Modeling CO₂ miscible flooding for enhanced oil recovery

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Abstract: The injection of fuel-generated CO₂ into oil reservoirs will lead to two benefits in both enhanced oil recovery (EOR) and the reduction in atmospheric emission of CO₂. To get an insight into CO₂ miscible flooding performance in oil reservoirs, a multi-compositional non-isothermal CO₂ miscible flooding mathematical model is developed. The convection and diffusion of CO₂-hydrocarbon mixtures in multiphase fluids in reservoirs, mass transfer between CO₂ and crude, and formation damages caused by asphaltene precipitation are fully considered in the model. The governing equations are discretized in space using the integral finite difference method. The Newton-Raphson iterative technique was used to solve the nonlinear equation systems of mass and energy conservation. A numerical simulator, in which regular grids and irregular grids are optional, was developed for predicting CO₂ miscible flooding processes. Two examples of one-dimensional (1D) regular and three-dimensional (3D) rectangle and polygonal grids are designed to demonstrate the functions of the simulator. Experimental data validate the developed simulator by comparison with 1D simulation results. The applications of the simulator indicate that it is feasible for predicting CO₂ flooding in oil reservoirs for EOR.

Key words: Compositional simulator, CO₂ flooding, mathematical model, irregular grids

1 Introduction

Since 1750, the CO₂ concentration in the atmosphere has increased from 280 ppm to 368 ppm in 2000, and 388 ppm in 2010 (Rackley, 2010). Chinese annual CO₂ emission was 5.1 billion tonnes at 2005, and it will reach 8.6 billion tonnes at 2020 (Wang et al, 2011).

The CO₂ emission is increasing at an average rate of 4.5% per annum. The increase in atmospheric emission of CO₂ with the attendant global warming and environmental degradation are driven by global energy demand.

Depleted or mature oil and gas fields may provide favorable sites for storing CO₂ in porous and permeable reservoirs (Wells et al, 2007; Özkilic and Gumrah, 2009; Yang et al, 2010). In most oil reservoirs, CO₂ exists as a supercritical fluid under reservoir conditions, which is a favorable flooding agent for enhanced oil recovery (EOR). Studies (Adewusi, 1998; Farajzadeh et al, 2009) show that CO₂ flooding for EOR in oil fields can improve oil recovery significantly. Miscible CO₂ flooding is capable of mixing in any ratio without separation of CO₂ and oil phases,

and immiscible CO₂ flooding leads to CO₂ and oil phases because of CO₂ cannot be completely dissolved in oil. Miscible flood is better than immiscible flood for CO₂ as it has more displacement efficiency for crude oil in a miscible (supercritical) state. CO₂ has been injected into the oil formations of many oil fields in the world for EOR (Orr et al, 1982; Mungan, 1992; Barnhart and Coulthard, 2000; Dahaghi et al, 2008).

During the CO₂ miscible flooding process in oil reservoirs, the main mechanism includes 1) miscible displacement, 2) convection and diffusion, 3) phase behavior of in-situ fluids on flow and mass transfer, 4) heavy organic precipitation and its effects on porosity and permeability, and 5) reducing oil viscosity.

Song (2008) studied the main factors that influence CO₂ miscible displacement using numerical simulation. However, the research is not based on his own simulator, and no mathematical model was presented in his work. More recently, Su et al (2011) developed a one-dimensional mathematical model for CO₂ miscible displacement with CO₂ adsorption. However, energy transfer was not considered in this model, and the oil is treated as one component. Therefore, the model is not a compositional model.

In this paper, the authors develop a non-isothermal

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compositional mathematical model. The changes in porosity and permeability caused by asphaltene precipitation are considered in the model. The integral finite difference method that is used to discretize in space and time is discretized as a fully implicit finite-difference. A reservoir simulator is developed to predict CO₂ miscible flooding behavior. Two simulation samples are designed to demonstrate the functions of the simulator. It is found that the predicted recovery from CO₂ injection under miscible conditions has a good match with the slim tube experimental recovery.

