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# Modeling of capacitance flow behavior in EOS compositional simulation

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## ABSTRACT

Gas injection is a widely used method for enhanced oil recovery. Oil bypassing by gas occurs at different scales because of micro and macroscopic heterogeneities, gravity segregation, and front instability. Part of the bypassed oil can be recovered by crossflow between the bypassed and flowing regions. This characteristic of reservoir flow is referred to as capacitance flow behavior in the literature. Modeling of such flow behavior at the sub-grid scale is challenging in the conventional flow simulation since fluids are perfectly mixed and in equilibrium within individual grid blocks under the local equilibrium assumption.

This research investigates capacitance flow behavior in compositional reservoir simulation. An efficient two-step method is presented to model bypassed oil recovery in multiphase compositional flow simulation of gas floods. The oil bypassing is first quantified by use of the dual-porosity flow with two dimensionless groups; bypassed fraction and throughput ratio. To represent bypassed oil recovery in single-porosity flow, a new flow-based fluid characterization is applied to part of the heavy fractions of the fluid model used. Properties for pseudo components can be determined based on the throughput ratio estimated in the dual-porosity flow. Case studies for various reservoir/fluid properties show that single-porosity flow with the new method reasonably represents bypassed oil recovery observed in core floods and fine-scale heterogeneous simulations.

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## 1. Introduction

Gas injection is a widely used method for enhanced oil recovery. The interplay of fluid flow with phase behavior can yield multicontact miscibility between reservoir oil and injection gas (Johns, 1992; Dindoruk, 1992; Orr, 2007). Therefore, design of gas injection processes often requires compositional simulation that can accurately model properties of equilibrium phases by use of a cubic equation of state (EOS) (Coats, 1980; Watts, 1986; Collins et al., 1992). Compositional simulation attempts to consider various complexities that exist in actual reservoir processes by increasing the generalization level of the conservation equations. (Chang et al., 1990; Cao, 2002). Fundamental assumptions always made include the local equilibrium assumption, where fluids are perfectly mixed and in equilibrium within individual continua (i.e., grid blocks) (Lake, 1989).

The continuum assumption is made to calculate large-scale fluid flow in porous media with a finite-difference scheme, in which grid blocks are greater than a representative elementary

volume (REV) (Lake, 1989; Hill, 1963). The local discontinuities of an actual porous medium are not taken into account under the continuum assumption. The grid-block scales in a practical finite-difference reservoir simulation are much greater than the REV (Salehi et al., 2013). Fluid properties in a grid block at each time step are then calculated with the local equilibrium assumption, where the thermodynamic equilibrium is calculated for a given set of overall composition, pressure, and temperature.

Oil bypassing by gas occurs at different scales because of micro and macroscopic heterogeneities, gravity segregation, and front instability. It has been observed in various types of experiments and field applications of gas injection. Flow-visualization experiments (Stalkup, 1970; Chatzis et al., 1983; Campbell and Orr, 1985; Bahralolom et al., 1988; Stern, 1991) showed that microscopic oil bypassing was related to pore structures with bimodal or wide pore-size distributions. Shielding of oil by water films in pores can also hinder the contact between the bypassed oil and injection gas in the region with high water saturations (Shelton and Schneider, 1975; Spence et al., 1980; Wylie and Mohanty, 1997; Wylie and Mohanty, 1999). These results clearly indicate that oil bypassing is present even at the microscopic scale smaller than a REV.

At macroscopic scales greater than a REV, gas channeling creates slow-flow or stagnant regions in heterogeneous reservoirs (Cinar et al., 2006; Al-Wahaibi et al., 2007). Thin shales with a thickness of only a

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<b>Nomenclature</b>		$x_D$	Dimensionless distance
<i>Roman Symbols</i>		$z_i$	Overall mole fraction of component i
$A$	Area	<i>Abbreviations</i>	
$A_m$	Dimensionless attraction parameter for mixtures	DPF	Dual-porosity flow
$a_i$	Attraction parameter for component i in a cubic equation of state	EOS	Equation of state
$B$	Bypassed fraction	MMP	Minimum miscibility pressure
$b_i$	Covolume parameter for component i in a cubic equation of state	PC	Pseudo component
$C_{Dh}$	Dimensionless volume-shift parameter of introduced pseudo heavy components	PR	Peng-Robinson
$c_{hi}$	Volume-shift parameter of component hi	PVI	Pore-volume injected
$e$	Coefficient defined for permeability correlation	SPF	Single-porosity flow
$f$	Exponent defined for permeability correlation	<i>Greek symbols</i>	
$K$	Permeability	$\varphi$	Porosity
$\vec{n}$	Outward unit normal vector	$\rho_j$	Molar density of phase j
$n_c$	Number of components	$\gamma_a$	Attraction-parameter index
$n_p$	Number of phases	$\gamma_h$	Molar-ratio index
$P_{C_T}$	Critical pressure	<i>Subscripts/superscripts</i>	
$\vec{q}_{ij}$	Molar flux vector of component i in phase j from the flowing fraction to the bypassed fraction	B	Bypassed fraction
$R_T$	Throughput ratio	D	Dimensionless
$S$	Surface area	F	Flowing fraction
$S_C$	Surface area of coarse-scale grid block	hi	Introduced heavier oil component i
$S_j$	Saturation of phase j	i	Component i
$t$	Time	j	Phase j
$t_D$	Dimensionless time	m	Mixture
$T_C$	Critical temperature	oi	Original oil component i
$\vec{U}_j$	Flow velocity of phase j	T	Transverse direction
$V$	Volume		
$V_C$	Volume of coarse-scale grid block		
$x_{ij}$	Mole fraction of component i in phase j		

few inches can cause marked oil bypassing by gas (McGuire et al., 1995). Front instability can also lead to oil bypassing, if the mobility ratio between the injection gas and reservoir oil is large (Gardner and Ypma, 1984; Brock and Orr, 1991).

Part of bypassed oil can be recovered by the transverse mass flux between the bypassed and flowing regions as reported by a number of researchers (Pande, 1992; Pande and Orr, 1994a, 1994b; Burger et al., 1994, 1996; Burger and Mohanty, 1997; Zhou et al., 1997; Cinar et al., 2006; Al-Wahaibi et al., 2007). The transverse flux between the two regions can occur because of diffusion, dispersion, viscous forces, and capillarity [Pande, 1992; Pande and Orr, 1994a, 1994b]. Gradual migration of oil from the bypassed region to the flowing region can cause the resulting composition profile to deviate from the one without the transverse mass flux (Brock and Orr, 1991; Pande and Orr, 1994a; 1994b; Zhou et al., 1997). High residual oil saturations were observed in dominant flow paths due to the interaction of phase behavior with oil bypassing (Gardner and Ypma, 1984; Campbell and Orr, 1985; Bahralolom et al., 1988; Mohanty and Johnson, 1993). These results indicate the importance of considering the effects of oil bypassing on oil recovery.

The degree of miscibility between oil and gas also affects the level of bypassing in gas floods (Mohanty and Johnson, 1993; Burger and Mohanty, 1997). Experimental results (Burger et al., 1994) showed that the bypassed-oil fraction was smaller for less miscible processes. It was stated that the optimum gas enrichment can be below the minimum miscibility enrichment for a secondary gas flood with a high-viscosity ratio, where the sweep and local displacement efficiencies take a balance. In the mechanistic

investigation of bypassed-oil recovery in CO<sub>2</sub> injection (Khosravi et al., 2014), a maximum recovery was achieved at sub-miscible conditions, where the oil swelling and vaporization enhanced the recovery of bypassed oil significantly. Also, it is not always economical or technically feasible to inject a gas that is miscible with oil (Bardon et al., 1994; Al-Wahaibi et al., 2007; Ren et al., 2011). In this research, the focus is on gas floods at sub-miscible (or immiscible) conditions.

The key characteristic of reservoir flow with oil bypassing is that the oil held in the bypassed (slow-flow or stagnant) region is gradually migrated to the flowing region through the transverse mass flux between the bypassed and flowing regions. This flow behavior has been referred to as capacitance. The capacitance flow behavior observed in core floods has been studied by use of mathematical models since late 1950s. The capacitance flow was observed as earlier breakthrough of the displacing component and longer tailing of the effluent-concentration history for the displaced component (Coats and Smith, 1964; Barker, 1977). The convection-dispersion model (Aronofsky and Heller, 1957) was confirmed to be incapable of reproducing the asymmetrical effluent-concentration histories of core-flood experiments (Coats and Smith, 1964; Barker, 1977; Zhang, 2014).

Deans (1963) proposed a capacitance model for single-phase flow, in which the pore volume was divided into the flowing and bypassed fractions. The longitudinal convection occurred only in the flowing fraction. Effective mass transfer coefficients were used to model the local transverse mass flux between the two regions. Coats and Smith (1964) included the longitudinal dispersion for the flow fraction on the basis of the capacitance model of Deans

(1963). The dispersion–capacitance model was successful in matching the asymmetrical effluent–concentration histories of core–flood experiments. The key dimensionless groups in the dispersion–capacitance model are flowing fraction, Péclet number, and Damköhler number. Damköhler number is the dimensionless mass–transfer rate expressed as a ratio of characteristic times for transverse mass transfer and longitudinal convection (Dai and Orr, 1987). The dispersion–capacitance model was extended and applied to study various non–uniform flow problems (Salter and Mohanty, 1982; Dai and Orr, 1987; Smith and Jikich, 1994; Nguyen et al., 2009). However, it has not yet been applied in compositional reservoir simulation.

Reservoir simulation can consider explicitly the level of heterogeneity at the scale of grid blocks and greater. However, modeling of capacitance flow behavior caused by sub–grid physics is challenging in reservoir simulation. The oil bypassing caused by front instability in gas floods was modeled by empirical viscous–fingering models (Koval, 1963; Todd and Longstaff, 1972; Young, 1990; Fayers et al., 1992; Blunt and Christie, 1994; Barker and Evans, 1995). However, such a model was not entirely satisfactory without the diffusion/dispersion term in large amplitude heterogeneities with a short correlation length (Fayers et al., 1992).

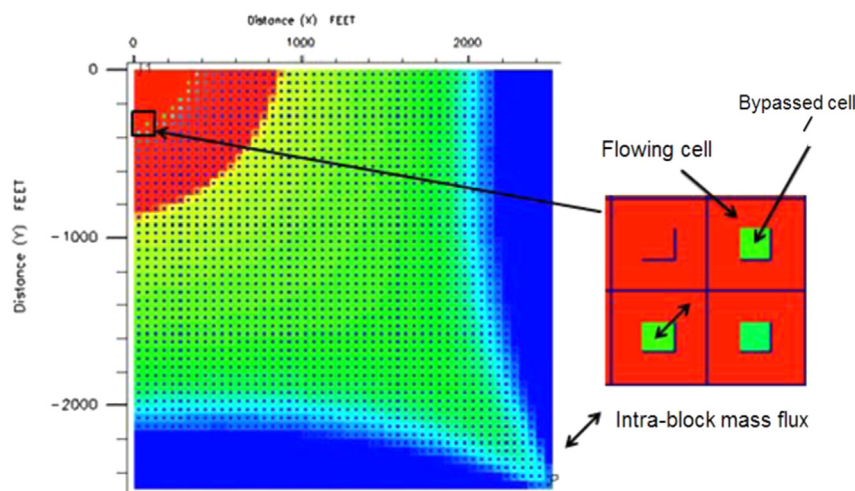
Modeling of capacitance flow behavior in compositional reservoir simulation is important since compositional simulation with a detailed geological model is computationally expensive (Salehi et al., 2013; Iranshahr et al., 2014). Various modeling methods relevant to this technical issue can be categorized into four types, although the demarcation cannot be entirely clear. A first type is the  $S_{orm}$  method, which is available in commercial simulators to model oil–bypassing (Hiraiwa and Suzuki, 2007; Lizuka et al., 2012). It excludes the immobile oil from flash calculations so that this part of oil cannot be recovered. The main disadvantage of this method is that no mass flux is allowed between the bypassed and flowing fractions. The  $S_{orm}$  method is equivalent to assigning zero to the Damköhler number in the dispersion–capacitance model. Thus, although oil bypassing can be considered, the bypassed oil is unrecoverable.

A second type is the method of Barker and Fayers (1994), which has been implemented in commercial simulators. This method uses the transport coefficients (alpha factors) to adjust the components' flux in compositional reservoir simulation. Barker et al. (2005) mentioned that this is a purely numerical concept; it is physically impossible to control the mass flux of certain components in a phase in given region of a reservoir. The alpha–factor method has been used

to retain a desired amount of residual oil in history matching for predominantly single–phase flow (Ballin et al., 2002). Pseudo relative permeabilities are required at sub–miscible conditions. The presence of more phases yields more non–linearity and severer non–uniqueness of the history matching process with the alpha factors (Barker and Fayers, 1994; Christie and Clifford, 1998; Barker et al., 2005; Bourgeois et al., 2011, 2012). Christie and Clifford (1998) combined the alpha–factor method with streamline techniques, and re–calculated the boundary conditions for certain grid blocks to deal with the potential error in multidimensional cases.

Modeling of capacitance at the sub–grid scale is difficult because the mass conservation equations used in compositional reservoir flow simulation do not consider the bypassed fraction and the mass transfer between the bypassed and flowing fractions. A third type of methods is to introduce one more continuum to represent a bypassed fraction of the reservoir volume. The mass flux between the flowing and bypassed fractions can represent the non–equilibrium behavior at the sub–grid scale. Fayers et al. (1989) proposed the dual–zone–mixing procedure, in which a gridblock is split into the contacted and bypassed zone with separate flash calculations performed. Nghiem and Sammon (1997) developed a non–equilibrium EOS compositional simulator, and introduced a transfer term to represent the diffusion process at the oil–gas interface. Compositional flow using the dual–porosity model is likely the most straightforward representation of oil bypassing and recovery of the bypassed oil (i.e., capacitance) in gas injection (Coats et al., 2007). The dual–porosity method was used to track the changes in the compositions of the trapped and mobile fluids in WAG injection (Brown et al., 2013). However, the dual–porosity model may be too time–consuming to be used for field–scale applications (Coats et al., 2007). Apart from the computational efficiency, a single–porosity model may be preferred in terms of the computational robustness; in Peng et al. (2009), for example, the dual–porosity model had convergence issues in simulating strongly heterogeneous reservoirs.

