

SPE SPE-145096-PP

A Practical Compositional Method for Simulation of CO₂ Flooding in Porous and Fractured Petroleum Reservoirs

Yuan Di, Peking University; Yu-Shu Wu, SPE, Colorado School of Mines; Binshan Ju, China University of Geosciences; Jishun Qin and Xinmin Song, PetroChina RIPED

Copyright 2011, Society of Petroleum Engineers

This paper was prepared for presentation at the SPE Asia Pacific Oil and Gas Conference and Exhibition held in Jakarta, Indonesia, 20-22 September 2011.

This paper was selected for presentation by an SPE program committee following review of information contained in an abstract submitted by the author(s). Contents of the paper have not been reviewed by the Society of Petroleum Engineers and are subject to correction by the author(s). The material does not necessarily reflect any position of the Society of Petroleum Engineers, its officers, or members. Electronic reproduction, distribution, or storage of any part of this paper without the written consent of the Society of Petroleum Engineers is prohibited. Permission to reproduce in print is restricted to an abstract of not more than 300 words; illustrations may not be copied. The abstract must contain conspicuous acknowledgment of SPE copyright.

Abstract

 CO_2 flooding is one of the most effective and used methods for enhanced oil recovery (EOR) approaches. The number of CO_2 flooding projects has increased rapidly in China and around the world. Compositional simulation is required for evaluating CO₂ flooding in EOR operations, especially for miscible or nearly miscible flooding when black-oil simulation is no longer adequate. The simulation method proposed here is a multi-dimensional, three-phase, and compositional modeling approach, which is applicable to both porous and fractured reservoirs. In the model formulation, a generalized multi-continuum approach is adopted to handle flow and transport in naturally fractured reservoirs and the mass flux of each mass component is contributed by advection and diffusion processes. In addition, precipitation of heavy oil components and absorption of CO_2 on the solid grains are modeled based on reversible linear or nonlinear isotherms. The governing partial differential equations for conservation of each component are discretized using a finite volume method and the resulting discrete equations are solved fully implicitly by Newton-Raphson iteration. The equation of state (EOS) by Soave-Redlich-Kwong is used to calculate the physical properties of fluids. Research has shown that the flash calculations with EOS in compositional simulation are computationally intensive and may not be reliable at near critical conditions. Therefore, a K-value based approach, improved by Almehaideb et al. (2002), is used for partitioning of oil components and CO_2 between oil and CO_2 phases. In addition, the laboratory measured oil and CO₂ phase compositional data can be used alternatively to account for compositional effect in this model. Two numerical examples are presented to show that the proposed modeling method is efficient for simulation of CO_2 flooding processes in EOR operations.

Introduction

 CO_2 flooding has been used as a commercial process for enhanced oil recovery (EOR) for over 40 years and is the secondmost applied EOR process in the world (Jarrell et al., 2002). Both laboratory studies and field applications have established that CO_2 can be an efficient oil-displacing agent. CO_2 injection in mature hydrocarbon fields has also been considered as a favourable option to reduce accumulation of atmospheric CO_2 and thus mitigate greenhouse effects on climate (Bradshaw and Cook, 2001). As the results, a number of CO_2 flooding projects has increased rapidly in China and around the world. Numerical simulation is the most common technique in the oil industry to better understand, predict, design, and manage a CO_2 -EOR project. Miscibility between oil and CO_2 will occur when pressure is high enough to compress the CO_2 to a density at which it becomes a good solvent for the lighter hydrocarbons in the crude oil. Compositional simulation is required for modeling the complex interaction of flow in CO_2 -EOR operations, especially for miscible or nearly miscible flooding when black-oil simulation is no longer adequate. In recent years, we have seen more CO_2 application in naturally fractured reservoirs. Due to the large permeability contrast between the matrix and the fracture in fractured reservoirs, injected fluids such as CO_2 or water easily move toward the production well and result in bypassing of the matrix oil and poor sweep efficiency. Early gas or water breakthrough becomes problematic in the secondary oil recovery stage in most fractured reservoirs.

Among the commonly used conceptual models for analyzing flow through fractured rock, dual-continuum models, i.e., double- and multi-porosity, and dual-permeability, are perhaps the most popular approaches used in fractured reservoir modeling studies (Barenblatt et al., 1960; Warren and Root, 1963; Kazemi, 1969). A more general and efficient method for multi-continuum, named multiple-interacting-continua (MINC) method, was proposed (Pruess and Narasimhan, 1985; Wu and Pruess, 1988). The TOUGH2 family of multiphase flow numerical simulators (Pruess, 2004) has a long recognized record of

applications in different fields of mass and heat transport in porous media and fractured reservoirs. Within the TOUGH2 family, TMVOC (Pruess and Battistelli, 2002) is a compositional simulator that was developed to model the migration of three-phase multi-component inorganic gases and hydrocarbons mixtures for environmental applications. However, because Henry's law and Raoult's law were adopted for phase equilibrium calculations, TMVOC is not applicable for conventional hydrocarbon reservoirs.