2 Mathematical model and governing equations

2.1 Assumption and consideration in the model

CO₂ flow and transport in porous media are simulated using a conceptual model of multiphase fluid flow and multi-component transport within oil and water. The CO₂-EOR mathematical model is based the following assumptions:

- 1) Heterogeneity of the oil formation and compressibility are considered.
- 2) Heat transfer in porous media is considered.
- 3) Flow and transport mechanisms include multiphase Darcy flow and multi-component diffusion, subject to adsorption and precipitation.
- 4) Mass components include CO₂, H₂O, and oil with some pseudo-oil components.
- 5) The flooding process is miscible.
- 6) CO₂ adsorption on pore walls of the oil formation is considered.
- 7) Formation damage induced by asphaltene deposition on pore walls is considered.

2.2 Governing equations

The physical processes associated with CO₂, oil, and water flow and transport in porous media are governed by the same fundamental conservation laws. Conservation of mass, momentum, and energy govern the behavior of fluid flow and heat transfer in rock. These physical laws are often represented mathematically on the macroscopic level by a set of partial differential or integral equations. We assume that these processes can be described using a continuum approach within a representative elementary volume (REV) in a porous medium.

2.2.1 Mass conservation equations

According to the mass conservation law, a conservation equation of mass components in the porous media can be written as follows:

$$\frac{\partial A^k}{\partial t} = F^k + q^k \quad (1)$$

where superscript k is the index for the components, $k = 1, 2, 3, \dots, N_c$, with N_c being the total number of mass components; A^k is the accumulation term of component k , kg/m³; q^k is an external source/sink term for mass component k , kg/(s·m³); and F^k is the “flow” term of mass, or diffusive and dispersive mass transport, kg/(s·m³).

The accumulation terms in Eq. (1) for component k is

written as

$$A^k = \phi \sum_{\beta} (\rho_{\beta} S_{\beta} X_{\beta}^k) + R_s^k \quad (k = 1, 2, 3, \dots, N_c) \quad (2)$$

where subscript β is an index for fluid phase ($\beta = g$ for gas phase, $= w$ for aqueous phase, $= o$ for oil phase); ϕ is the porosity of porous media; ρ_{β} is the density of phase β , kg/m³; and S_{β} is the saturation of phase β ; X_{β}^k is the mole fraction of component k in fluid β ; R_s^k is the adsorption term of component k on rock solids, kg/m³.

The adsorption term in Eq. (2) is used mainly for incorporating possible CO₂ adsorption and may be described using a K_d approach,

$$R_s^k = \int_0^t \rho_{\beta} \frac{\partial \delta^k}{\partial t} = \int_0^t \rho_{\beta} \alpha_d^k v_o X_{\beta}^k dt \quad (k = 1, 2, 3, \dots, N_c) \quad (3)$$

where α_d^k is a capture rate constant of component k at pore walls, kg/m; v_o is the flow velocity of the oil phase, m/s; δ^k is the volume of component k deposited on the pore surfaces per unit bulk volume. Some heavy components such as asphalt and asphaltene have more opportunity to attach on pore walls, which leads to formation damage.

The mass component transport is governed in general by processes of advection, diffusion and dispersion. The total mass flow term (Scheidegger, 1961; Wu and Pruess, 2000) for a component k , by advection and dispersion, is written as

$$F^k = -\sum_{\beta} \nabla \cdot (\rho_{\beta} X_{\beta}^k v_{\beta}) + \sum_{\beta} \nabla \cdot (\underline{D}_{\beta}^k \cdot \nabla (\rho_{\beta} X_{\beta}^k)) \quad (k = 1, 2, 3, \dots, N_c) \quad (4)$$

where v_{β} is a vector of volumetric flow rate for fluid flow, defined by Darcy's law to describe the multiphase flow as,

$$v_{\beta} = -\frac{\kappa \kappa'_{r\beta}}{\mu_{\beta}} (\nabla P_{\beta} - \rho_{\beta} g \nabla z) \quad (5)$$

where P_{β} (Pa), μ_{β} (Pa·s), and g (m/s²) are pressure, viscosity of fluid phase β , and gravitational constant, respectively; z is the vertical coordinate; κ is the absolute or intrinsic permeability, m²; and $\kappa'_{r\beta}$ is the relative permeability to phase β . In Eq. (4), $\underline{D}_{\beta}^k$ is the hydrodynamic dispersion tensor accounting for both molecular diffusion and mechanical dispersion for component k in phase β , m²/s, defined by an extended dispersion model (Scheidegger, 1961) to include multiphase effects (Wu and Pruess, 2000) as,

