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## Nonlinear simulation of miscible displacements with concentrationdependent diffusion coefficient in homogeneous porous media



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#### HIGHLIGHTS

- Highly accurate numerical simulation of miscible viscous fingering is presented.
- First time to examine miscible concentration-dependent diffusion coefficient (CDDC).
- Both mobility and diffusion contrasts result in complicated frontal instabilities.
- The CDDC case shows quite different characteristics with widely used constant case.
- The CDDC is non-negligible and should be considered in miscible displacements.

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#### ABSTRACT

The nonlinear dynamics of miscible flow displacements in homogeneous porous media are examined for the special case of concentration-dependent diffusion coefficient (CDDC) models. Highly accurate numerical methods are used to simulate the time evolution of fingering with both mobility and diffusion coefficient contrasts of two components in a fully miscible solution system. The simulations revealed that, when compared with a constant diffusion coefficient (CDC), the CDDC models show drastically different viscous fingering structures and mixing of the two components. In particular, for a pure diffusion process with a stable front, using a CDDC results in less mixing, with a non-symmetric concentration gradient. While for the unstable displacements with relatively large mobility contrasts, it is found that using a CDDC tends to trigger fingers at the very beginning of the displacements. The diffusion-dominated period is therefore very short and can nearly be neglected. Moreover, the fingers reach the downstream boundary much earlier with fingering structures about 2-4 times more complex than the CDC case. Quantitative analysis indicates that the exponential CDDC models can enhance the mixing by shortening the diffusive regime but not change the growth rate of mixing in the convective regime. In addition, in contrast with the CDC case, the time required for the appearance of fingers for the CDDC seems to be independent of Peclet number Pe at a relatively large log mobility ratios R. As Pe increases for the CDDC cases, more complex dynamics of the fingers are observed, which can only be found at very high Pe and R values for the CDC case. In addition, a small increase in R is able to significantly enhance the instabilities since it can result in not only larger mobility contrast but also a steeper diffusion gradient. © 2017 Elsevier Ltd. All rights reserved.

### 1. Introduction

The instability in a flow displacement within a porous media is widely encountered in a series of industrial processes such as enhanced oil recovery, groundwater flows, CO<sub>2</sub> sequestration, chromatographic separation, fixed bed regeneration and soil remediation. It is a time evolution process with the contact area of two

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or more components becoming unstable when a high-viscosity fluid is displaced by a low viscosity one. It is therefore referred to as viscous fingering (VF) because of its finger-like patterns at the contact zone.

Depending on the actual situations, VF may be desired, but most often it is to be avoided. For instance, in the water flooding enhanced oil recovery (EOR) process, the VF is undesirable. Once it happens the injected water tends to bypass oil and reaches the production wells quickly, resulting in low sweep efficiency and oil recovery. However, in other conditions such as cyclic solvent

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#### Nomenclature Α aspect ratio under-relaxation factor $\boldsymbol{\varpi}$ concentration of fluid С и viscosity concentration base state $\bar{c}$ . β constant C'perturbations of concentration porosity φ D diffusion coefficient stream function absolute average rate of concentration change for conω vorticity $I_{conv}$ vection absolute average rate of concentration change for diffu- $I_{diff}$ **Superscripts** sion dimensionless form of a parameter K permeability current time step Lx length of porous media lth level of iteration 1 width of porous media Ly P pressure Subscripts Ре Peclet number the displacing fluid 1 R log mobility ratio, or log viscosity ratio, or viscosity ratio 2 the displaced fluid Re Reynolds number the ith grid point in x direction i characteristic time Tcthe jth grid point in y direction i time t the derivative of time t $T_c$ characteristic time x derivative x constant injection velocity U v derivative two-dimensional Darcy's velocity vector u

injection (CSI) and CO<sub>2</sub> huff-n-puff EOR processes, VF is desirable and enhances the mass transfer between solvent and oil by increasing the mixing area between the two components during the injection process. This increased mixing area is also beneficial during the followup soaking stage of the process, where additional time is provided for the solvent-oil mass transfer to occur through diffusion and convective dispersion. The viscosity of crude oil can therefore be significantly reduced in the solvent diluted oil regions. The diluted oil will be more mobile and easily driven to producers during in the production stage. In this case, the VF is desired and a deeper understanding of the miscible VF in the solvent-based processes is very meaningful.