Phase equilibrium calculation is important for the transfer or partitioning of species between the phases to account for the effect of phase composition change on fluid properties. There are two methods to calculate equilibrium compositions and phase molar fractions in compositional simulation: K-value approach and equation-of-state (EOS) based on flash calculation. The most common way in compositional simulation was to perform a two-phase flash calculation. Rachford and Rice derived a simple objective function, Rachford-Rice function, to determine the phase mole fractions and phase compositions for a fixed overall composition and set of specified K-values (Rachford and Rice, 1952). The Rachford-Rice method has been extended by Li and Nghiem (1982) to negative flash calculations, where the overall composition can be outside the two-phase zone. Whitson and Michelsen (1989) proposed a more robust method by specifying a window in which the correction root of the objective function should lie. Although there have been significant progress and advance in two-phase equilibrium calculations with EOS, flash calculations in compositional simulation are computational intensive and may not be reliable near critical regions. Three-phase equilibrium calculations for CO₂-water-hydrocarbon mixtures are required in compositional reservoir simulation despite a large number of publications on the subject (Haugen et al., 2007). The compositional reservoir simulations are computationally very expensive primarily due to three-phase flash calculations, leading to the use of small number of grid blocks and high numerical dispersion, hence full-field compositional simulation usually is not possible.

Although the K-value approach may not automatically satisfies the thermodynamic consistency requirements, the compositional simulation based on K-value approach is robust and efficient, and the parameters for phase equilibrium calculations are directly related to the experimental data of crude oil. Wilson (1968) proposed a general correlation for K-values from experimental data. This simplified expression was modified by Whitson and Torp (1983) to accommodate the compositional effects at high pressures. K-value charts and the according polynomial equation for light hydrocarbons vs. pressure and temperatures that are valid up to around 6,000 psi pressures or more, are presented by DePriester (1953) and McWilliams (1973), respectively. Based on their work and experimental results, a new correlation for computing K-values for high-pressure systems was proposed by Almehaideb et al. (2002).

The main objective of this work is to propose a robust, efficient, compositional and implicit method for numerical simulation of CO_2 flooding in multiphase, three dimensional, porous and fractured reservoirs. In this compositional simulation method, the K-value correlation improved by Almehaideb et al. (2002), is used for partitioning of CO_2 and oil components in CO_2 -water-hydrocarbon mixtures. The multiphase fluid flow is described by Darcy equation, and the diffusion and mechanical dispersion of multicomponent are described by an extended model based on Fick's law. Adsorption of CO_2 on the rock grains, and precipitation of heavy component are considered to obey a linear or nonlinear isotherm. A residual based Newton-Raphson algorithm is used to solve the governing equations.

Mathematical Model

It is assumed that the multicomponent fluids are in local chemical and thermal equilibrium, and no chemical reactions take place. Multiphase fluid flow, multicomponent transport, and heat transfer through porous and fractured media are governed by the fundamental conservation laws mass, momentum, and energy. The model formulations are presented in this section.

Multiphase Flow

Darcy's law proposed originally for single-phase flow has been extended to describe the flow of multiple, immiscible fluids (Scheidegger, 1974). The generalized Darcy's law for the simultaneous flow of immiscible fluids in a multiphase system is given as

$$\mathbf{v}_{\beta} = -\frac{k \, k_{r\beta}}{\mu_{\beta}} \Big(\nabla P_{\beta} - \rho_{\beta} \mathbf{g} \nabla \mathbf{z} \Big) \tag{1}$$

where \mathbf{V}_{β} is a vector of the Darcy's velocity, or volumetric flow rate, of phase β , with β being fluid phase index ($\beta = g$ for CO₂; = w for water; and = n for oil); P_{β} , μ_{β} , ρ_{β} , and g are pressure, viscosity and density (all mass densities in this paper are expressed in molar units) of fluid phase β , and gravitational constant, respectively; z is the vertical coordinate; k is absolute or intrinsic permeability; and $k_{r\beta}$ is the relative permeability to fluid phase β .