A fourth type of methods is to adjust thermodynamic properties of components to match fine–scale fluxes in a coarse–scale simulation. Camy and Emanuel (1977) applied pseudo  $K$ –values obtained from a 1–D representative model for gas flooding. It also required pseudo gas–oil relative permeability and components' correction factors to reduce the deviation of coarse–scale results from fine–scale results. Recently, a novel upscaling algorithm was developed on the basis of non–equilibrium thermodynamics



**Fig. 1.** Schematic of 2-D dual–porosity flow (DPF). Each grid block consists of the flowing and bypassed fractions. The bypassed fraction does not contribute to the longitudinal convection. The intra–block mass flux allows for the gradual migration of the bypassed oil to the flowing fraction.

(Iranshahr et al., 2014). Phase-equilibrium constraints were adjusted to correct the difference in phase behavior between the coarse- and fine-scale models. The thermodynamically-consistent alpha-factor method was then developed using their non-equilibrium approach to upscale near-miscible gas injection processes (Salehi et al., 2013).

This paper presents a two-step method, which combines the third and fourth types of methods, to efficiently model the sub-grid-scale capacitance by use of the conventional compositional simulation. The first step is to quantify capacitance flow behavior in a reservoir by use of the dual-porosity flow (DPF) model with two dimensionless groups. The second step is to correct the fluid model used in the simulation for the quantified capacitance flow behavior using a flow-based fluid characterization method. Case studies are presented to show that SPF with the two-step method can quantitatively reproduce capacitance flow behavior present in core floods and fine-scale simulations. The main novelty of the research lies in the way of representing capacitance flow behavior by controlling components' in-situ propagation through EOS-related parameters.

## 2. Quantification of capacitance flow behavior by use of dual-porosity flow

This section describes dual-porosity flow (DPF) and its application for capturing capacitance flow behavior in heterogeneous fine-scale simulations. Capacitance flow behavior occurs when the oil held in the bypassed (slow-flow or stagnant) region is gradually migrated to the flowing (fast-flow) region (Coats and Smith, 1964; Barker, 1977). Modeling of capacitance flow behavior at the sub-grid scale is difficult in single-porosity flow (SPF) simulation due to the local equilibrium assumption within individual grid blocks.

One way to capture such flow behavior is to use DPF simulation (Coats et al., 2007), where the primary- and secondary-pore systems represent the flowing and bypassed fractions, respectively. Oil in the flowing fraction is directly displaced by the injectant. The bypassed fraction has no contribution to the longitudinal convection. The two fractions have intra-block mass flux in the transverse direction within individual grid blocks. The DPF model is capable of representing the flow characteristics of the dispersion-capacitance model, since the bypassed oil held up in the secondary-pore volume (the bypassed fraction) is gradually migrated to the primary-pore volume (the flowing fraction) through intra-block mass flux. Fig. 1 schematically shows a 2-D DPF model.

**Table 1**  
Reservoir properties for 1-D dual porosity simulation.

Dimensions (F*/B*)	2 × 900 × 50 ft <sup>3</sup> /2 × 100 × 50 ft <sup>3</sup>
Number of grid blocks	500 × 2 × 1
Porosity	0.3
Permeability (F*/B*)	2000 md (X,Z), 2000 md(Y)/0.0 md(X,Z), 0.2 md (Y)
Reservoir pressure	1015.27 psia
Reservoir temperature	158°F
Injection pressure	1025.27 psia
Production pressure	1015.27 psia
Relative permeability model	Corey
Residual saturation (Oil/Gas)	0.24/0.0
Endpoint relative permeability (Oil/Gas)	1.0/0.6
Exponent (Oil/Gas)	2.1/1.8
Initial saturation (Oil/Gas)	1.0/0.0
Molecular diffusion coefficients in oil phase (C <sub>1</sub> /C <sub>2</sub> /C <sub>10</sub> )	0.002575/0.001465/0.000625 ft <sup>2</sup> /day
Molecular diffusion coefficients in gas phase (C <sub>1</sub> /C <sub>2</sub> /C <sub>10</sub> )	25.75/14.65/6.25 ft <sup>2</sup> /day
*F: Flowing grid block; *B: Bypassed grid block.	

### 2.1. Material balance equations

A DPF model for capturing capacitance flow behavior can be explained by comparing material balances applied to SPF and DPF. The molar balance for component *i* for a grid block with volume *V* and surface area *S* in SPF is

$$\frac{d}{dt} \int_V \left( \varphi \sum_{j=1}^{n_p} x_{ij} \rho_j S_j \right) dV + \int_S \sum_{j=1}^{n_p} \left[ \vec{n} \cdot (x_{ij} \rho_j \vec{U}_j) \right] dA = 0 \quad (1)$$

where  $i=1, 2, \dots, n_c$ , and  $j=1, 2, \dots, n_p$ .  $n_c$  and  $n_p$  are the numbers of components and phases, respectively. The first term is the accumulation term, and the second term is the convective flux term. The physical diffusion/dispersion term is neglected in the equation. Symbols are defined in the nomenclature section.

Suppose that grid blocks are grouped into a coarse-scale grid block with volume  $V_C$  and surface area  $S_C$  (i.e.,  $V_C > V$ ). This grid block consists of the flowing and bypassed fractions; that is, a dual-porosity model is applied. The volume and surface area are split into two fractions;  $V_{CF}$  and  $S_{CF}$  for the flowing fraction and  $V_{CB}$  and  $S_{CB}$  for the bypassed fraction. Then, the molar balance for component *i* for this coarse-scale grid block is

$$\frac{d}{dt} \left[ \int_{V_{CF}} \left( \varphi \sum_{j=1}^{n_p} x_{ij} \rho_j S_j \right) dV + \int_{V_{CB}} \left( \varphi \sum_{j=1}^{n_p} x_{ij} \rho_j S_j \right) dV \right] + \int_{S_{CF}} \sum_{j=1}^{n_p} \left[ \vec{n} \cdot (x_{ij} \rho_j \vec{U}_j) \right] dA = 0. \quad (2)$$

The flux term is only for the flowing fraction since the bypassed fraction does not contribute to the inter-block flux.

The molar balance for component *i* for the bypassed fraction of the coarse-scale grid block ( $V_{CB}$ ) is

$$\frac{d}{dt} \int_{V_{CB}} \left( \varphi \sum_{j=1}^{n_p} x_{ij} \rho_j S_j \right) dV - \int_{S_{CB}} \sum_{j=1}^{n_p} \left( \vec{n} \cdot \vec{q}_{ij}^T \right) dA = 0, \quad (3)$$

where  $\vec{q}_{ij}^T$  in the second term is the molar flux vector of component *i* in phase *j* from the flowing fraction to the bypassed fraction within this coarse-scale grid block. The positive direction

**Table 2**  
Properties for three-component n-alkane mixtures.

	Oil (mole fraction)	Gas (mole fraction)	Molecular weight (g/mol)	T <sub>c</sub> (°F)	P <sub>c</sub> (psia)	ω	Critical volume (ft <sup>3</sup> /lb-mol)
C <sub>1</sub>	0.2	0.0	16.043	-116.590	667.20	0.0080	1.59
C <sub>2</sub>	0.0	1.0	30.070	90.050	708.35	0.0980	2.37
C <sub>10</sub>	0.8	0.0	142.285	644.620	321.78	0.5032	9.66

for the intra-block flux was defined merely for a notational convenience. Using Eqs. (2) and (3), the molar balance of component  $i$  for the flowing fraction of the coarse-scale grid block ( $V_{CF}$ ) is written as

$$\frac{d}{dt} \int_{V_{CF}} \left( \varphi \sum_{j=1}^{n_p} x_{ij} \rho_j S_j \right) dV + \int_{S_{CF}} \sum_{j=1}^{n_p} [\vec{n} \cdot (x_{ij} \rho_j \vec{U}_j)] dA + \int_{S_{CB}} \sum_{j=1}^{n_p} (\vec{n} \cdot \vec{q}_{ij}^T) dA = 0. \quad (4)$$

The DPF model given in Eq. (4) will be able to reproduce the capacitance flow behavior that is present in the fine-scale model given in Eq. (1), if Eq. (4) matches the following balance equation for the group of fine-scale grid blocks:

$$\frac{d}{dt} \int_{V_C} \left( \varphi \sum_{j=1}^{n_p} x_{ij} \rho_j S_j \right) dV + \int_{S_C} \sum_{j=1}^{n_p} [\vec{n} \cdot (x_{ij} \rho_j \vec{U}_j)] dA = 0. \quad (5)$$

The net molar fluxes out of volume  $V_C$  in the DP and SP models (i.e., the second terms of Eqs. (4) and (5)) become identical if

$$\frac{d}{dt} \int_{V_C} \left( \varphi \sum_{j=1}^{n_p} x_{ij} \rho_j S_j \right) dV = \frac{d}{dt} \int_{V_{CF}} \left( \varphi \sum_{j=1}^{n_p} x_{ij} \rho_j S_j \right) dV + \int_{S_{CB}} \sum_{j=1}^{n_p} (\vec{n} \cdot \vec{q}_{ij}^T) dA. \quad (6)$$

Eq. (6) indicates two important parameters for reproducing the coarse-scale flow behavior in the fine-scale SPF (i.e., Eq. (5)) by use of the coarse-scale DPF (i.e., Eq. (4)). One is the flowing fraction to define  $V_{CF}$  ( $=V_C - V_{CB}$ ) in the first term of the right-hand side of Eq. (6). The other is the intra-block molar flow rate, the second term of the right-hand side of Eq. (6).

One could attempt to satisfy Eq. (6) for each of the coarse-scale grid blocks if the bypassed fractions and intra-block molar flow rates were known for the grid blocks. This is similar to the capacitance-dispersion model, where Damkhöler number can control the intra-block mass-transfer rate locally. However, such information is usually unavailable. In this research, therefore, capacitance flow behavior is characterized at the scale of flow of interest; i.e., the core scale in core floods and the well-pattern scale in reservoir simulations. Then, Eq. (6) is applied to the entire volume at the flow scale, yielding two dimensionless parameters associated with capacitance flow behavior, which are bypassed fraction ( $B$ ) and throughput ratio ( $R_T$ ) as defined below.

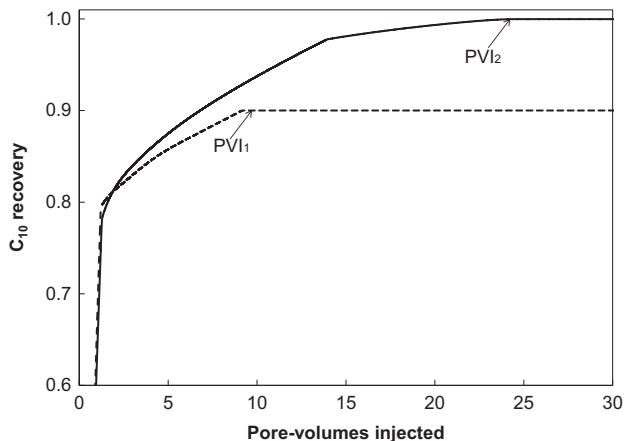


Fig. 2.  $C_{10}$  recovery predictions for 1-D DPF with/without the intra-block mass flux.  $PVI_1$  and  $PVI_2$  represent the pore-volumes injected required for the ultimate recovery without/with the intra-block mass flux in DPF, respectively. Tables 1 and 2 give the simulation conditions and fluid properties, respectively.

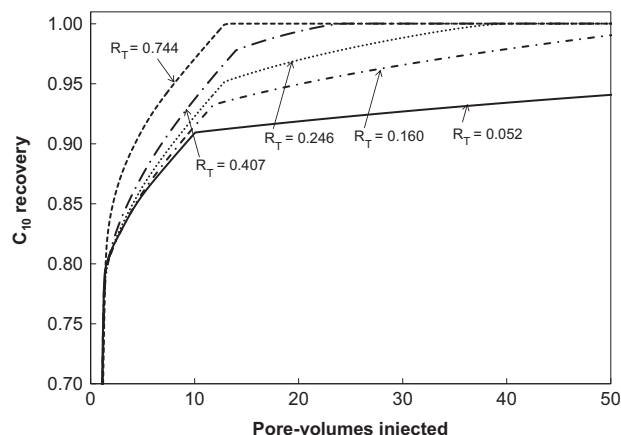


Fig. 3.  $C_{10}$  recovery predictions for 1-D DPF with different values of the throughput ratio ( $R_T$ ) from 0.052 to 0.744. Oil recoveries with different levels of capacitance are well characterized by  $R_T$  for a given bypassed fraction. Tables 1 and 2 give the simulation conditions and fluid properties, respectively. For simulations with different  $R_T$  values, the intra-block mass flux was adjusted by multiplying the diffusion coefficients by different constants as described in Zhang (2014).

## 2.2. Dimensionless groups

Bypassed fraction ( $B$ ) is  $V_B/V$ , where  $V_B$  is the bypassed volume within volume  $V$ . The same definition was used in the literature (Stern, 1991; Lange, 1998). Lange (1998) presented a correlation for estimating the bypassed fraction based on gas solubility in oil, gas density, and average molecular weight of oil. Note that a single value of  $B$  is determined to a given flow in this research since flow characterization is made globally at the flow scale.

Throughput ratio ( $R_T$ ) is defined as  $PVI_1/PVI_2$ , where  $PVI_1$  and  $PVI_2$  are the pore-volumes injected (i.e., throughputs measured in pore volumes) required for ultimate oil recovery without and with intra-block flux in the DPF, respectively.  $R_T$  is zero for no intra-block mass flux, which corresponds to SPF with the  $S_{orm}$  method.  $R_T$  becomes unity as the intra-block mass flux approaches infinity. Thus, SPF without the  $S_{orm}$  method has a limiting  $R_T$  of unity since equilibrium is instantaneously achieved within individual grid blocks with the local equilibrium assumption.