There is a long history of attempts to model and understand VF in porous media. The earliest study where VF was referred to as channeling was conducted by Hill (1952). Since then, a large number of works has been performed for various aspects of such instability. Several authors had conducted very comprehensive and extensive literature reviews on this topic and can be found in Homsy (1987), McCloud and Maher (1995), Casademunt (2004).

Despite the considerable research effort applied to VF, most of the studies were based on a very important assumption that the diffusion coefficient of two components in the miscible displacements is constant. This assumption is somewhat valid in the case where the concentration of the solvent in the oil phase is small (Das and Butler, 1996). However, in other situations, a varying diffusion coefficient which is dependent on concentration has to be taken into account. For instance, in the solvent-based process such as vapor extraction (VAPEX) in EOR, Das and Butler (1996) considered an exponential relation between diffusivity and viscosity or concentration, proposed by Hayduk and Cheng (1971), to determine the diffusivity of propane and butane in Peace River bitumen. They also pointed out that diffusion plays a vital role and neglecting the dependence of diffusivity on concentration may result in unrealistic results. This was proved later by Das (2005) who found the production rate and contact profile of solvent and in-situ oil cannot be matched simultaneously while using a CDC. Meanwhile, to match the oil production rate, very high coefficients in the order of  $10^{-2}$  to  $10^{-3}$  cm<sup>2</sup>/s are needed, which is surely unrealistic as mentioned by the author. In the same year with Das and Butler (1996), the experiments conducted by Petitjeans and Maxworthy

(1996) showed that the diffusion coefficient of water and glycerin is strongly dependent on the local concentration and varied by a factor of about 30 (Chen and Meiburg, 1996).

Considering the importance of concentration-dependent diffusion coefficient (CDDC) in EOR as well as in a variety of industrial processes, researchers have conducted experimental studies to determine the concentration dependency of diffusion coefficient. Using a pressure-decay method in a closed system, Upreti and Mehrotra (2000) investigated the concentration-dependent diffusivity of carbon dioxide in Athabasca bitumen. An algorithm method based on functional minimization was developed for the determination of gas diffusivity. It was found that the diffusivity of carbon dioxide was a unimodal function of its concentration in bitumen. Later, the same methods were used in the measurement of CDDC for carbon dioxide, methane, ethane, and nitrogen in two different Athabasca bitumen samples (Upreti and Mehrotra, 2002). The similar unimodal function of gas concentration in bitumen was reported and the values of diffusivity generally increased with gas concentration at the fixed temperature and pressure. Using the experimental data by Upreti and Mehrotra (2000, 2002), Sheikha et al. (2005) developed two graphical methods to estimate the diffusion coefficient of carbon dioxide, methane and nitrogen in bitumen. Analytical solutions were obtained and the calculated diffusion coefficient was in a good agreement with that reported in previously experimental studies. Jamialahmadi et al. (2006) measured the diffusivities of methane and carbon dioxide in liquid hydrocarbons over a wide range of pressure and temperatures. The diffusion coefficients were determined using continuity equation with finite-domain boundary conditions. An incubation period was reported in which the diffusion coefficient was controlled by convection and molecular diffusion, while after this period, its value was independent of concentration. A new and rapid approach was developed by Civan and Rasmussen (2009) for simultaneous determination of the diffusion coefficients of single-component gas in liquid hydrocarbons as well as other three parameters. In the same year, Okazawa (2009) introduced a concept of the average flow fraction of bitumen to analytically study the influence of CDDC in VAPEX process. The fractional Stokes-Einstein law was used for CDDC to accurately determine the bitumen rate. The obtained analytical expression considering CDDC can

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