Transport of Diffusion and Mechanical Dispersion

The combined effects of diffusion and mechanical dispersion are often called hydrodynamic dispersion and are described using the Fick's law for transport through a single-phase porous medium (Scheidegger, 1961; Bear, 1972). Fick's law has been generalized to describe the transport of components in multiphase, miscible, or immiscible fluid systems (Corapcioglu and

$$\mathbf{f}_{\beta}^{k} = -\underline{D}_{\beta}^{k} \nabla \left(\rho_{\beta} x_{\beta}^{k} \right) \tag{2}$$

where superscript k is an index for mass components (for CO₂, water, oil); $\mathbf{f}_{\beta}^{\mathbf{k}}$ is the dispersive mass flux vector of component k within fluid β ; x_{β}^{κ} is the mole fraction of component k in fluid β ; and $\underline{D}_{\beta}^{k}$ is the hydrodynamic dispersion tensor

accounting for both molecular diffusion and mechanical dispersion for component k in phase β. The general dispersion model (Scheidegger, 1961) was improved to include multiphase fluid effects as (Wu and Pruess, 2000),

$$\underline{D}_{\beta}^{k} = \alpha_{T}^{\beta} \left| \mathbf{v}_{\beta} \right| \delta_{ij} + \left(\alpha_{L}^{\beta} - \alpha_{T}^{\beta} \right) \frac{\mathbf{v}_{\beta} \mathbf{v}_{\beta}}{\left| \mathbf{v}_{\beta} \right|} + \phi S_{\beta} \tau d_{\beta}^{k} \delta_{ij}$$
(3)

where α_T^{β} and α_L^{β} are transverse and longitudinal dispersivities, respectively, in fluid β of porous media; ϕ is the effective porosity of the porous medium; S_{β} is saturation of fluid β ; τ is tortuosity of the porous medium; d_{β}^{k} is the molecular diffusion coefficient of component k within fluid β ; and δ_{ij} is the Kronecker delta function ($\delta_{ij} = 1$ for i = j, and $\delta_{ij} = 0$ for $i \neq j$) with i and j being coordinate indices.

Heat Transfer

Heat transfer in porous media is in general a result of both convective and conductive processes. Heat convection is contributed by thermal energy carried mainly by bulk flow of all fluids as well as by dispersive mass fluxes. On the other hand, heat conduction is driven by temperature gradients and may follow Fourier's law. Then the overall heat flux vector may be described as,

$$\mathbf{F}^{\mathbf{T}} = \sum_{\beta} \left(h_{\beta} \rho_{\beta} v_{\beta} \right) - \sum_{\beta} \sum_{k} \left(h_{\beta}^{k} \underline{D}_{\beta}^{k} \bullet \nabla \left(\rho_{\beta} x_{\beta}^{k} \right) \right) - \left(K_{T} \nabla T \right)$$

$$\tag{4}$$

where \mathbf{F}^{T} is the combined heat flux vector, including both advective and conductive heat flow in a multiphase, multicomponent system; h_{β} and h_{β}^{k} are specific enthalpies of fluid phase β and of component k in fluid β , respectively; K_{τ} is the overall thermal conductivity, which is a function of fluid saturations; and T is temperature.

Absorption of CO₂ and Precipitation of Heavy Oil Components

Adsorption of CO_2 component onto solid grains is a kinetic process. If the rate of adsorption and desorption is fast relative to other processes occurring in the reservoirs, adsorption of CO_2 can be modeled as reversible instantaneous sorption isotherms.

The equilibrium adsorption may be related to the concentration of component k (CO₂) in phase β as,

$$M_{ads}^{k} = (1 - \phi)\rho_{s}K_{d,\beta}^{k}\rho_{\beta}x_{\beta}^{k}$$
⁽⁵⁾

where M_{ads}^k is the mass of component k adsorbed per unit reservoir volume; ρ_s is the density of rock solids; $K_{d,\beta}^k$ is the distribution coefficient of component k between the phase β and rock solids to account for adsorption effects, it is treated as a

constant for the linear isotherm, or as a function of the concentration or mole fraction in a fluid phase and a maximum sorptive capacity when the non-linear Langmuir isotherms are considered.

Precipitation of heavy oil components from reservoir fluids during CO_2 injection is a serious problem, because it can plug the formation, cause permeability reduction and alteration of rock wettability from water wet to oil wet. In order to avoid fourphase equilibrium calculations, it is assumed that precipitation of heavy oil components on the solid grains can be modeled as the absorption isotherms (See Eq. (5)), whereas the distribution coefficient should be also a function of mole fraction of CO_2 in the fluid phase.