$R_T$  represents the ratio of characteristic time for intra-block mass flux and mass flux in the longitudinal direction in DPF. This is a gross form of Damkhöler number in the dispersion–capitance model; i.e.,  $R_T$  is measured for the entire flow system of interest (e.g., a core, and a reservoir volume at a drive-pattern scale), and Damkhöler number is defined locally. Unlike the traditional SPF models with and without the  $S_{orm}$  method, the DPF model can represent capacitance flow behavior with any  $R_T$  value between 0.0 and 1.0 for a given bypassed fraction.

For further description of  $R_T$ , simple 1-D simulations are used here. Table 1 shows the reservoir properties used for the 1-D DPF simulations. For the 1-D SPF simulations, the bypassed fraction is simply set to zero while keeping the reservoir dimensions. Phase behavior of the ternary system given in Table 2 is calculated using the Peng–Robinson (PR) EOS (Peng and Robinson, 1976) with the van der Waals mixing rules.  $C_2$  is injected to displace the reservoir oil consisting of 20%  $C_1$  and 80%  $C_{10}$ . The reservoir temperature and pressure are 158°F and 1015.27 psia, respectively. The pressure is fixed at 1025.27 psia for the injector and at 1015.27 psia for the producer to control the effects of pressure on phase behavior. The minimum miscibility pressure (MMP) for this displacement is calculated to be 1174.27 psia using the tie-line approach within the PVTsim software (PVTsim, 2011). Viscosity calculations are based on the Lohrenz–Bray–Clark method (Lohrenz et al., 1964). The Wilke–Chang correlation (Wilke and Chang, 1955) is used to

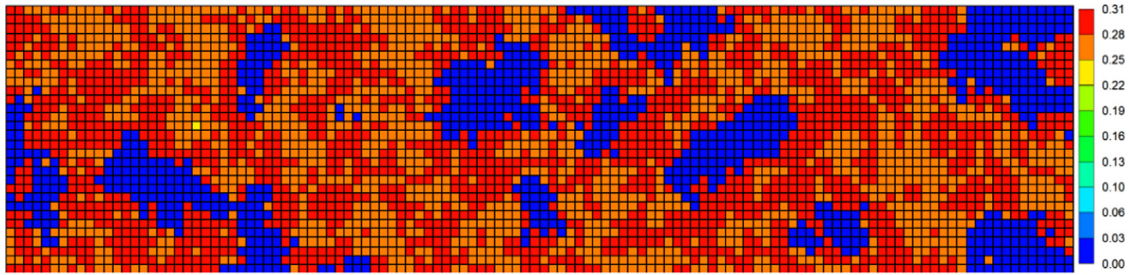


Fig. 4. Porosity distribution for the areal 2-D reservoir. The reservoir consists of 20% shale and 80% sandstone with a correlation length of 10 ft. Gas is injected along the left edge of the reservoir model.

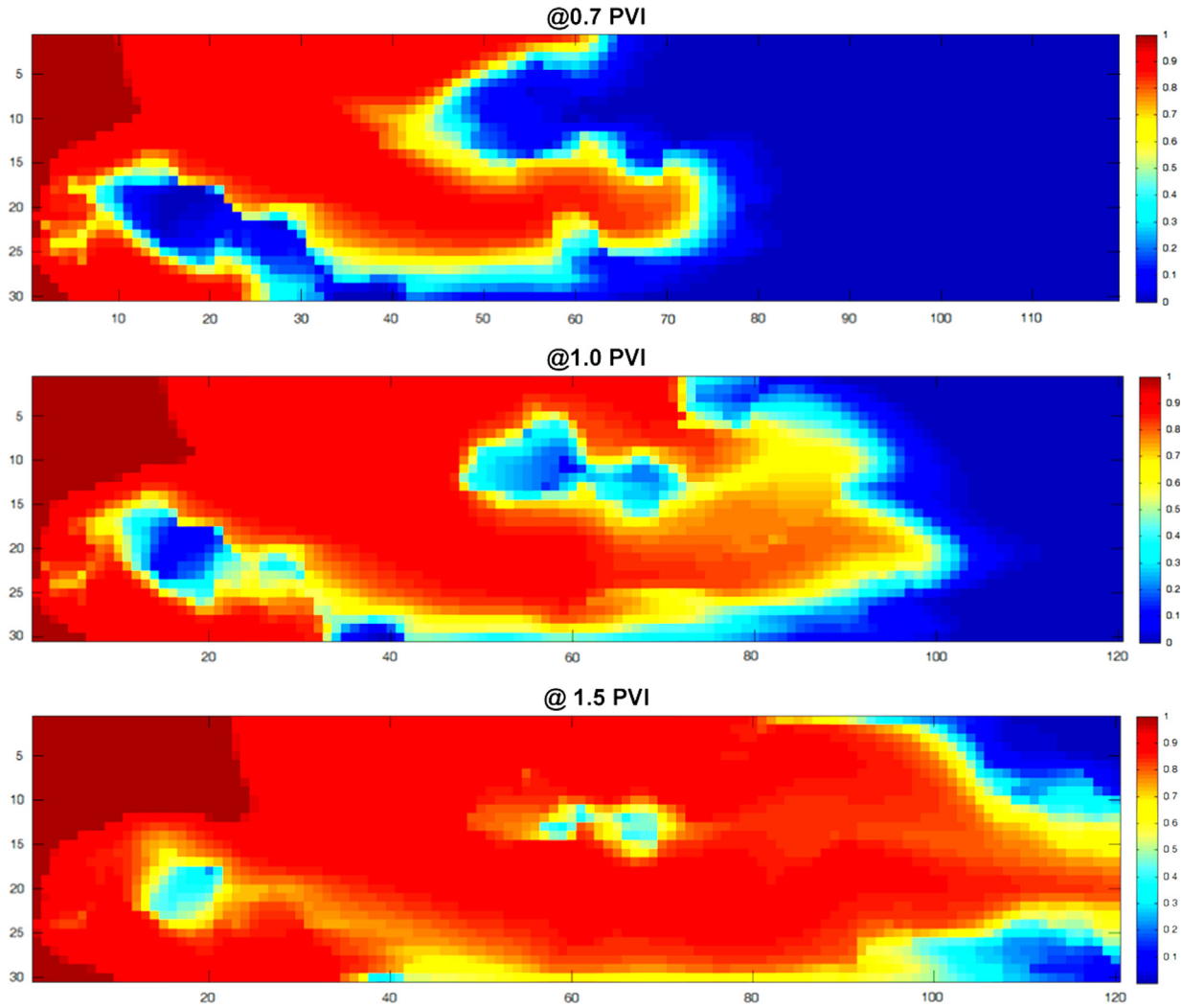


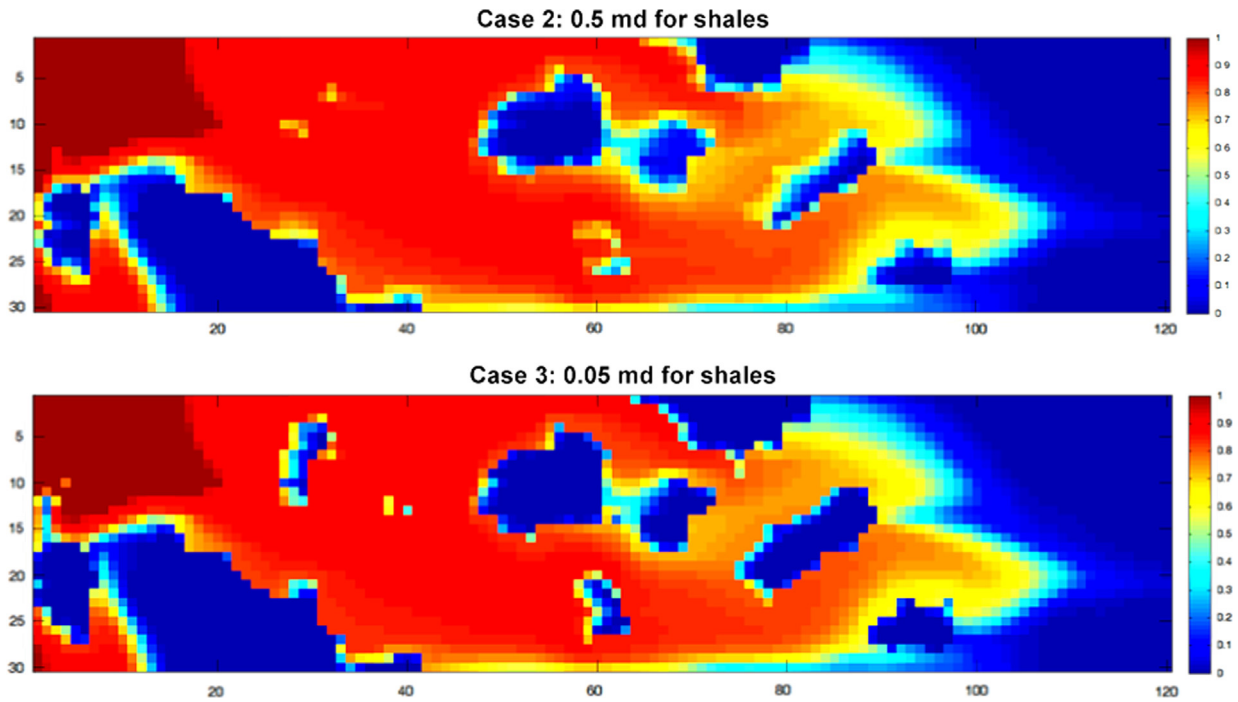
Fig. 5.  $C_2$  concentration distributions in the fine-scale simulation case 1 at different PVIs. The fluid model used is presented in Table 2. Oil bypassing due to channeling is observed at 0.7 PVI, and the bypassed oil is gradually recovered at later times.

estimate the diffusion coefficients listed in Table 1. All flow simulations in this research are performed using Eclipse 300 of Schlumberger (Eclipse 300, 2010) with the fully implicit scheme with the single-point upstream weighting for relative mobilities.

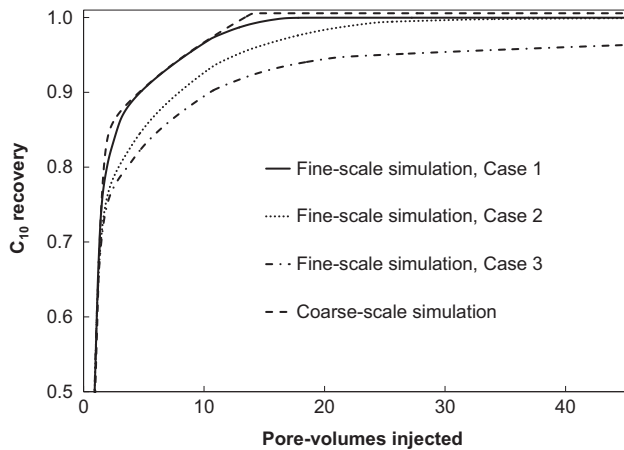
Fig. 2 shows  $C_{10}$  recoveries in the 1-D DP model with and without intra-block mass flux. In this example,  $PVI_1$  and  $PVI_2$  are 9.93 and 24.34, respectively.  $R_T$  is then calculated to be 0.408. Fig. 3 presents  $C_{10}$  recoveries with different  $R_T$  values. Oil recoveries with

different degrees of capacitance are well characterized using  $R_T$ . These different  $R_T$  values are generated by multiplying the intra-block diffusion coefficients (see Table 2) by factor C (e.g., C is zero for  $R_T=0$ ). This method of controlling  $R_T$  is also used in the subsequent sections.

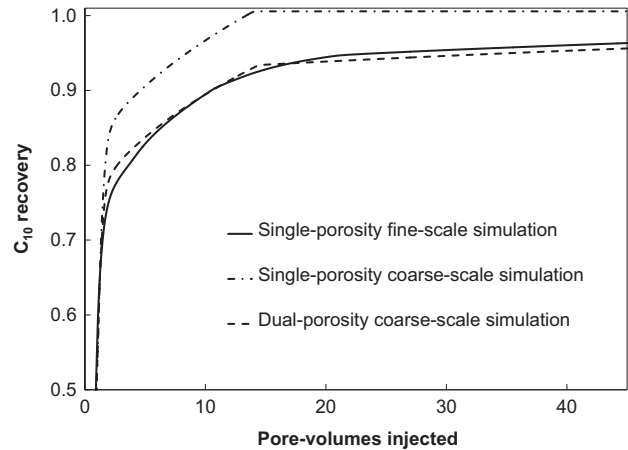
In this research, the longitudinal dispersion is controlled by the number of grid blocks using a uniform time step and grid block size. The longitudinal Péclet number is approximated to be  $2/(\Delta x_D + \Delta t_D)$



**Fig. 6.**  $C_2$  concentration distributions in the fine-scale simulation cases 2 and 3 at 1.0 PVI. The fluid model used is presented in Table 2. The oil recovery from the bypassed (or slow-flow) regions is dependent on the shale permeability that affects the mass flux between the slow-flow and fast-flow regions. This can be confirmed by comparing with case 1 (5 md for shales) given in Fig. 5.



**Fig. 7.** Oil recovery predictions for the fine-scale simulation cases 1, 2, and 3 compared with the coarse-scale simulation. The fluid model used is presented in Table 2. The permeability of the shale region greatly affects the oil recovery from the bypassed (slow-flow) region. The coarse-scale simulation overestimates the oil recovery because it cannot consider the sub-grid scale capacitance flow behavior.



**Fig. 8.** Oil recovery predictions for the fine-scale simulation case 3 and the coarse-scale DPF and SPF simulations. The fluid model used is presented in Table 2. The DPF greatly improve the recovery prediction for the coarse-scale simulation because it accommodates the sub-grid scale capacitance flow behavior. The resulting throughput ratio and bypassed fraction are 0.14 and 0.08, respectively.

in the fully implicit simulations in this research, where  $\Delta x_D$  is the dimensionless grid-block size and  $\Delta t_D$  is the dimensionless time-step size measured in pore volumes (Lantz, 1971).

### 2.3. Capacitance flow behavior in fine-scale simulation

This subsection presents capacitance flow behavior observed in example fine-scale simulations. The DPF is then used to quantify the capacitance flow behavior.