$$\underline{D}_{\beta}^k = \alpha_T^{\beta} |v_{\beta}| \delta_{ij} + (\alpha_L^{\beta} - \alpha_T^{\beta}) \frac{v_{\beta} v_{\beta}}{|v_{\beta}|} + \phi S_{\beta} \tau d_{\beta}^k \delta_{ij} \quad (k = 1, 2, 3, \dots, N_c) \quad (6)$$

where α_T^{β} and α_L^{β} are the transverse and longitudinal dispersivities, respectively, in fluid β of porous media, m; τ is the tortuosity of the porous medium; d_{β}^k is the molecular diffusion coefficient of component k within fluid β , m²/s; 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.

2.2.2 Energy conservation equations

Heat transfer in porous media is in general a result of both convective and conductive heat-transfer processes (Scott, et al 2005; Dabagh et al, 2009), and radiation may be ignored in most cases. These heat-transfer processes are complicated by interactions between multiphase fluids, multicomponents, and associated changes in phases, internal energy, and enthalpy. The combined, overall heat flux term, from convection, conduction and radiation in a multiphase, multicomponent, porous medium system, may be described as,

$$\begin{aligned} \frac{\partial}{\partial t} \left\{ \sum_{\beta} (\phi \rho_{\beta} S_{\beta} U_{\beta}) + (1-\phi) \rho_s U_s \right\} - q^T = \\ - \sum_{\beta} \nabla \cdot (h_{\beta} \rho_{\beta} \mathbf{v}_{\beta}) + \sum_{\beta} \sum_k \nabla \cdot (h_{\beta}^k \underline{D}_{\beta}^k \cdot \nabla (\rho_{\beta} X_{\beta}^k)) \\ + \nabla \cdot (C_T \nabla T) \end{aligned} \quad (7)$$

where ρ_s is the density of rock solids, kg/m³; and U_{β} and U_s are the internal energies of fluid β and rock solids, respectively, J/kg; q^T are external source/sink terms for component k and energy, W/(s·m³); h_{β} and h_{β}^k are specific enthalpies of fluid phase β and of component k in fluid β , respectively, J/kg; C_T is the overall thermal conductivity, W/(m·°C); and T is the temperature, °C.

2.2.3 Constitutive relationships

To complete the mathematical description of multiphase flow and heat transfer in porous media, the mass and energy-balance equation needs to be supplemented with a number of constitutive equations. The constitutive correlations are expressed as follows.

Constraint on summation of total fluid saturation in porous media satisfies as

$$\sum_{\beta} S_{\beta} = 1 \quad (8)$$

Constraint on mole fractions within phase β is written as

$$\sum_k X_{\beta}^k = 1 \quad (9)$$

2.2.4 Description of formation damage

The adsorption of heavy components on pore surfaces may lead to the changes in the local porosity and permeability of the oil formation (Ju et al, 2009). The instantaneous porosity is expressed by

$$\phi = \phi - \Delta\phi \quad (10)$$

where $\Delta\phi$ denotes the variation of porosity by retention of heavy components in porous media, and it is expressed by

$$\Delta\phi = \sum \delta^k \quad (11)$$

The change in permeability in this study is caused by asphaltene release and mobilization. According to the literature (Ju et al, 2007), the expression for instantaneous permeability changed by release and retention of asphaltene is given by

$$\kappa = \kappa_0 [(1-f)\lambda_f + f\phi/\phi_0]^n \quad (12)$$

in which κ_0 and ϕ_0 are the initial permeability (m²) and porosity; κ and ϕ are the instantaneous local permeability (m²) and porosity of porous media; and λ_f is a constant for fluid seepage allowed by the plugged pores. The range of index n is from 2.5 to 3.5. f is a flow efficiency factor (Ju et al, 2002).

3 Numerical solution scheme

3.1 Selection of primary variables and variable switching

There are a total of N_c mass conservation equations to solve for an isothermal reservoir; and N_{c+1} equations to solve for a non-isothermal system. The selection of primary variables lists in Table 1.