Governing Equations

The multiphase system consists of three fluid phases, CO_2 , water, and oil, and each fluid in turn consists of a number of mass components. A combination of mass and energy conservation principle with Eqs. (1-4) gives rise to a set of governing equations described below. The mass conservation equations of each component k in the porous continuum can be written as follows:

(A)

$$\frac{\partial}{\partial t} \left\{ \phi \sum_{\beta} \left(\rho_{\beta} S_{\beta} x_{\beta}^{k} \right) + (1 - \phi) \sum_{\beta} \rho_{s} \rho_{\beta} x_{\beta}^{k} K_{d,\beta}^{k} \right\} + \lambda_{k} \left\{ \phi \sum_{\beta} \left(\rho_{\beta} S_{\beta} x_{\beta}^{k} \right) + (1 - \phi) \sum_{\beta} \rho_{s} \rho_{\beta} x_{\beta}^{k} K_{d,\beta}^{k} \right\} - q^{k} - R^{k} = -\sum_{\beta} \nabla \bullet \left(\rho_{\beta} x_{\beta}^{k} \mathbf{v}_{\beta} \right) + \sum_{\beta} \nabla \bullet \left(\underline{\mathbf{D}} \bullet \nabla \left(\rho_{\beta} x_{\beta}^{k} \right) \right) \tag{6}$$

and the energy conservation equation is:

$$\frac{\partial}{\partial t} \left\{ \sum_{\beta} \left(\phi \, \rho_{\beta} S_{\beta} U_{\beta} \right) + \left(1 - \phi \right) \, \rho_{s} U_{s} \right\} - q^{T} - R^{T} = -\sum_{\beta} \nabla \bullet \left(h_{\beta} \, \rho_{\beta} \, \mathbf{v}_{\beta} \right) \\
+ \sum_{\beta} \sum_{k} \nabla \bullet \left(h_{\beta}^{k} \underline{\mathbf{D}} \bullet \nabla \left(\rho_{\beta} x_{\beta}^{k} \right) \right) + \nabla \bullet \left(K_{T} \nabla T \right)$$
(7)

where k is the index for the components, $k = 1, 2, 3, ..., N_c$, with N_c being the total number of mass components; ρ_s is the density of rock solids; λ_k is the radioactive decay constant of component k; $\underline{\mathbf{D}}$ is the hydrodynamic dispersion tensor; q^k and q^E are external source/sink terms or fracture-matrix exchange terms for component k and energy; R^k and R^T is the internal generation term for component k and for energy, respectively; and U_β and U_s are the internal energies of fluid β and rock solids, respectively.

Constitutive Relationships and Fluid Properties

For a flow system consisting of N_c components and N_p phases, the total number of primary thermodynamic variables is $N_c + 1$. The constitutive correlations express inter-relations and constraints of physical processes, variables, and parameters, and allow the evaluation of thermophysical properties as functions of the primary unknown variables.

Saturation and Mass Fraction Constraints

For fluid saturations,

$$\sum_{\beta} \mathbf{S}_{\beta} = 1 \tag{8}$$

The mass fractions of component k within phase β are subject to

$$\sum_{k} x_{\beta}^{k} = 1 \tag{9}$$

Capillary Pressure and Permeability

In a multiphase system, the capillary pressure relates pressures between the phases. When dealing with a three-phase system of gas (CO_2) , water, and oil, water- and gas-phase pressures are related by

$$P_{w} = P_{g} - P_{cgw} \left(S_{w}, S_{g} \right) \tag{10}$$

where P_{cgw} is the gas-water capillary pressure. The oil phase pressure is related to the gas phase pressure through

$$P_n = P_g - P_{cgn}(S_w, S_n) \tag{11}$$

where P_{cgn} is the gas-oil capillary pressure in a three-phase system. The oil-water capillary pressure, P_{cnw} , in a three-phase system can be derived from,

$$P_{cnw} = P_{cgw} - P_{cgn} = P_n - P_w \tag{12}$$

The relative permeabilities of a fluid phase in a three-phase system are normally assumed to be functions of fluid saturation only as

$$k_{r\beta} = k_{r\beta} \left(S_w, S_g \right) \tag{13}$$

The functions of capillary pressure and relative permeability are generally determined from laboratory and field studies for a given site in a tabulated form.

From the mass balances, the precipitation of heavy oil components is obtained. The volume fraction of precipitated heavy oil components in the original pore volume can be calculated, the remaining void space is available for fluid flow. The impact of porosity change on formation permeability depends not only on the overall reduction of porosity but on details of the pore space geometry and the distribution of precipitate within the pore space. Several models of permeability reduction can be selected (Pruess et al, 1999).

Properties of Gas Phase

Density of CO_2 as a function of pressure at various temperatures (Hendriks and Blok, 1993) and viscosity of CO_2 as a function of pressure at various temperatures (Goodrich, 1980) are adopted in this paper.