The areal 2-D reservoir model consists of 120 grid blocks in the  $x$  direction and 30 grid blocks in the  $y$  direction. The dimensions of each grid block are  $1.0 \times 1.0 \times 1.0 \text{ ft}^3$ . The porosity field has been generated by use of S-GeMS ver. 2.1 (S-GeMS V2.1), assuming a bimodal distribution consisting of 80% sandstone and 20% shale.

The average porosity is 0.280 for sandstone and 0.019 for shale. The variance is 0.00012 for sandstone and 0.00002 for shale. The average porosity is 0.227, and the variance is 0.0118 for the 2-D reservoir model. The correlation length is 10.0 ft in the  $x$  and  $y$  directions. The porosity distribution used is shown in Fig. 4. The shales are shown in blue. Gas is injected along the left edge, and oil is produced along the right edge of the reservoir model.

Permeability distributions are calculated using the following widely-used correlation (Leung and Srinivasan, 2011; Leung and Srinivasan, 2012):  $K = e\phi^f$ , where  $K$  is permeability in mD and  $f$  is 1.2 in this research. Different values are used for  $e$  as follows:

Case 1.  $e = 1200$  mD for sandstone and shale

Case 2.  $e = 1200$  mD for sandstone and 120 mD for shale

Case 3.  $e = 1200$  mD for sandstone and 12 mD for shale.

The three cases have the same porosity distribution and sandstone permeability.

The ternary fluid system given in Table 2 is used again. The reservoir temperature and pressure are 158°F and 1015.27 psia, respectively.  $C_2$  is injected into the heterogeneous reservoir at partially miscible conditions. The oil and gas relative permeabilities are taken from Bardon et al. (1994).

Fig. 5 presents the  $C_2$  concentration distributions for case 1 at different PVI. The injected  $C_2$  channels through the sandstone, and the oil near the shales is bypassed as shown at 0.7 PVI. The bypassed oil is gradually recovered because of the mass flux between the bypassed and flowing regions as shown at later PVI. The recovery of bypassed oil is relatively fast in case 1 because of the relatively high permeability assigned to the shales (5 mD). Gas breakthrough occurs after 1.0 PVI because of the significant volume change on mixing in this fluid system.

$C_2$  concentration distributions for cases 2 and 3 at 1.0 PVI are presented in Fig. 6. Recovery of the bypassed oil depends substantially on the shale permeability used, because it controls the mass flux between the bypassed and flowing regions. For case 3 with the lowest shale permeability (0.05 mD), the bypassed oil was clearly observed even at 10.0 PVI in Figure 3.24 of Zhang (2014). Thus, modeling of bypassed oil recovery can greatly affect oil recovery predictions in gas injection simulation.

As well known in the literature, simplistic upscaling of a fine-scale reservoir model results in erroneous gas-flooding simulation results (Barker and Fayers, 1994). To confirm this, the fine-scale model was upscaled into a coarse-scale reservoir model with  $12 \times 3$  grid blocks. The porosities of the coarse-scale model were calculated by the arithmetic mean in the corresponding regions of the fine-scale model. The permeability distribution for the coarse-scale model was then calculated by use of the equation  $K = 1200\phi^{1.2}$  based on the upscaled porosity distribution.

Fig. 7 presents  $C_{10}$  recovery predictions from the fine-scale simulation cases 1, 2, and 3 along with the coarse-scale simulation with the upscaling presented previously. The simplistic upscaling gives a reasonable prediction only if the level of capacitance is insignificant (i.e., case 1). It substantially overestimates the oil recovery for cases 2 and 3.

As shown in Section 2.1, one way to improve the issues associated with the subgrid-scale capacitance is to use the DPF simulation. A DPF model with the coarse-scale reservoir model was fitted to the fine-scale simulation case 3 with the bypassed fraction of 0.08 and throughput ratio of 0.14. Fig. 8 shows that the resulting DPF model agrees well with the fine-scale simulation in terms of  $C_{10}$  recovery. The DPF parameters, such as  $B$  and  $R_T$ , are useful to quantify the capacitance flow behavior. The DPF parameters have been successfully applied to other cases, such as core floods, capillary dominant cases, and viscous dominant cases.

The uniform distribution of a bypassed fraction is sufficient to reproduce oil recovery as a function of throughput, as shown above. However, distribution of different bypassed fractions can be helpful in reproducing local concentration distributions by use of the coarse-scale DPF model. A detailed explanation of how to distribute different bypassed fractions can be found in Zhang (2014).

### 3. Flow-based fluid characterization

Section 2 presented that key characteristics of a given capacitance flow can be quantified by DPF with single average values of bypassed fraction ( $B$ ) and  $R_T$ . However, it may be unacceptably time-consuming to run a DPF model for field-scale applications (Coats et al., 2007). Convergence issues may occur more often with

highly heterogeneous reservoir models (Peng et al., 2009). Efficient modeling of capacitance flow behavior is a long-existing technical issue as pointed out by Burger et al. (1994).

As shown in Section 2, oil recovery with capacitance flow behavior takes more throughput than without it to achieve the same level of oil recovery. This was the fundamental idea used in the definition of  $R_T$ , which successfully quantifies the delayed oil recovery. Efficient modeling of sub-grid capacitance using a SPF model inevitably requires adjustment of components' propagation with respect to throughput in reservoir simulation. It is well-understood from the gas injection theory (Orr, 2007) that components' properties affect the dimensionless velocities (i.e., distances traveled at one pore volume injected) along the composition path for a partially miscible oil displacement by gas. Thus, one way to control components' propagation rates in reservoir simulation is to adjust their properties in the fluid model used.

The objective of flow-based fluid characterization in this research is to represent oil recovery that takes additional throughput in the presence of capacitance by adjusting components' properties in the fluid model used. The method attempts to minimize the deviation from the original fluid model of interest in terms of phase behavior predictions. Ideally, such deviation should be kept within the level of uncertainty inherent in characterization of reservoir oils.

#### 3.1. Methodology

Properties are adjusted for some of the oil components; typically heavy pseudo components representing a plus fraction (e.g.,  $C_{7+}$ ). Each of adjusted components is split into two components; one with the original properties and the other with altered properties. This splitting is useful to retain the well-defined limiting properties in the case of no capacitance (i.e.,  $R_T = 0$ ).

Adjustment of components' properties considers representation of DPF (Eqs. (2) or (4)) by use of SPF with the same coarse-scale grid blocks (with  $V_C$  and  $S_C$ ), but with an altered fluid model. Here, it is assumed that capacitance flow behavior in the fine-scale model has been already reproduced by the coarse-scale DPF model (Eqs. (2) or (4)) by a certain set of bypassed fraction and  $R_T$ .

Oil component  $i$  is split into components "oi" and "hi" while retaining the total mass of the fluid of interest. Components oi and hi have the same molecular weight as the original oil component  $i$ . Component oi also has the same properties as the original oil

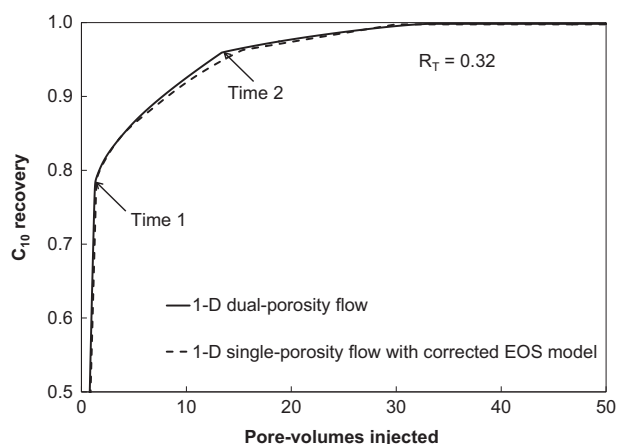


Fig. 9.  $C_{10}$  recovery predictions for the 1-D DPF and 1-D SPF with a corrected fluid model. Time 1 is the breakthrough time. Time 2 is the PVI when the evaporation wave in the flowing region reaches the outlet. After Time 2, the recovery comes from the bypassed oil. Tables 1 and 2 present the simulation conditions and fluid properties used, respectively.



component  $i$ . However, component  $hi$  has properties of a heavier component than component  $oi$  (and the original oil component  $i$ ). The molar balance of component  $i$ , which now consists of  $oi$  and  $hi$ , for the coarse-scale grid block (with  $V_C$  and  $S_C$ ) is

$$\frac{d}{dt} \int_{V_C} \left[ \varphi \sum_{j=1}^{n_p} (x_{ojj} + x_{hij}) \rho_j S_j \right] dV + \int_{S_C} \sum_{j=1}^{n_p} \left\{ \vec{n} \cdot [(x_{ojj} + x_{hij}) \rho_j \vec{U}_j] \right\} dA = 0. \quad (7)$$

The molar fluxes out of volume  $V_C$  in Eqs. (4) and (7) become identical if

$$\frac{d}{dt} \int_{V_C} \left[ \varphi \sum_{j=1}^{n_p} (x_{ojj} + x_{hij}) \rho_j S_j \right] dV = \frac{d}{dt} \int_{V_{CF}} \left( \varphi \sum_{j=1}^{n_p} x_{ij} \rho_j S_j \right) dV + \int_{S_{CB}} \sum_{j=1}^{n_p} \left( \vec{n} \cdot \vec{q}_{ij}^T \right) dA. \quad (8)$$

Using Eq. (3), it is easy to show that Eq. (8) is equivalent to

$$\frac{d}{dt} \int_{V_C} \left[ \varphi \sum_{j=1}^{n_p} (x_{ojj} + x_{hij}) \rho_j S_j \right] dV = \frac{d}{dt} \left[ \int_{V_{CF}} \left( \varphi \sum_{j=1}^{n_p} x_{ij} \rho_j S_j \right) dV + \int_{V_{CB}} \left( \varphi \sum_{j=1}^{n_p} x_{ij} \rho_j S_j \right) dV \right] \quad (9)$$

Properties of component  $hi$  are adjusted to approximately satisfy Eq. (9). The right-hand side of Eq. (9) shows that oil component  $i$  is held in  $V_{CB}$  that does not contribute to interblock fluxes. The left-hand side attempts to represent this capacitance by making the apparent properties of component  $i$  less volatile through component  $hi$ .

The thermodynamic model used in this research is the PR EOS with the van der Waals mixing rules. It is assumed that only one EOS fluid model is used for a given reservoir simulation. The attraction parameters of components  $hi$ 's are adjusted through the attraction-parameter index  $\gamma_a$  defined as

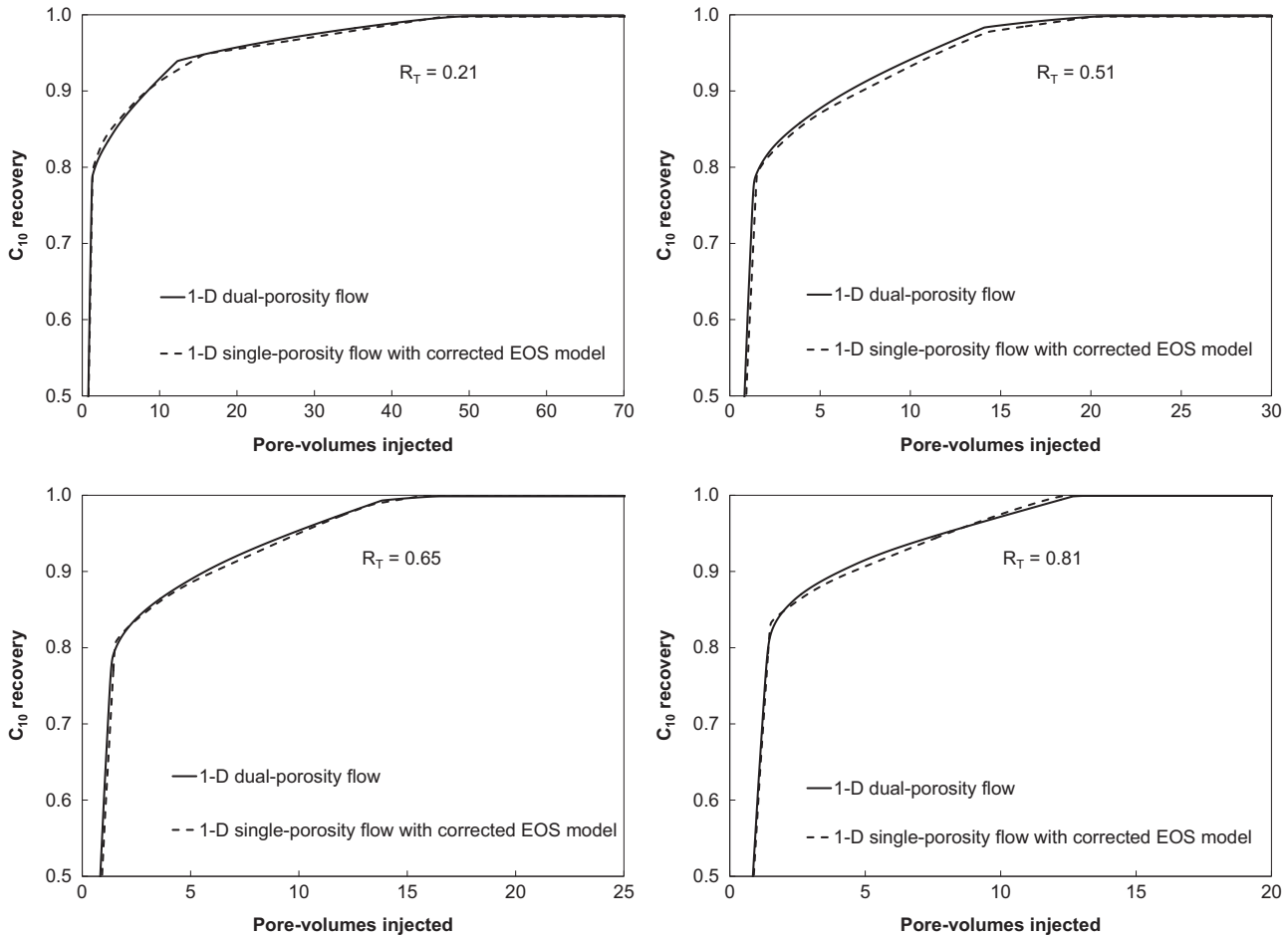
$$\gamma_a = (a_{hi} - a_i) / (a_{hi} + a_i), \quad (10)$$

where  $a_{hi}$  and  $a_i$  are the attraction parameter of component  $hi$  and that of component  $i$ , respectively. The  $\gamma_a$  index is zero when  $a_{hi} = a_i$ , and tends to unity as  $a_{hi}$  becomes higher. Kumar and Okuno (2013) described the behavior of the PR attraction parameter for different carbon numbers and different levels of aromaticity. It monotonically increases with increasing carbon number for a fixed aromaticity level. A single value of  $\gamma_a$  is uniformly applied for all  $hi$ 's in this research.

