1}$, $D = 0.00056 \text{ cm}^2\text{s}^{-1}$ and the critical velocity $u_{gc} = 0.00046 \text{ cm s}^{-1}$. The nanoparticles diameter is taken as 40 nm. Fig. 3 shows the normalized water saturation with nanoparticles after 2 month of injection. One may note that nanoparticles in CO_2 reduce the saturation significantly. Fig. 4 shows the distribution of the nanoparticles concentration after 2 month of injection. From this figure, it is can be seen that the concentration of the nanoparticles decreases. In Fig. 5, the ration of the variation of the porosity to the initial porosity is plotted. Also, variation of the permeability ration is plotted in Fig. 6. It is interesting to note that both figures indicate that nanoparticles injection reduces both and permeability.

Fig. 3: CO₂ saturation after 2 month of injection

Fig. 4: CO₂ concentration after 2 month of injection

Fig. 5: Porosity ratio φ/φ_0 variation after 2 month of injection

Fig. 6: Permeability ratio K / K_0 variation after 2 month of injection

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