The Soave-Redlich-Kwong (SRK) equation (Redlich and Kwong, 1949; Soave, 1972) of state is used to describe the PVT properties of gas phase. For a pure component the cubic equation may be written in the form

$$Z^{3} - Z^{2} + (A^{*} - B^{*} - (B^{*})^{2})Z - A^{*}B^{*} = 0$$
⁽¹⁴⁾

where the largest root Z is the gas compressibility factor; $A^* = aP/R^2T^2$ and $B^* = bP/RT$; *a* and *b* are parameters that depend on critical pressure P_c , critical temperature T_c and Pitzer's acentric factor ω ; with *R* the universal gas constant.

$$a = \frac{0.42748R^2 T_c^2}{P_c} [1 + (0.48 + 1.574\omega - 0.176\omega^2)(1 - [T/T_c]^{1/2})]^2$$
(15)

$$b = \frac{0.08664RT_{\rm c}^2}{P_c}$$
(16)

For a multicomponent mixture, if the mixing rules recommended by Reid et al. (1987) are adopted, the two parameters are written as,

$$a_m = \left(\sum_k x_g^k \sqrt{a_k}\right)^2 \tag{17}$$

$$b_m = \sum_k x_g^k b_k \tag{18}$$

The molar density of the gas phase is given by

$$\rho_g = P(RTZ_g) \tag{19}$$

Using the Chapman-Enskog kinetic theory, gas phase viscosity μ_g is obtained as a function of pure component viscosities

 μ_k .

$$\mu_g = \sum_{k=1}^{N} \frac{x_g^k \mu_k}{\sum_{\lambda=1}^{N} x_g^\lambda \Phi_{k\lambda}}$$
(20)

The $\boldsymbol{\Phi}_{k\lambda}$ are binary interaction parameters given by

$$\boldsymbol{\varPhi}_{k\lambda} = \frac{\left(1 + \sqrt{\mu_k/\mu_\lambda} \sqrt[4]{M_\lambda/M_k}\right)^2}{\sqrt{8(1 + M_k/M_\lambda)}}$$
(21)

where M_k is the molecular weight of component k.

Properties of Oil Phase

The molar density of the oil phase is given by

$$\rho_{0} = P(RTZ_{0}) \tag{22}$$

where Z_o is the compressibility factor of oil phase, and can be calculated from Eq. (14) for hydrocarbon mixture.

The viscosity of a pure hydrocarbon component is calculated as a function of temperature from an equation due to Yaws et al. (1976).

$$\ln \mu = A' - \frac{B'}{T} + C'T + D'T^2$$
(23)

where A'B'C'D are the constants, and their values can be found in Ref. by Reid et al. (1987).

The mixture viscosity of the oil phase is obtained approximately in terms of the pure component viscosities as

$$\mu_o = \prod_{k=1}^{N_c} \mu_k^{x_o^k} \tag{24}$$

Properties of Water Phase

Effects on thermodynamic properties of water phase from dissolution of hydrocarbon and CO_2 are neglected. Therefore density and viscosity of the water phase are taken to depend only on pressure and temperature, and can be calculated by the steam table equations issued by the International Formulation Committee (IFC, 1967).

Phase Partitioning and K-Value approach

In a multicomponent system, the equilibrium ratio, $K_{\alpha\beta}^k$, of a given component k is defined as the ratio of the mole fraction of the component in the phase α to the mole fraction of the component in the phase β .

$$K_{\alpha\beta}^{k} = \frac{x_{\alpha}^{k}}{x_{\beta}^{k}}$$
(25)

For the water-oil equilibrium, the solubility of water in oil phase and the dissolution of hydrocarbon components in water phase are generally small. The equilibrium constants for water-oil partitioning are

$$K_{wo}^n = x_w^{n,sol} \tag{26}$$

$$K_{wo}^{w} = \frac{1}{x_{o}^{w,sol}}$$
(27)

where the superscripts n and w denote hydrocarbon components and water, respectively. $x_w^{n,sol}$ is the solubility of hydrocarbon component in water phase and $x_o^{w,sol}$ is the solubility of water in oil phase. The solubility is an increasing or decreasing function of temperature (Adenekan et al., 1993).

For the gas-water equilibrium, dissolution of CO_2 in water phase can be calculated by Henry's law and the gas mixture is assumed to obey Dalton's law.

$$K_{gw}^{CO_2} = \frac{K_H}{P_g}$$
(28)

$$K_{gw}^{H_2O} = \frac{P_{vap}^{H_2O}}{P_g}$$
(29)

where K_H is the Henry's coefficient for CO₂ dissolution in water phase, and can be computed from a polynomial fit to experimental data as a function of temperature (Battistelli et al.,1997). $P_{vap}^{H_2O}$ is the saturated vapor pressure of water at the given temperature.