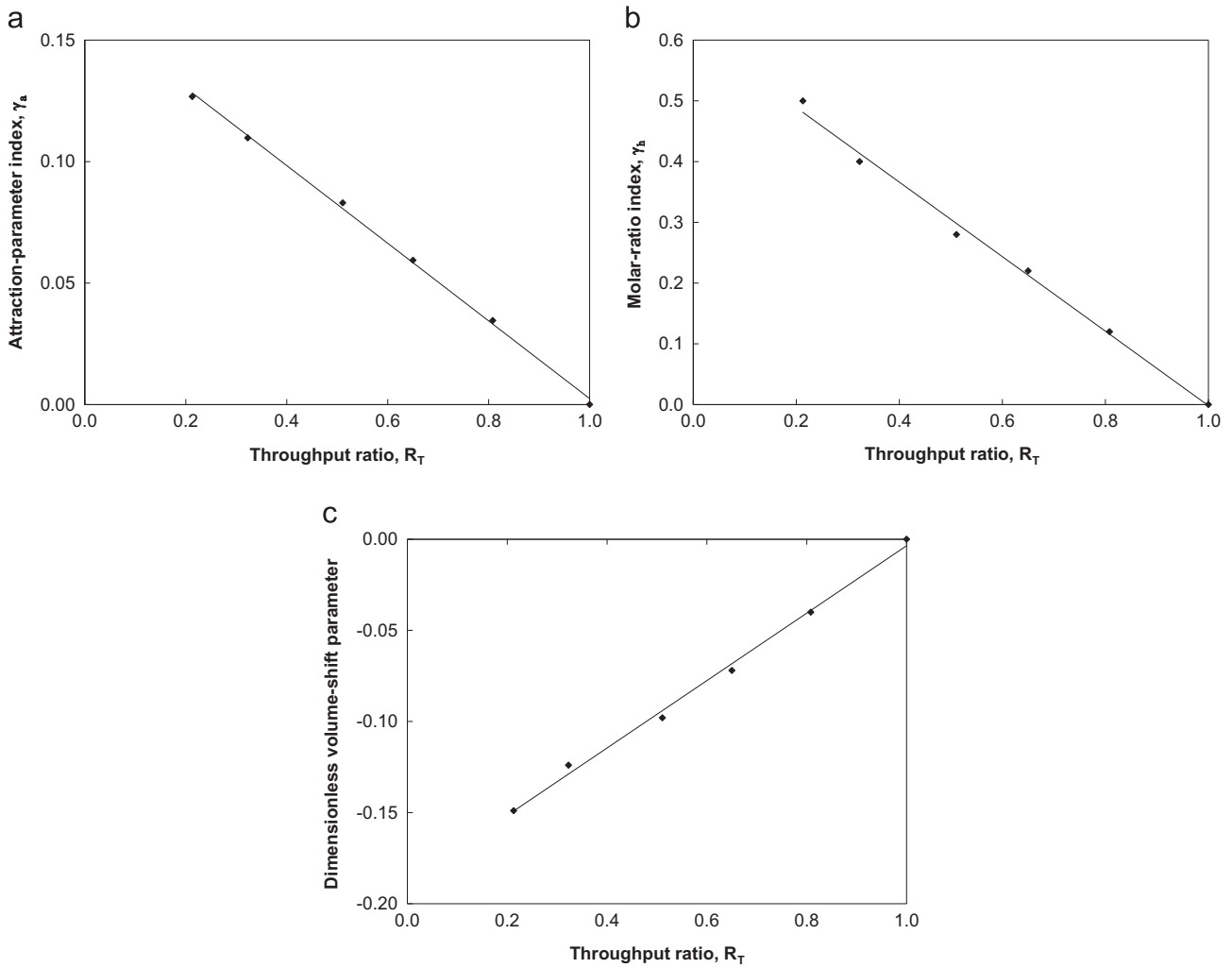
A more general approach is to adjust the attraction and covolume parameters of the PR EOS for components  $hi$ 's. However, adjustment of the attraction parameters alone has been found to be sufficient to achieve the objective of the flow-based fluid characterization method in this paper. It is also desirable in reducing the deviation of phase behavior predictions from the original fluid model.

Once the properties of  $hi$ 's are set through  $\gamma_a$ , the amounts of  $hi$ 's relative to the original components are determined by adjusting the molar-ratio index  $\gamma_h$  defined as

$$\gamma_h = Z_{hi} / (Z_{oi} + Z_{hi}) = Z_{hi} / Z_i. \quad (11)$$



**Fig. 10.**  $C_{10}$  recovery predictions for 1-D DPF and 1-D SPF simulations with a corrected fluid model. The throughput ratios for the 1-D DPF simulations are 0.21, 0.51, 0.65, and 0.81. Tables 1 and 2 present the simulation conditions and fluid properties used, respectively. For simulations with different throughput ratios, the intra-block mass flux was adjusted by multiplying the diffusion coefficients by different constants as described in Zhang (2014).



**Fig. 11.** Relationship between the throughput ratio ( $R_T$ ) and three adjustment parameters: (a) Attraction-parameter index ( $\gamma_a$ ) decreases with increasing  $R_T$ , (b) Molar-ratio index ( $\gamma_h$ ) decreases with increasing  $R_T$ , and (c) Dimensionless volume-shift parameter ( $c_{Dh}$ ) increases with  $R_T$ .

In Eq. (11),  $z_i$  is the mole fraction of component  $i$ , which is the summation of the mole fractions of components  $oi$  and  $hi$ ,  $Z_{oi}$  and  $Z_{hi}$ . The  $\gamma_h$  index is zero when  $Z_{hi}=0$ , and tends to unity as  $Z_{hi}$  becomes higher. A single value of  $\gamma_h$  is uniformly applied for all adjusted components in this research.

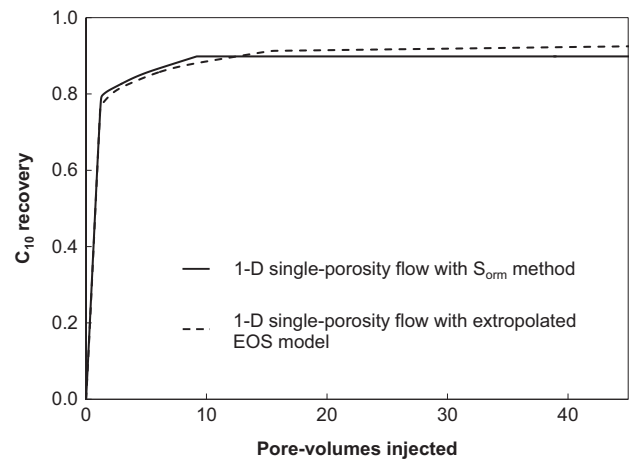
Use of  $\gamma_h > 0$  with  $\gamma_a \neq 0$  gives the flexibility in compositional phase behavior predictions, which enables to control components' propagation in reservoir simulation. However, it also alters volumetric phase behavior (i.e., phase densities), and viscosity predictions through conventional viscosity models, such as the one by Lohrenz et al. (1964) as used in this research. It is possible to retain volumetric and viscosity predictions by use of volume shift. The dimensionless volume-shift parameter of component  $hi$  is

$$c_{Dh} = c_{hi}/b_i, \tag{12}$$

where  $c_{hi}$  is the volume-shift parameter of component  $hi$ , and  $b_i$  is the covolume parameter of component  $i$ . A single value of  $c_{Dh}$  is uniformly applied for all introduced components  $hi$ 's in this research.

### 3.2. Algorithm

To explain the algorithm for the flow-based fluid characterization method, the example DPF with the ternary fluid system presented previously is used. Tables 1 and 2 give the simulation conditions and fluid properties used, respectively. The DPF with a throughput ratio of



**Fig. 12.**  $C_{10}$  recovery prediction for the SPF simulation with the  $S_{orm}$  method is compared to that with a corrected fluid model extrapolated to  $R_T$  of zero. The linear extrapolation of the adjustment parameters to  $R_T$  of zero (see Fig. 11) gives reasonable representation of the limiting capacitance behavior, where the bypassed oil is unrecoverable as in the  $S_{orm}$  method. Tables 1 and 2 present the simulation conditions and fluid properties used, respectively.

0.32 is considered, for which Fig. 9 presents the oil recovery prediction. Time 1 is the PVI at the breakthrough, and Time 2 is when the evaporation wave reaches the outlet in the flowing fraction.

The first step is to split  $C_{10}$  into  $C_{o10}$  and  $C_{h10}$ . A value of  $\gamma_a$  is estimated by matching the  $C_{10}$  recovery after Time 2. In this example,  $\gamma_a$  is 0.11. The dimensionless volume-shift parameter for  $C_{h10}$  is determined to retain the original oil density. The dimensionless volume-shift parameter for the injected gas component  $C_2$  can be also adjusted to retain the oil recovery at the breakthrough time (Time 1 in Fig. 9). The last step is to determine  $\gamma_h$  to match the oil recovery between Time 1 and Time 2. For this selected case,  $\gamma_h$  is 0.4. Fig. 9 shows that the SPF with the corrected fluid model accurately matches the recovery prediction of the DPF model with a throughput ratio of 0.32.

A step-wise description of the algorithm for a general multi-component case is as follows:

Step 1. Split the pseudo components (representing the plus fraction) in the fluid model of interest into two fractions; one with the original properties and the other with altered properties. That is, pseudo component  $i$  is split into components “oi” and “hi.” The mass of component  $i$  is retained;  $Z_i = Z_{oi} + Z_{hi}$ , and molecular weights of oi and hi are the same as that of  $i$ .  
Step 2. Adjust the  $\gamma_a$  index by matching the oil recovery prediction from DPF after Time 2, when the behavior of delayed oil recovery is easily captured.

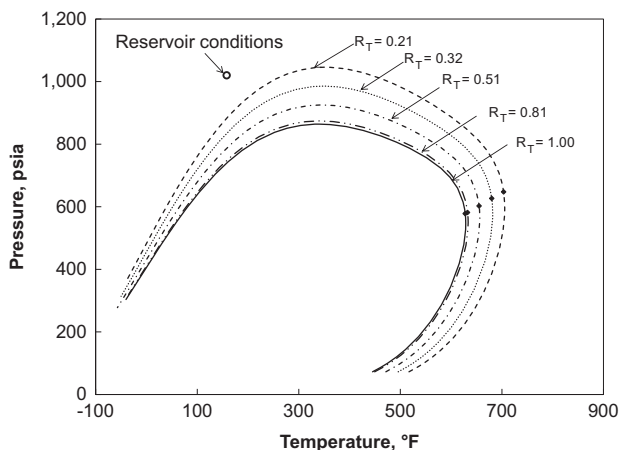


Fig. 13. Two-phase envelopes predicted for the oil (given in Table 2) with corrected fluid models with different throughput-ratio ( $R_T$ ) values from 0.21 to 1.0. The deviation of the two-phase envelope increases with decreasing  $R_T$ .

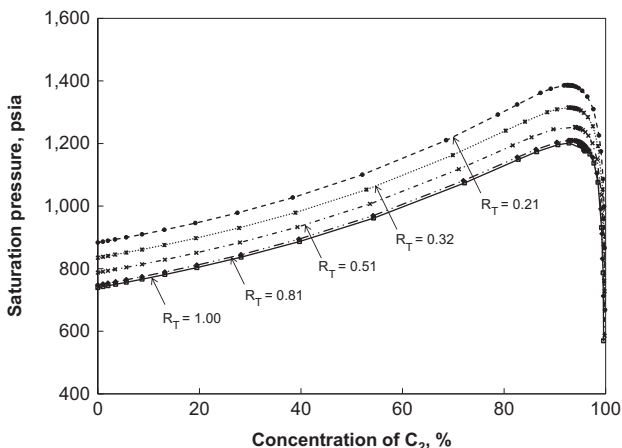


Fig. 14. Saturation pressure predictions for the oil- $C_2$  mixtures with corrected fluid models with different throughput-ratio ( $R_T$ ) values from 0.21 to 1.0. The predicted saturation pressures deviate from the original one ( $R_T$  of 1.0) as  $R_T$  is decreased. Table 2 gives the fluid model parameters used.

Step 3. Adjust the  $c_{Dh}$  to match the original oil density and viscosity.

Step 4. Adjust the volume-shift parameters of injected gas components to match the oil recovery at breakthrough (Time 1).

Step 5. Adjust the  $\gamma_h$  index to match the oil recovery between Times 1 and 2.

This algorithm has been used successfully for various cases, part of which will be presented in Section 4.

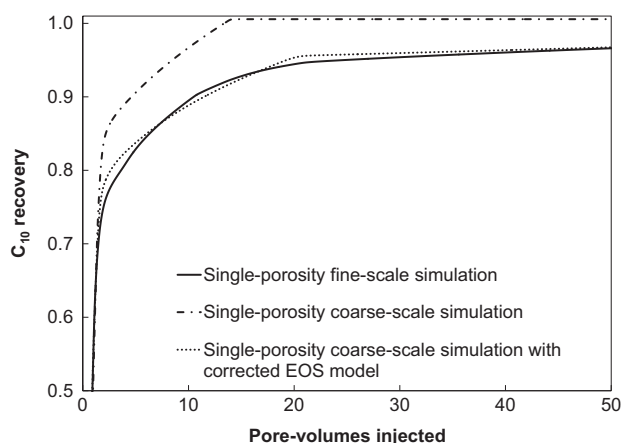
### 3.3. Relationship between the adjustment parameters and $R_T$

The three main adjustment parameters,  $\gamma_a$ ,  $\gamma_h$ , and  $c_{Dh}$ , exhibit monotonic trends with respect to  $R_T$ . Interestingly, applications of the characterization method for various different cases have indicated that their trends are somewhat linear with respect to  $R_T$ , when  $R_T$  is not close to zero.