Table 1 Primary parameters and variables in the Jacobian matrix

Index	1	2	3	4	...	m	...	N_c-1	N_c	N_c+1
Parameters	P_o	X_o^3	X_o^4	X_o^5	...	...	...	$X_o^{N_c}$	S_w	T
Variables in the Jacobian matrix	x_1	x_2	x_3	x_4	...	x_m	...	x_{N_c-1}	x_{N_c}	x_{N_c+1}

In Table 1, subscript o denotes the phase index for oil; and X_o^k is the mole fraction of component k in the oil phase.

3.2 Discretization and numerical solution procedure

Time discretization is carried out using a backward, first-order, fully implicit finite-difference scheme and the integral finite-difference method (Pruess et al, 1999) is used for spatial discretization. The discrete nonlinear equations for the mass and heat of component k at node i can be written in a general form:

$$\left\{ A_i^{k,n+1} - A_i^{k,n} \right\} \frac{V_i}{\Delta t} = \sum_j flow_{ij}^{k,n+1} + Q_i^{k,n+1} \quad (13)$$

where $k = 1, 2, 3, \dots, N_c, N_c+1$ (N_c+1 denotes energy equation), and $i = 1, 2, 3, \dots, N$.

There are a number of numerical solution techniques that have been developed in the literature over the past few decades to solve the nonlinear, discrete equations of reservoir simulations. The predominant approach is to use a fully implicit scheme. This is due to the extremely high nonlinearity inherent in those discrete equations which causes convergence difficulties. The discrete non-linear equation (Eq. (13)) can be written in a residual form:

$$R_i^{k,n+1} = \left\{ A_i^{k,n+1} - A_i^{k,n} \right\} \frac{V_i}{\Delta t} - \sum_j flow_{ij}^{k,n+1} - Q_i^{k,n+1} = 0 \quad (14)$$

In terms of the primary variables, the residual equation (Eq. (14)) at node i is regarded as a function of the primary variables at not only node i , but also at all its direct neighboring nodes j . The Newton iteration scheme gives rise to:

$$\sum_m \frac{\partial R_i^{k,n+1}(x_{m,p})}{\partial x_m} (\delta x_{m,p+1}) = -R_i^{k,n+1}(x_{m,p}) \quad (15)$$

where x_m is the primary variable m with $m = 1, 2, 3, \dots, N_{c+1}$, respectively, at node i and all its direct neighbors; p is the iteration level; and $i = 1, 2, 3, \dots, N$. The primary variables in Eq. (15) need to be updated after each iteration:

$$x_{m,p+1} = x_{m,p} + \delta x_{m,p+1} \quad (16)$$

The Newton iteration process continues until the residuals $R_i^{k,n+1}$ or changes in the primary variables $\delta x_{m,p+1}$ over an iteration are reduced below preset convergence tolerances.

4 Numerical results and discussion

This section will demonstrate the functions of the simulator and validate the mathematical model that predicts CO₂ miscible flooding.

4.1 The comparison between simulation and slim tube experimental data

The simulation result of one-dimensional miscible flooding was compared with the slim tube experimental data. The main parameters used in numerical simulation are shown in Table 2. The minimum miscible pressure (MMP) of the CO₂-oil system is 27.9 MPa, which was also obtained by slim tube experiments in the laboratory. The crude oil used in MMP and CO₂ flooding experiments was sampled from well H75-29-5 in the Honggang Oil Field. The viscosity and density at reservoir conditions were 1.67 mPa·s and 0.7464 g/

cm³. The initial model pressure and flow pressure at the outlet (the 30th grid) were set at 32.50 MPa and 31.90 MPa, which keep miscible flooding during the simulation. The conditions such as pressure and temperature were kept the same in the numerical run and experiments.

Fig. 1 shows that the oil recovery increases approximately linearly with continuous injection of CO₂ until 0.90 pore volume (PV) of CO₂ has been injected. Then the increase in the oil recovery slows down because of CO₂ breakthrough at the outlet of the model. The oil recoveries obtained by the simulation match well with experimental data. There is only a small deviation between the numerical and experimental results, which validates the reliability of the mathematical model.