For the gas-oil equilibrium, the K-value correlation improved by Almehaideb et al. (2002) is adopted.

$$K_{go}^{i} = \left(\frac{p_{ci}}{p_{k}}\right)^{A-1} \left(\frac{p_{ci}}{p}\right) \exp\left(AK_{i}^{*}\right)$$
(30)

$$A = 1 - \left(\frac{p - 14.7}{p_k - 14.7}\right)^{0.6} \tag{31}$$

$$K_{i}^{*} = \frac{a_{\text{T1}}}{T^{2}} + \frac{a_{\text{T2}}}{T} + a_{\text{T3}} + a_{\text{p1}} \ln p + \frac{a_{\text{p2}}}{p^{2}} + \frac{a_{\text{p3}}}{p} + \frac{a_{\omega}}{\omega}$$
(32)

where the superscripts *i* denote hydrocarbon components or CO₂. *p* is the system pressure (psia), p_k is the convergence pressure (psia), p_{ci} is the critical pressure of component *i* (psia), *T* is the system temperature (${}^{\circ}R$), ω is the acentric factor, a_{T1} , a_{T2} , a_{T3} , a_{p1} , a_{p2} , a_{p3} , a_{ω} are constants for component *i* from experimental data.

Numerical Algorithm and Numerical Examples

The governing equations (Eqs. 6 and 7) are solved using a fully implicit method. A kind of finite volume method, the integral finite difference method (Narasimhan and Witherspoon, 1976; Pruess, 1991) is used as the spatial discretization scheme. The integral finite difference method has the flexibility of finite element method and no predetermined limit on the number of neighbors that a grid block can have. The time discretization is carried out using a backward, first-order finite-difference scheme. Finally, the discretized formulae of component mass and energy balance equations are solved iteratively by Newton-Raphson method.

Depending on pressure, temperature and relative abundance of the different components, the fluids may exist in three different phase combinations, each of the phase may appear and disappear in a grid block during the simulation. The phases of each grid block are checked for the thermodynamic compatibility with the new values of the primary variables at the end of every Newton-Raphson iteration. The numerical algorithm for the treatment of phase appearance and disappearance (Adenekan et al., 1993) is adopted, the primary variables in the grid block are switched accordingly when there is a phase appear or disappear.

A compositional simulator is developed on the basis of the method proposed in this paper. Two numerical examples are simulated. The first one is a one-dimensional homogeneous isothermal geological model with one injection well of CO_2 and one production well of oil, as shown in Fig. 1. The fluid mixture has five pseudo-oil components and the fluids properties are listed in Table 1. The injection rate is constant and the production well bottomhole pressure is maintained at the initial pressure of the model. The relative permeability curves are shown in Fig. 2. The capillary pressures are assumed to be negligible and the input data are summarized in Table 2. The oil recoveries obtained from the simulation results with different bottomhole pressures are shown in Fig. 3. It can be seen that the simulated minimum miscibility pressure is of the order of 21.8MPa.

In the second example, the CO₂ flooding in a two dimensional cross sectional synthetic model is simulated. The reservoir is considered to be a dual-continuum system. The grid is shown in Fig. 4 with $50 \times 1 \times 10$ grid blocks and initially saturated by oil. The fluids properties and the relative permeability are same as that of the first example, and the capillary pressures are also assumed to be negligible. Boundaries of the model domain are no-flow. The initial pressure is 20MPa. The injected fluid is

 CO_2 at a rate of $3.1m^3/day$, located at Grid (1, 1). The producing well is located at Grid (1, 50) and the production pressure

is 10MPa. The summarized input data are given in Table 3. The distributions of oil saturation in matrix and fracture continua after CO_2 injection of 60 days are shown in Fig. 5 and Fig. 6, respectively. The result shows that the injection CO_2 fluids easily move toward the production well and result in bypassing of the matrix oil and poor sweep efficiency. This is mainly due to the large permeability contrast between the matrix and the fracture in this model.

Conclusions

A three-dimensional, three-phase compositional modeling method for simulation of CO_2 flooding has been implemented and tested. Because the proposed method is based on a generalized multi-continuum approach, it is applicable to both porous and fractured reservoirs. The multiphase fluid flow is described by Darcy equation, the diffusion and mechanical dispersion of multicomponent are described by an extended Fick's law. Adsorption of CO_2 on the rock grains, and precipitation of heavy component are considered to obey a linear or nonlinear isotherm. The governing partial differential equations for conservation of each component are discretized using a finite volume method and the resulting discrete equations are solved fully implicitly by Newton-Raphson iteration. The K-value approach improved by Almehaideb et al. (2002), is used for partitioning of oil components and CO_2 between oil and gas phases. The simulated minimum miscibility pressure is presented by a one-dimensional homogeneous example. The numerical results of a two-dimensional dual-continuum example shows that injection CO_2 fluids can easily move toward the production well in the fractured reservoirs, early gas breakthrough occurs and results in bypassing of the matrix oil and poor sweep efficiency.