To show this, the algorithm is applied to the previously-mentioned DPF with the ternary fluid system, but with different  $R_T$  values, 0.21, 0.51, 0.65, and 0.81. Tables 1 and 2 give the simulation conditions and fluid properties used, respectively. Fig. 10 presents that the  $C_{10}$  recovery is successfully reproduced by SPF with a corrected fluid model for each of the different  $R_T$ 's. Fig. 11 shows the resulting values of  $\gamma_a$ ,  $\gamma_h$ , and  $c_{Dh}$  at different  $R_T$  values. Both  $\gamma_a$  and  $\gamma_h$  monotonically decrease with increasing  $R_T$ . These adjustment parameters become zero at  $R_T=1$  because there is no need to split the oil components in such a case. The oil density from a corrected fluid model will be greater than the original density when  $\gamma_h$  and  $\gamma_a$  are positive. Therefore, negative values of  $c_{Dh}$  are obtained to retain the original oil density when  $R_T \neq 1$ . Fig. 11 shows that  $c_{Dh}$  monotonically increases with increasing  $R_T$ , and is zero for  $R_T$  of unity. The linear trend lines correlate well the behavior of  $\gamma_a$ ,  $\gamma_h$ , and  $c_{Dh}$  with respect to  $R_T$  in this case.

The adjustment parameters at  $R_T=0$  are estimated by extrapolating the linear trends given in Fig. 11. As mentioned in Section 2.2,  $R_T$  of zero corresponds to SPF with the  $S_{orm}$  method. Therefore, comparison of the oil recovery from the SPF with these extrapolated parameters to that from the SPF with the  $S_{orm}$  method can serve as a severe test of the linear correlations. Fig. 12 shows that at earlier PVIs, the linear extrapolations to  $R_T$  of zero give a reasonable representation of the limiting capacitance flow behavior, where the bypassed oil is unrecoverable as in the  $S_{orm}$  method. However, they deviate as PVI increases. This is because the extrapolated  $\gamma_a$  index is not high enough to represent immobile components at  $R_T$  of zero. Nevertheless, the linear correlations of  $\gamma_a$ ,  $\gamma_h$ , and  $c_{Dh}$  with respect to  $R_T$  are reasonable when  $R_T$  is not close to zero (see Fig. 11). Although these linear correlations are purely empirical within this research, the monotonic variations with respect to  $R_T$  are qualitatively consistent with the roles of the adjustment parameters in the flow-based fluid characterization method.

Linear correlations of  $\gamma_a$  and  $\gamma_h$  with respect to  $R_T$  can be useful; once values for  $\gamma_a$  and  $\gamma_h$  are obtained for a given non-zero  $R_T$  by applying the algorithm described in Section 3.2 to the capacitance flow of interest, linear correlations can be established and used for estimating  $\gamma_a$  and  $\gamma_h$  for different  $R_T$  values. It is straightforward to determine the corresponding  $c_{Dh}$  value for a given set of  $\gamma_a$  and  $\gamma_h$ , since step 3 does not require flow simulations (see Section 3.2). Therefore, although  $c_{Dh}$  has also exhibited linear correlations with respect to  $R_T$  for the cases tested (e.g., Fig. 11), we consider that the linearity of  $\gamma_a$  and  $\gamma_h$  with respect to  $R_T$  is of more fundamental importance.



**Fig. 15.**  $C_{10}$  recovery predictions in the areal 2-D heterogeneous reservoir simulations. The recovery prediction from the fine-scale simulation can be reproduced with the coarse-scale simulation when the fluid model is corrected for sub-grid scale capacitance. The coarse-scale simulation erroneously overestimates the oil recovery without correction of the fluid model. Table 2 gives the fluid properties used. The porosity distribution for the fine-scale model is given in Fig. 4.

**Table 3**  
Properties of the Shengli oil.

	Oil (mole fraction)	Gas (mole fraction)	Molecular weight (g/mol)	$T_c$ (°F)	$P_c$ (psia)	$\omega$	Critical volume (ft <sup>3</sup> /lb-mol)
N <sub>2</sub>	0.003	0.000	28.01	-232.51	492.26	0.0400	1.44
CO <sub>2</sub>	0.005	1.000	44.01	87.89	1069.80	0.2250	1.51
C <sub>1</sub>	0.244	0.000	16.04	-116.59	667.18	0.0080	1.59
C <sub>2</sub>	0.023	0.000	30.07	90.05	708.37	0.0980	2.37
C <sub>3</sub>	0.031	0.000	44.10	205.97	615.83	0.1520	3.25
C <sub>4</sub>	0.030	0.000	58.12	305.69	551.15	0.1930	4.08
C <sub>5</sub>	0.038	0.000	72.15	385.61	489.36	0.2510	4.87
C <sub>6</sub>	0.069	0.000	86.18	453.65	430.62	0.2960	5.93
PC1	0.215	0.000	122.99	775.74	510.68	0.1761	10.11
PC2	0.153	0.000	173.09	927.18	406.40	0.2776	11.94
PC3	0.114	0.000	231.28	1056.90	334.17	0.3975	14.6
PC4	0.076	0.000	350.53	1229.94	251.21	0.6096	17.38

### 3.4. Deviation of compositional phase behavior from the original fluid model

As mentioned in Section 3.1, the deviation of compositional phase behavior from the original fluid model of interest can be suppressed by not adjusting the covolume parameters. Nevertheless, compositional phase behavior is inevitably altered in the flow-based fluid characterization when  $\gamma_a \neq 0$ . There is no deviation of compositional phase behavior from the original fluid model when  $\gamma_a = 0$  at  $R_T = 1.0$ .

The ternary fluid system is used here again, to show how much deviation of the corrected fluid model from the original model occurs in terms of compositional behavior predictions for different  $R_T$  values. Fig. 13 shows two-phase envelopes predicted in  $P$ - $T$  space for the ternary oil with corrected fluid models at different  $R_T$  values. The two-phase envelope becomes greater in  $P$ - $T$  space with increasing  $R_T$ . The original bubble-point pressure is 738.6 psia at 158°F. However, it is increased to 752.6 psia, 785.5 psia, and 887.3 psia at  $R_T$ 's of 0.81, 0.51, and 0.21, respectively. The respective deviations for these  $R_T$  values are +1.9%, +6.0%, and +16.8%.

Fig. 14 presents saturation pressure predictions at 158°F for the pseudo binary of the oil and gas given in Table 2. The saturation

**Table 4**  
Reservoir properties for 1-D SPF simulation of the Shengli oil core flood.

Dimensions	0.0123 × 0.8723 × 0.8723 in <sup>3</sup>
Number of grid blocks	500 × 1 × 1
Porosity	0.1529
Permeability	19.49 md (X, Y, Z)
Reservoir pressure	2842.65/3263.36/3727.48 psia
Reservoir temperature	258.80°F
Injection rate	4.39 in <sup>3</sup> /min
Production pressure	2842.65/3263.35/3727.48 psia
Relative permeability model	Corey
Residual saturation (Oil/Gas)	0.1/0.0
Endpoint relative permeability (Oil/Gas)	1.0/0.5
Exponent (Oil/Gas)	1.5/3.0
Initial saturation (Oil/Gas)	1.0/0.0

pressure becomes systematically higher with decreasing  $R_T$ . For example, the saturation pressure for the equimolar pseudo binary mixture is 739.7 psia at  $R_T = 1.0$ . It is increased to 747.7 psia at  $R_T$  of 0.81, 787.7 psia at  $R_T$  of 0.51, and 883.4 psia at  $R_T$  of 0.21. The corresponding deviation is +1.1% at  $R_T$  of 0.81, +6.5% at  $R_T$  of 0.51, and +19.4% at  $R_T$  of 0.21. However, this level of deviation of compositional phase behavior predictions from experimental data is often observed when a cubic EOS with the van der Waals mixing rules is used with a fixed set of binary interaction parameters [for example, see Kumar and Okuno (2012) for nine different binary mixtures C<sub>1</sub>-C<sub>16</sub>, C<sub>1</sub>-C<sub>20</sub>, C<sub>2</sub>-C<sub>16</sub>, C<sub>2</sub>-C<sub>20</sub>, C<sub>2</sub>-C<sub>22</sub>, C<sub>2</sub>-C<sub>24</sub>, C<sub>6</sub>-C<sub>16</sub>, C<sub>6</sub>-C<sub>24</sub>, and C<sub>6</sub>-C<sub>36</sub>].

The MMP is calculated to be 1174.2 psia at 158°F for the original oil and gas properties given in Table 2. The MMP is 1180.9 psia at  $R_T$  of 0.81, 1214.4 psia at  $R_T$  of 0.51, and 1303.4 psia at  $R_T$  of 0.21. The corresponding deviation is +0.6% at  $R_T$  of 0.81, +3.4% at  $R_T$  of 0.51, and +11.0% at  $R_T$  of 0.21. The deviations may be within or similar to the level of uncertainties inherent to reservoir oil characterization using an EOS, depending on the level of capacitance, or  $R_T$ .

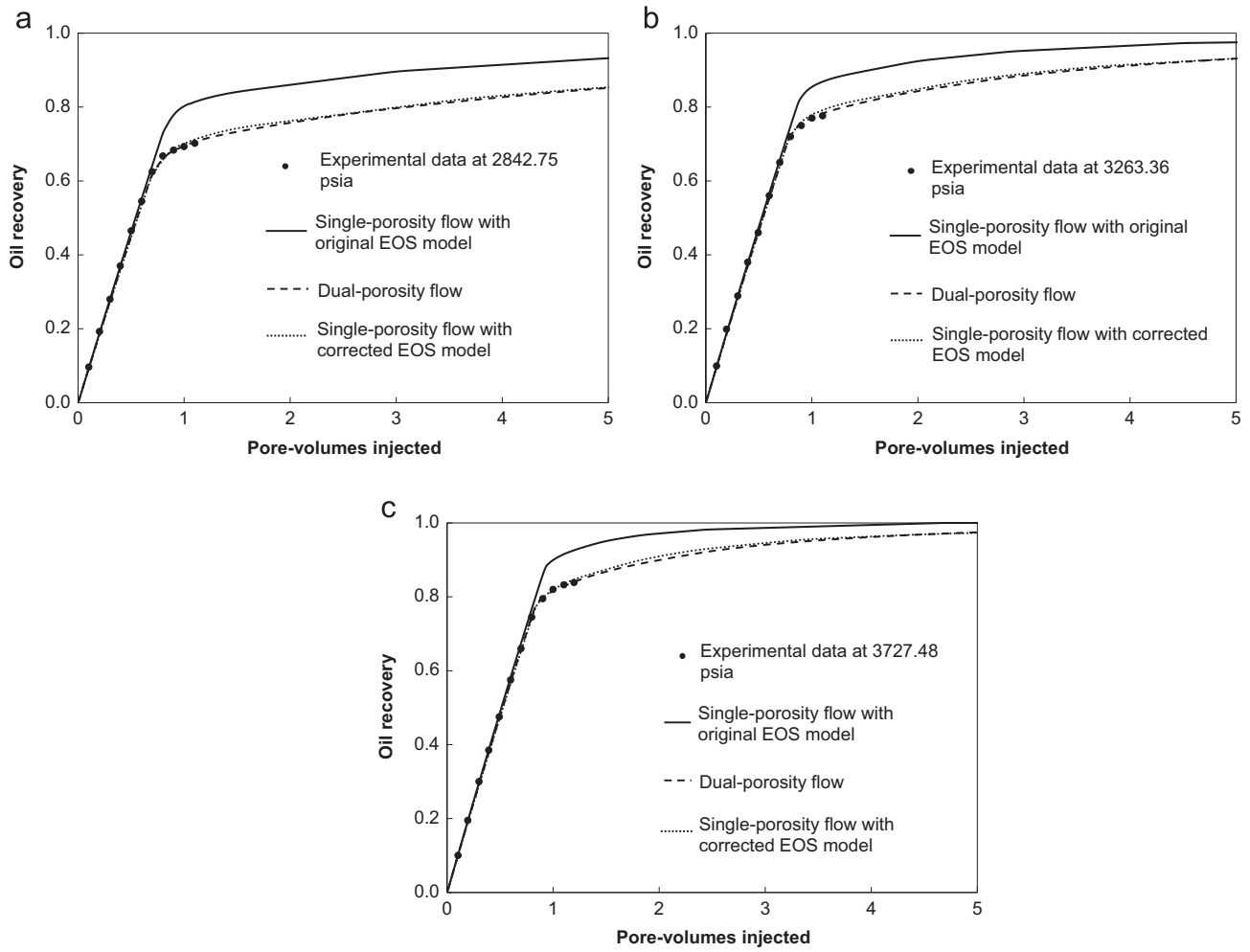
### 3.5. Representation of capacitance flow behavior observed in the fine-scale simulation

In Section 2.3, capacitance flow behavior was explained by use of a fine-scale simulation. A coarse-scale DPF simulation was then fitted successfully to the fine-scale simulation results. This subsection shows the application of the flow-based fluid characterization method for representing this capacitance flow behavior by use of efficient SPF simulation. Fine-scale simulation case 3 is considered. The DPF model fitted to case 3 resulted in the bypassed fraction of 0.08 and the throughput ratio of 0.14 (see Fig. 8). These dimensionless numbers indicate the importance of properly modeling capacitance flow behavior in this case.