Fig. 1 A comparison between numerical results and experimental data

Fig. 2 shows the distribution of CO₂ in the oil phase along the model from the inlet to the outlet. This indicates that CO₂ arrives at the outlet before 0.90 PV of CO₂ has been injected. Fig. 3 demonstrates the distributions of each component (five pseudo-components for hydrocarbon) along the model when 0.33 PV of CO₂ is injected. This implies that the hydrocarbon components are displaced from the locations where the CO₂ has swept. There is a relative flat displacement front for the diffusion phenomenon. The simulation results imply that CO₂ flooding is piston-like displacement in the miscible state, which leads to a high displacement efficiency. Zhao et al (2011) drew a similar conclusion from flooding experiments.

Fig. 2 CO₂ distribution in the oil phase at different injection volumes

Table 2 Main parameters of the example

Parameters	Value
The length of the slim tube, m	18.30
The node numbers	30
The size of grid of x , m	0.61
Temperature, °C	108.30
Initial pressure, MPa	32.50
Number of pseudo-components of crude oil	5
Cross-section area of the model, 10 ⁻⁵ m ²	1.169
Initial oil saturation	0.77
Connate water saturation	0.23
Initial gas saturation	0
Porosity	0.39
Permeability, μm ²	3.20
CO ₂ injection rate, 10 ⁻⁸ kg/s	2.5
Wellhole flow pressure, MPa	31.90

Fig. 3 Distributions of each component in the oil phase after 0.33 PV of CO₂ injected

4.2 Three dimensional sample

This section is designed to demonstrate the grid types and their effects on CO₂ distribution in the oil phase. Due to the application of the integral finite difference technique in the discretization for the governing equation, the regular grid (cuboids) or flexible irregular grid type (polygonal, PEBI, hybrid, etc.) is optional for a simulation. Fig. 4 shows the two types of grid used as demonstration examples for CO₂ miscible flood for EOR in a five-spot well pattern. Fig. 4 (a) is a regular cuboidal grid model and Fig. 4 (b) is a hybrid grid system with locally refined grids around injection and production wells. The geological and other parameters such as reservoir fluids are completely the same except for grid discretization for the two demonstrations (see Table 3).

Fig. 4 Grid types used in simulation sample

Table 3 Main parameters of the two demonstrations

Parameters	Value	Parameters	Value
The length of the geological model <i>X</i> , m	220	Initial oil saturation	0.449
The width of the geological mode <i>Y</i> , m	220	Initial water saturation	0.551
The thickness of the geological mode <i>Z</i> , m	20	Porosity	0.185
Initial reservoir temperature, °C	99	Permeability for all grids at all direction, 10 ⁻³ μm ²	90
Initial reservoir pressure, MPa	30.18	CO ₂ injection rate of each injection well, kg/s	0.08
Numbers of pseudo-components of oil	5	Wellbore flow pressures for four production wells, MPa	30.01

Fig. 5(a) shows that the apparent distribution of CO₂ in the oil phase is affected by the grid direction. The contours of CO₂ mole fractions around the injection well look like squares. The transport velocities of CO₂ in the oil formation reach a maximum in the *X* and *Y* directions, which demonstrates a numerical pseudo-phenomenon for

the cuboidal grid model. The contours of CO₂ mole fractions around the injection well look like circles in Fig. 5(b). The characteristic of the contours reflects radial flow behavior. This implies that the simulation results in this hybrid grid model are more accurate than that in the regular cuboidal grid model.

Fig. 5 The distribution of CO₂ in the oil phase after CO₂ injection of 400 days

5 Conclusions

A nonisothermal multi-compositional mathematical model is developed for predicting CO₂ miscible flood in oil reservoirs for EOR. Physical and chemical processes such as heat transfer, multi-component convection-diffusion, adsorption, are fully considered during CO₂ flow and transport in porous media. The governing equations of CO₂ miscible flood are discretized in space using an integral finite-difference method. The Newton-Raphson iterative technique is used to solve the numerical equation system. Slim tube experimental data are used to validate the model and simulator developed in this work. Two simulations of the 3D cuboidal and hybrid grid model demonstrate the optional functions for grid types and their effects on the modeled CO₂ distribution in oil. It is found that the hybrid grid system leads to more accurate prediction of CO₂ distribution than that of the cuboidal grid.

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