Acknowledgments

This work was supported by the Chinese National S&T Major Project (2008ZX05014), the Project 10932001 by NSFC, and by the PetroChina RIPED.

References

- Adenekan A.E., T.W. Patzek and K. Pruess (1993). Modeling of Multiphase Transport of Multicomponent Organic Contaminants and Heat in the Subsurface: Numerical Model Formulation, Water Resour.Res., Vol. 29, No. 11, pp. 3727-3740.
- Almehaideb R.A., Ashour I., and El-Fattah K.A., Improved K-value Correlation for UAE Crude Oil Components at High Pressures Using PVT Laboratory Data, SPE 78581, Abu Dhabi International Petroleum Exhibition and Conference, 13-16 October 2002, Abu Dhabi, United Arab Emirates.
- Barker J.W., Fayers F.J. (1991). Transport coefficients for compositional simulation with coarse grids in heterogeneous media. SPE 22591, Ann. Tech. Conf., Dallas, TX, Oct. 6-9.
- Barenblatt G.I., Zheltov I.P. and Kochina I.N. (1960). Basic concepts in the theory of seepage of homogeneous liquids in fissured rocks, PMM, Sov. Appl. Math. Mech., 24(5), 852-864.
- Battistelli A., C. Calore and K. Pruess (1997). The Simulator TOUGH2/EWASG for Modeling Geothermal Reservoirs with Brines and Non-Condensible Gas, Geothermics, Vol. 26, No. 4, pp. 437 464.
- Bradshaw J. and Cook P. (2001). Geological sequestration of carbon dioxide. Environmental Geosciences, 8, 149-151.
- Damilola O.O. and Kishore K.M. (2005). Compositional upscaling in fractured reservoirs during gas recycling. Journal of Petroleum Science and Engineering, 46, 1-21.
- DePriester C.L. (1953). Chemical Engineering Progress Symposium Series 7, 49:1-43.
- Goodrich, J.H. (1980). Review and Analysis of Past and ongoing Carbon Dioxide injection Field Test. SPE Paper 8832, Presented at the first joint SPE symposium on EOR, Tusla, 20-23 April.
- Haugen K.B., Sun L. and Firoozabadi A., Multiphase equilibrium calculations for compositional simulation. SPE 106045. Proceedings of the 2007 Reservoir Simulation Symposium, Feb. 26-28, Woodlands, TX.
- Hendriks C.A., Blok K. (1993). Underground storage of carbon dioxide. Energy Convers Mgmt, 34:949-957.
- International Formulation Committee (IFC). A Formulation of the Thermodynamic Properties of Ordinary Water Substance, IFC Secretariat, Düsseldorf, Germany, 1967.
- Jarrell P.M., Fox C.E., Stein M.H. and Webb S.L. (2002). Practical Aspects of CO2 Flooding. Monograph 22, Society of Petroleum Engineers, Richardson, TX, USA.
- Kazemi H. (1969). Pressure transient analysis of naturally fractured reservoirs with uniform fracture distribution. Soc. Pet. Eng. 451-62. Trans., AIME, 246.
- Li Y.K., and Nghiem L.X., The development of a general phase envelope construction algorithm for reservoir fluid studies. SPE 11198 presented at 1982 SPE Annual Technical Conference and Exhibition, 26-29 September 1982, New Orleans, Louisiana.
- McWilliams., Chemical Engineering, 1973;80(25):138-140.
- Narasimhan T.N. and Witherspoon P.A. (1976). An Integrated Finite Difference Method for Analyzing Fluid Flow in Porous Media, Water Resources Research, 12(1), pp. 57-64.
- Pruess K. and Narasimhan T.N. (1985). A practical method for modeling fluid and heat flow in fractured porous media, Soc. Pet. Eng. J., 25, 14-26.
- Pruess K. (1991) TOUGH2 A General-Purpose Numerical Simulator for Multiphase Fluid and Heat Flow, Report LBL-29400, Lawrence Berkeley National Laboratory, Berkeley, California.
- Pruess K. (2004). The TOUGH codes—a family of simulation tools for multiphase flow and transport processes in permeable media. Vadose Zone J. 3, 738–746.
- Pruess K., Battistelli, A. (2002). TMVOC, a Numerical Simulator for Three-Phase Non-Isothermal Flows of Multicomponent Hydrocarbon Mixtures in Saturated–Unsaturated Heterogeneous Media. LBNL Report 49375, Lawrence Berkeley National Laboratory, Berkeley, CA.
- Pruess K., C. Oldenburg and G. Moridis. TOUGH2 User's Guide, Version 2.0, Lawrence Berkeley National Laboratory Report LBNL-43134, Berkeley, CA, November 1999.
- Rachford H.H. and Rice J.D. (1952). Procedure for Use of Electronic Digital Computers in Calculating Flash Vaporization Hydrocarbon Equilibrium. Petroleum Transanctions AIME, 195, 237-238.
- Redlich O. and J.N.S. Kwong. (1949). On the Thermodynamics of Solutions. V An Equation of State. Fugacities of Gaseous Solutions, Chem. Reviews, Vol. 44, pp. 233 - 244.
- Reid R.C., J.M. Prausnitz, and B.E. Poling. The Properties of Gases and Liquids, McGraw-Hill, New York, 1987.
- Scheidegger A. E., The Physics of Flow through Porous Media, Third Edition, University of Toronto Press, Toronto, 1974.
- Soave G. (1972). Equilibrium Constants from a Modified Redlich-Kwong Equation of State, Chem. Eng. Sci., Vol. 27, No. 6, pp. 1197 1203.
- Whitson C.H. and Michelsen, L.M. (1989). The Negative Flash, Fluid Phase Equilibria, 53, 51-71.