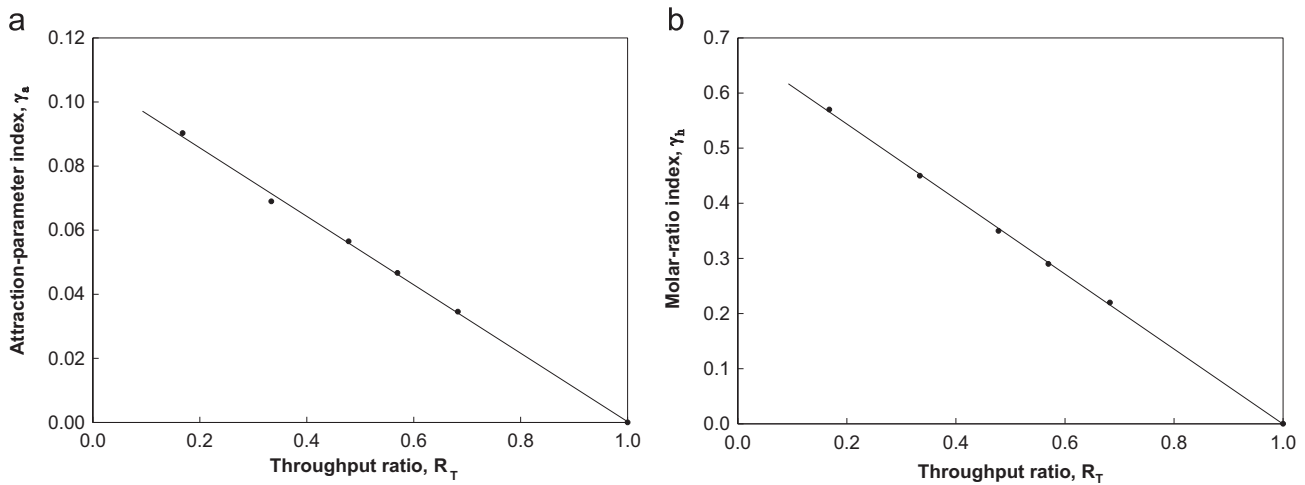
The flow-based fluid characterization method results in an estimated value of 0.487 for  $\gamma_a$ , 0.3125 for  $\gamma_h$ , and -0.09 for  $c_{Dh}$ . The resulting oil recovery prediction is compared with the original fine-scale simulation in Fig. 15. The SPF simulation with the corrected fluid model exhibits accurate representation of the capacitance flow behavior. It is not possible to reproduce the oil recovery using SPF if the flow-based fluid characterization method is not used.

## 4. Case studies

Sections 2.3 and 3.5 showed that capacitance flow behavior in a fine-scale simulation can be efficiently reproduced by the following two steps:



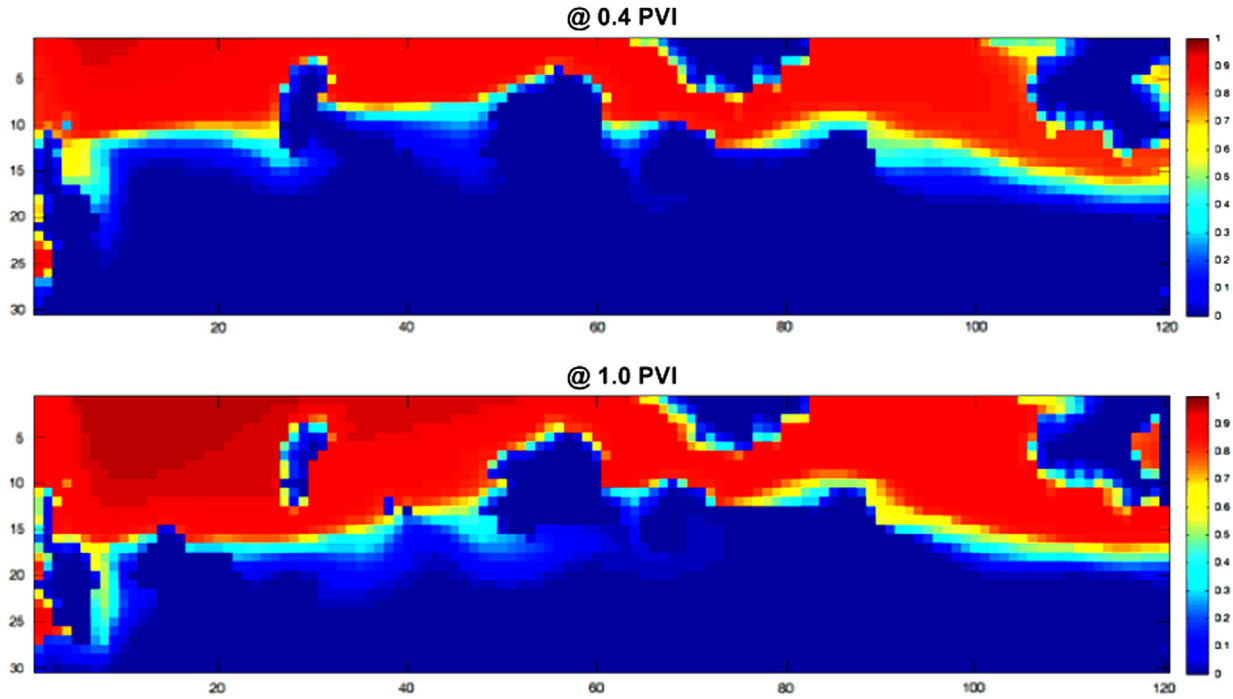
**Fig. 16.** 1-D DPF models fitted to core-flood data for the Shengli oil. (a) Bypassed fraction is 0.18 and throughput ratio is 0.48 at 2842.75 psia, (b) Bypassed fraction is 0.14 and throughput ratio is 0.48 at 3263.36 psia, and (c) Bypassed fraction is 0.14 and throughput ratio is 0.472 at 3727.48 psia. The recovery predictions from 1-D SPF simulations cannot reproduce the core-flood data unless the fluid model is corrected for capacitance. The fluid model characterized for 3263.36 psia is successfully applied at the other two pressures since the flow characteristics represented by the bypassed fraction and throughput ratio are similar to one another.



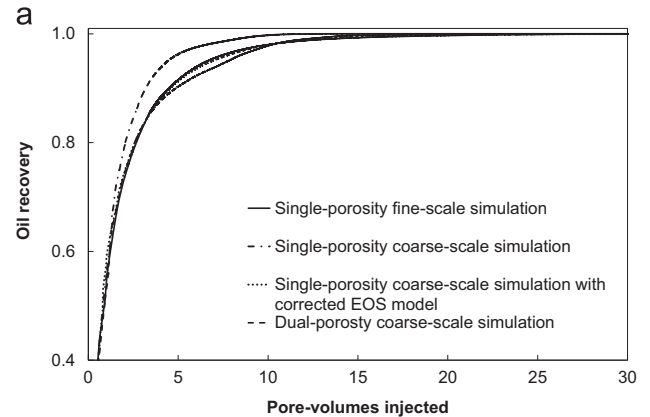
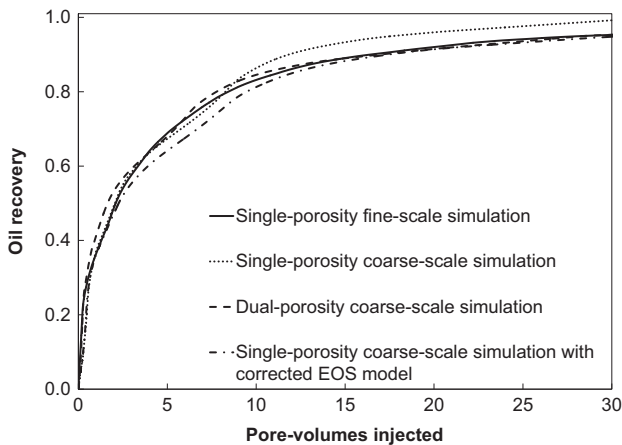
**Fig. 17.** Empirical linear relationship observed for the attraction-parameter index  $\gamma_a$  and the molar-ratio index  $\gamma_h$  with respect to  $R_T$  at 3263.36 psia. The core flooding case is at  $R_T$  of 0.48.

Step 1. Quantification of capacitance flow behavior by fitting a coarse-scale DPF model to the oil recovery from a fine-scale simulation. This gives certain values for bypassed fraction and throughput ratio ( $R_T^*$ ).

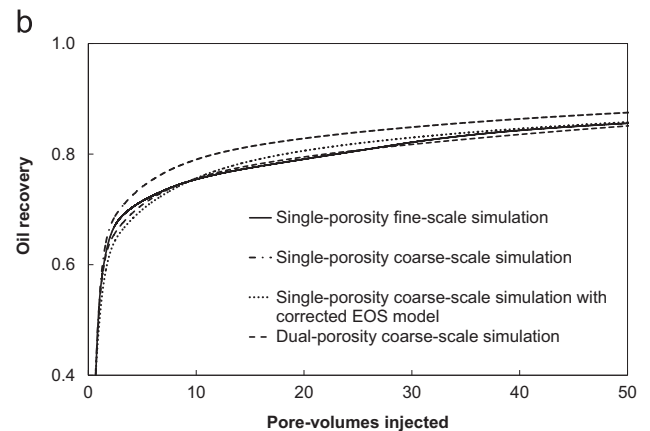
Step 2. Correction of the original fluid model for capacitance using the flow-based fluid characterization method. The coarse-scale DPF model is reduced to the corresponding SPF model with a corrected fluid model.



**Fig. 18.** CO<sub>2</sub> concentration distributions in the vertical 2-D fine-scale simulation at 0.4 PVI and 1.0 PVI. The channeling flow under gravity is observed. Table 3 gives the fluid properties used. The porosity distribution given in Fig. 4 was used in the vertical two dimensions.



**Fig. 19.** Oil recovery predictions for the vertical 2-D case. The DPF simulation successfully represents the capacitance flow behavior with a bypassed fraction of 0.10 and a throughput ratio of 0.22. The SPF simulation with a corrected fluid model is then used to reproduce the capacitance flow, which cannot be modeled using the coarse-scale SPF simulation. Table 3 gives the fluid properties used. The porosity distribution given in Fig. 4 was used in the vertical two dimensions.



**Fig. 20.** Oil recovery predictions for two layers from the SPE-10 problem. (a) Layer 15.  $B=0.10$ ,  $R_T=0.52$ ,  $\gamma_a=0.223$ ,  $\gamma_h=0.32$ , and  $c_{Dh}=-0.14$ . (b) Layer 80.  $B=0.05$ ,  $R_T=0.51$ ,  $\gamma_a=0.364$ ,  $\gamma_h=0.28$ , and  $c_{Dh}=-0.24$ .

For different  $R_T$  values anticipated in a specific application, the SPF model from Step 2 can be used with another fluid model that is based on linear correlations of  $\gamma_a$ ,  $\gamma_h$ , and  $c_{Dh}$  with respect to  $R_T$  between 1.0 and  $R_T^*$  (extrapolated if necessary).

This section presents case studies for capacitance flow in core floods and fine-scale simulations for the Shengli oil with CO<sub>2</sub>, and layers 15 and 80 from the SPE-10 problem (Christie and Blunt, 2001). The two-step method is applied for efficient representation of capacitance flow by use of SPF with a corrected fluid model.

#### 4.1. Core floods

Ren et al. (2011) conducted core floods of the Shengli oil by CO<sub>2</sub> at 258.8°F. Details of the core-flooding apparatus and core

properties are given in Ren et al. (2011). The MMP measured at the reservoir temperature 258.8°F was 3800 psia. Table 3 gives the EOS fluid model developed based on the data given in Ren et al.

(2011) and the characterization method of Kumar and Okuno (2013). Ren et al. (2011) described that the reservoir pressure dropped below the MMP after depletion in the G89 block of the Shengli oil field. Hence, the injection pressures tested in their core floods were set below the MMP in order to determine an optimal injection pressure.

In this research, a 1-D SPF model was first made as given in Table 4. The numerical Péclet number is estimated to be approximately 660 with uniform 500 grid blocks and 0.01-hour time step with the fully implicit scheme. The recovery predictions at three different pressures, 2842.65 psia, 3263.36 psia, and 3727.48 psia, were erroneously higher than the experimental results of Ren et al. (2011), as shown in Fig. 16. This is because the sub-grid scale capacitance flow behavior could not be captured in the 1-D SPF simulations with the conventional local equilibrium assumption. The two-step method is applied to these core-flooding data below.

The first step is to quantify the capacitance flow behavior using the 1-D DPF model. Fig. 16 shows that the 1-D DPF model is fitted well to the core-flooding data (black dots) at three different pressures. The resulting dimensionless groups associated with capacitance ( $B$ ,  $R_T$ ) are (0.18, 0.48) at 2842.75 psia, (0.14, 0.48) at 3263.36 psia, and (0.14, 0.472) at 3727.48 psia, where  $B$  and  $R_T$  are the bypassed fraction and throughput ratio, respectively.

In the second step, the flow-based fluid characterization method is applied with the DPF at 3263.36 psia. Fig. 16(b) shows that the SPF with a corrected fluid model can reproduce the oil recovery predic-

tions from the DPF. The resulting dimensionless groups associated with capacitance ( $\gamma_a$ ,  $\gamma_h$ ) are (0.12, 0.36), where  $\gamma_a$  and  $\gamma_h$  are the attraction-parameter index (Eq. (10)) and the molar-ratio index (Eq. (11)), respectively. The corresponding  $c_{Dh}$  is calculated to be  $-0.06$ . Since the levels of capacitance measured by  $B$  and  $R_T$  are similar at the three pressures, the corrected fluid model for 3263.36 psia is applied to the other pressures, 2842.75 psia and 3727.48 psia. Fig. 16 (a and c) shows that the resulting SPF simulations are still in good agreement with the corresponding DPF simulations and experimental results.

To see the relationship of  $\gamma_a$  and  $\gamma_h$  with  $R_T$ , four more cases are generated with the DPF at different  $R_T$ 's. Each of the DPF cases is reproduced by the corresponding SPF based on step 2, the flow-based fluid characterization method. Fig. 17 shows the resulting values of  $\gamma_a$  and  $\gamma_h$  for the five  $R_T$  values, including  $R_T$  of 0.48. They are correlated well with straight lines that go through zero at  $R_T$  of 1.0.

#### 4.2. Vertical 2-D fine-scale simulation

Capitance flow behavior observed in vertical 2-D fine-scale simulations is considered in this subsection. The porosity and permeability distributions used are the same as those in Section 2.3 (see Fig. 4), except that the original y direction is changed to the z (vertical) direction. The fluid properties used are given in Table 3; that is, the injection gas is pure  $\text{CO}_2$ . The reservoir pressure and temperature are 3263.36 psia and 258.8°F, respectively.

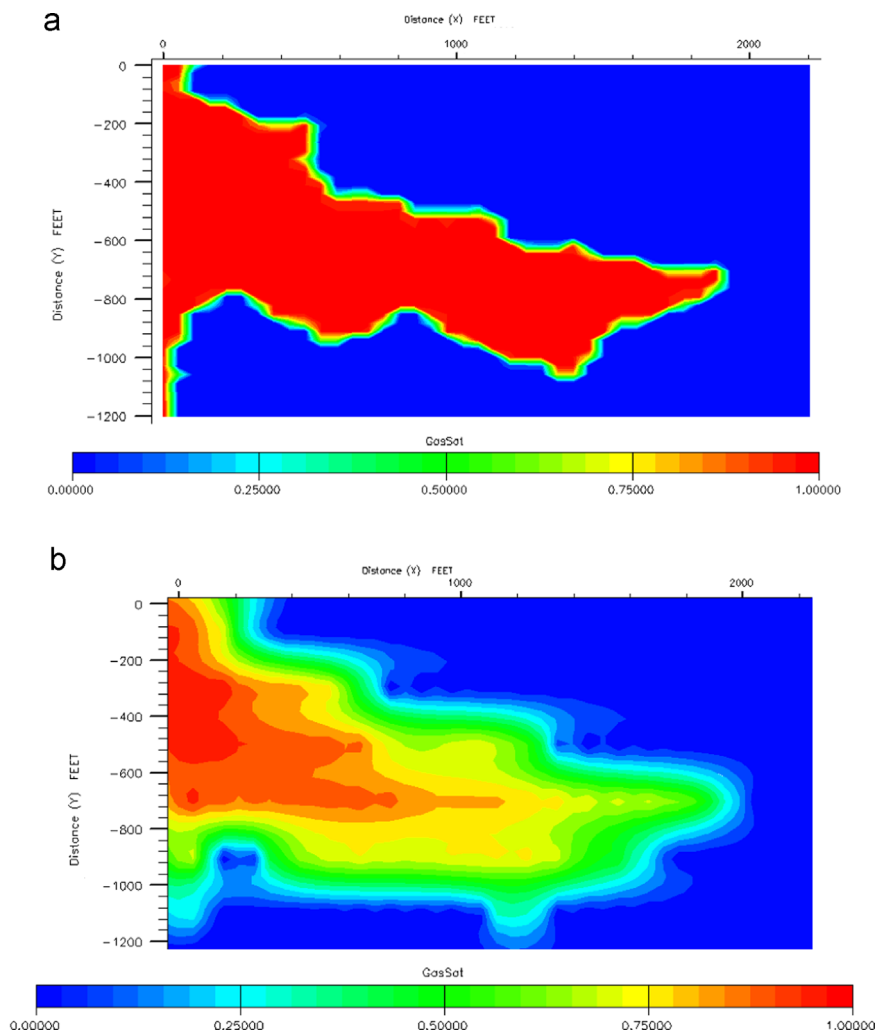
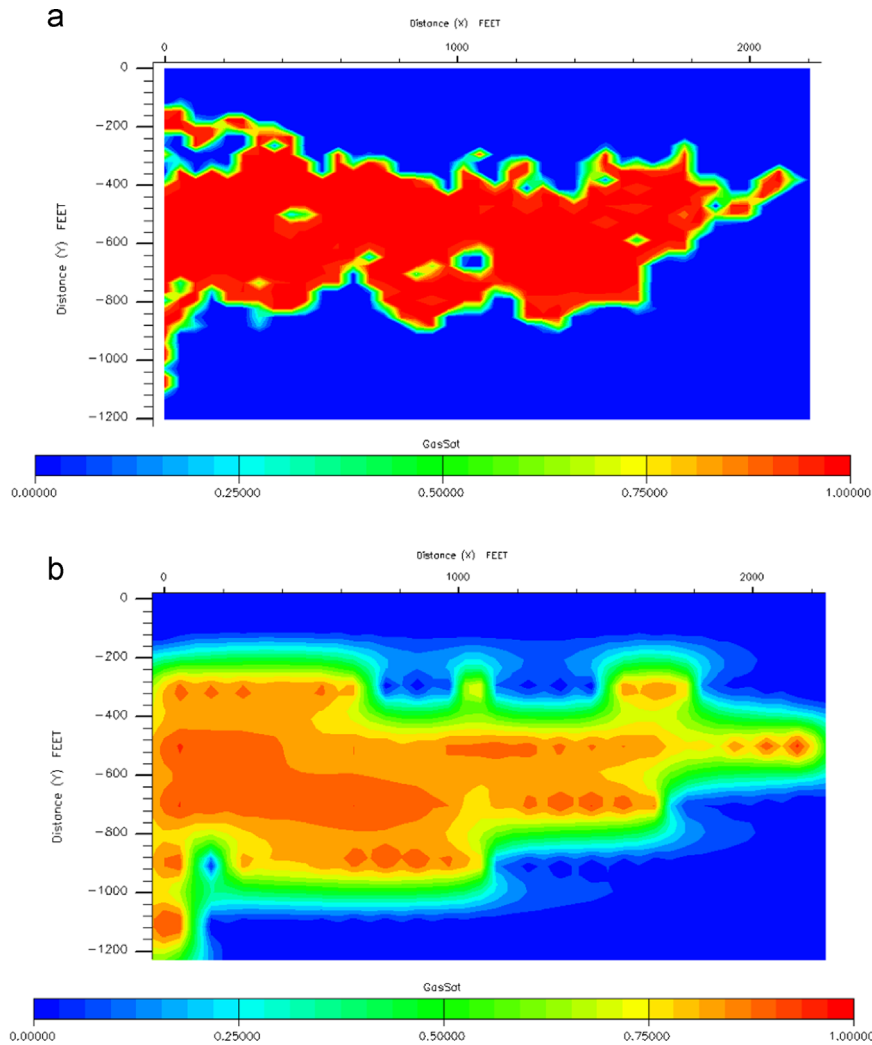
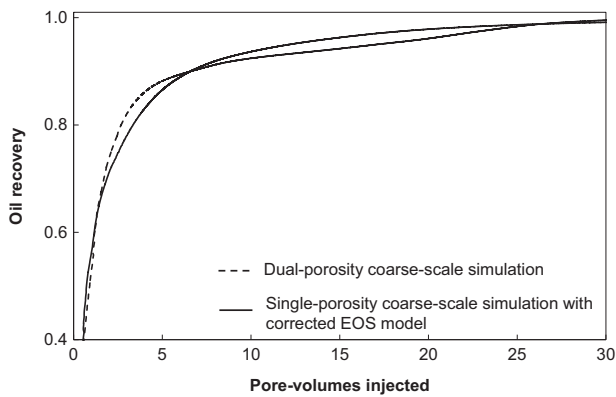


Fig. 21. Gas saturation contours at 0.74 PVI for layer 15 of the SPE-10 problem. (a) Original fine-scale simulation. (b) Coarse-scale simulation with the corrected fluid model. The root-mean-square deviation is 15.3%.



**Fig. 22.** Gas saturation contours at 0.98 PVI for layer 80 of the SPE-10 problem. (a) Original fine-scale simulation. (b) Coarse-scale simulation with the corrected fluid model. The root-mean-square deviation is 29.5%.



**Fig. 23.** Oil recovery predictions for layer 15 of the SPE-10 problem.  $B=0.10$  and  $R_T=0.33$ . The prediction from the linearly extrapolated SPF is in good agreement with the benchmark result from the DPF. The extrapolation gives  $(\gamma_a, \gamma_h, c_{Dh}) = (0.314, 0.45, -0.20)$  at  $R_T=0.33$ .

Fig. 18 illustrates the  $\text{CO}_2$  concentration distributions in the vertical 2-D fine-scale simulation at 0.4 PVI and 1.0 PVI. The channeling flow under gravity is clearly observed. In the first step, the original  $120 \times 30$  grid blocks are upscaled to  $12 \times 3$  coarse-scale grid blocks. The coarse-scale DPF model is fitted to the fine-scale simulation in terms of oil recovery, resulting in a bypassed

fraction of 0.10 and a  $R_T$  of 0.22 (Fig. 19). In step 2, the flow-based fluid characterization method is used to fit the coarse-scale SPF to the coarse-scale DPF, resulting in  $\gamma_a$  of 0.21,  $\gamma_h$  of 0.12, and  $c_{Dh}$  of  $-0.1$ . As shown in Fig. 19, the oil recovery predictions at later PVIs from the fine-scale simulation can be quantitatively reproduced by use of the coarse-scale SPF with the corrected fluid model.

#### 4.3. Layers 15 and 80 from SPE 10

In this subsection, the proposed two-step method is applied for upscaling of layers 15 and 80 from the SPE-10 problem (Christie and Blunt, 2001), in which methane is injected to displace the reservoir oil consisting of methane,  $\text{CO}_2$ , n-C<sub>4</sub>, and C<sub>10</sub> at 211.73° F. It is a partially miscible displacement. For each of the layers, the original fine-scale model of  $220 \times 60 \times 1$  is upscaled to a coarse-scale model of  $22 \times 6 \times 1$ ; i.e., the upscaling ratio is 100. These upscaling cases were used by Salehi et al. (2013) to demonstrate the applicability of their compositional upscaling method. The simulation conditions can be found in Christie and Blunt (2001) and Salehi et al. (2013), and are not duplicated here.

Quantification of the capacitance flow yields the DPF parameters ( $B, R_T$ ) of (0.10, 0.52) for layer 15, and (0.05, 0.51) for layer 80. Then, the resulting fluid-characterization parameters  $(\gamma_a, \gamma_h, c_{Dh})$  are (0.223, 0.32,  $-0.14$ ) for layer 15, and (0.364, 0.28,  $-0.24$ ) for layer 80. Fig. 20 shows oil recoveries from four different simulation runs



for each layer; i.e., the original fine-scale simulation, SPF with the original fluid model, DPF, and SPF with the corrected fluid model. In the DPF simulation and the SPF simulation with the corrected fluid model, the capacitance flow behavior that is present in the original fine-scale model is properly represented for each layer. This figure indicates that layer 15 is more challenging for the flow-based fluid characterization because the SPF with the original fluid model gives greater absolute deviations from the original fine-scale simulation in terms of oil recovery.

It was observed that the coarse-scale SPF with the corrected fluid model requires much less computational time than the original fine-scale simulation; e.g., it takes less than 2% of the total computational time taken by the fine-scale simulation for layer 15. For layer 80, the computational-time ratio is less than 1%. Similar levels of computational efficiency were achieved by Salehi et al. (2013) with their upscaling method.

Fig. 21 shows gas saturation contours in the original fine-scale simulation and the coarse-scale simulation with the corrected fluid model for layer 15 at 0.74 PVI (390 days). Gas saturation contours for layer 80 at 0.98 PVI (130 days) are given in Fig. 22. The root-mean-square deviation in gas saturation is calculated to be 15.3% for Fig. 21, and 29.5% for Fig. 22. Salehi et al. (2013) presented that their upscaling method resulted in the deviation of 8.3% for layer 15 at 390 days, and 10.2% for layer 80 at 130 days. Hence, the method of Salehi et al. (2013) exhibited higher accuracy for upscaling of the two layers at the tested PVI. This is expected because their method allows for local adjustment of compositional flow.

For layer 15, which is more challenging than the other layer, the applicability of linear extrapolations of  $\gamma_a$ ,  $\gamma_h$ , and  $c_{Dh}$  are examined. They are extrapolated to a  $R_T$  value of 0.33 to obtain  $(\gamma_a, \gamma_h, c_{Dh}) = (0.314, 0.45, -0.20)$ , on the basis of the linear correlations from the original case with  $(R_T, \gamma_a, \gamma_h, c_{Dh}) = (0.52, 0.223, 0.32, -0.14)$ . Fig. 23 shows that the linearly extrapolated SPF is in good agreement with the DPF with  $(B, R_T)$  of  $(0.10, 0.33)$ .

Unlike in local-upscaling methods, it is not the primary objective to reproduce local saturations/concentrations in the proposed two-step method. In the global upscaling method developed in the current paper, local saturations/concentrations are approximated indirectly by matching global flow behavior under capacitance. Nevertheless, the simplicity of the method developed in this research gives the following distinct features: (1) it can quantify the level of capacitance flow behavior observed in a flow experiment or fine-scale simulation in a simple, but physically meaningful manner by use of DPF with  $B$  and  $R_T$ ; (2) it can represent the quantified capacitance flow in coarse-scale SPF in a simple, systematic manner with no change in the conventional compositional-flow formulation. The simplicity owing to the selected parameters resulted in the finding that  $\gamma_a$ ,  $\gamma_h$ , and  $c_{Dh}$  have empirically linear correlations with  $R_T$ .

## 5. Conclusions

This paper presented capacitance flow behavior in compositional reservoir simulation. The two-step method was proposed to efficiently reflect in coarse-scale single-porosity simulation the capacitance flow behavior observed in core floods and fine-scale simulations. Conclusions are as follows:

1. Dual-porosity flow (DPF) can capture the characteristics of capacitance flow behavior. Quantification of the capacitance is possible with bypassed fraction and throughput ratio ( $R_T$ ).  $R_T$  is defined as the ratio of throughput required for ultimate oil recovery without intra-block mass flux to that with intra-block mass flux.  $R_T$  of zero corresponds to single-porosity flow (SPF)

with the  $S_{orm}$  method.  $R_T$  of unity corresponds to the traditional SPF with the local equilibrium assumption.

2. In the flow-based fluid characterization method developed in this research, the fluid model of interest is corrected for capacitance. It adjusts in-situ propagation rates of components through the attraction parameters. Two main adjustment parameters are the attraction-parameter index ( $\gamma_a$  defined by Eq. (10)) and the molar-ratio index ( $\gamma_h$  defined by Eq. (11)). These adjustment parameters decrease monotonically with increasing  $R_T$ . In the cases studied, they are well correlated with  $R_T$  using straight lines that go through zero at  $R_T$  of 1.0, where the fluid model naturally becomes the original one (i.e., no capacitance).
3. The two-step method presented requires no change in the governing equations in compositional reservoir simulation. It can be easily applied with the existing reservoir simulators.

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