Wilson G. (1968). A modified Redlich-Kwong equation of state applicable to general physical data calculations, Paper No.15C, 65th AICHE National meeting, Cleveland, Ohio, May 4-7.

Whitson C.H. and Torp S.B., Evaluation of constant-volume depletion data, Journal of Petroleum Technology, March 1983, 610-620.

Warren J.E. and Root P.J. (1963). The behavior of naturally fractured reservoirs, Soc. Pet. Eng. J., Trans., AIME, 228, 245-255.

Wu Y.S. and Pruess K. (1988). A multiple-porosity method for simulation of naturally fractured petroleum reservoirs, SPE Reservoir Engineering, 3, 327-336.

Wu, Y. S. and Pruess K. (2000). Numerical simulation of non-isothermal multiphase tracer transport in heterogeneous fractured porous media, Advances in Water Resources, Vol. 23, 699-723.

Yaws C.L., J.W. Miller, P.N. Shah, G.R. Schorr and P.M. Patel. (1976). Correlation Constants for Chemical Compounds, Chem. Eng. Sci., Vol. 83, No. 24, pp. 153 - 162.

Component name	$p_c(^{o}R)$	$T_c(psia)$	ω	a _{T1}	a _{T2}	a _{T3}	a _{p1}	a _{p2}	a _{p3}	a _ø	Mole fraction
CO ₂	1071.0	547.90	0.2250	-292859	-0.01414	16.2443	-0.564467	48.8616	-1331.41	0.0	0.0
Comp-1	667.8	343.37	0.0104	-292865	-0.00518	5.92040	0.009982	35.2435	54.8676	0.0	0.18
Comp-2	707.8	550.09	0.0986	-970689	0.0	-3.56546	0.622591	5.09279	688.0477	0.0	0.18
Comp-3	616.3	666.01	0.1524	-1481582	0.0	-6.38713	0.968672	-3.39020	747.110	0.0	0.22
Comp-4	490.4	829.10	0.2223	-1778903	0.0	-8.45991	1.159219	-5.06920	873.201	0.0	0.22
Comp-5	320.3	1139.40	0.5069	-1778901	0.01436	-6.00502	-1.10606	-1.03540	-376.926	0.0	0.20

Table 1. Initial composition and oil properties

Table 2. Summary of input data for one-dimensional model

Parameter	Value
Dimension	10×1×1
Grid block size	$1m \times 1m \times 1m$
Initial temperature	90 <i>°C</i>
Porosity	0.3
Permeability	16.0 <i>md</i>

Table 3. Summary of input data for two-dimensional sectional model

Parameter	Value
Dimension	50×1×10
Grid block size	$2m \times 1m \times 2m$
Initial temperature	90°C
Matrix porosity	0.25
Fracture porosity	0.05
Matrix permeability	16.0 <i>md</i>
Fracture permeability	1600md



Fig. 1. A one-dimensional homogeneous isothermal geological model



V																													
																													_
																													_
		1						F	F		F														t	1			_
	1							F	F	F	F	F	F	F	F	F	F												_
																													ł





Fig. 5. Oil saturation for fracture continua of the two-dimensional vertical section model after CO₂ injection of 60 days



Fig. 6. Oil saturation for matrix continua of the two-dimensional vertical section model after CO₂ injection of 60 days