

Numerical Solution of CO₂-Hydrocarbon Convective Mixing

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Introduction

Storage of carbon dioxide (CO₂) in geological formations is a means to reduce atmospheric emissions of greenhouse gases. CO₂ capture and storage with utilization in enhanced oil recovery (EOR), or CCUS, is perceived as the most cost-effective method of disposing captured CO₂ emissions. CO₂-EOR has been performed for many decades with a focus on hydrocarbon recovery. With CCUS, CO₂ storage will be emphasized in order to meet greenhouse gas emissions targets. Increased storage efficiency relies on the ability to manage reservoir dynamics at the large-scale. However, field-scale impacts are driven by fine-scale interactions between CO₂ and hydrocarbons that determine miscibility, mobility, and fluid properties of mixtures. Mixing of CO₂ and hydrocarbons is governed by complex physics occurring at sub-centimeter-scale and relies on highly accurate mathematical and property models. In this paper, we investigate gravity-driven mixing using high-resolution simulation of different CO₂-hydrocarbon mixtures.

CO₂-hydrocarbon mixtures properties

Under typical reservoir conditions, pure CO₂ is typically lighter than oil, but heavier than gas. As CO₂ mixes with oil (and gas) through diffusion and dispersion, the density and viscosity of the mixture will change. Many oils exhibit non-monotonic density variation with increasing CO₂ concentration. In Figure 1, the Peng-Robinson (PR) model shows significant non-monotonicity of neo-pentane and octane mixtures. Characteristics of these curves are given in Table 1. The shape the curves will vary according to temperature and pressure. Viscosity of these mixtures decreases linearly with increasing CO₂ concentration. We note that the PR model differs from other models (e.g. GERG-2008) in the prediction of mixture density. It is uncertain which mixture model is most accurate since the availability of data is poor. If existing models are shown to be insufficient, improved cubic EOS can be developed through modification of the EOS model coefficients, which is the subject of ongoing work.

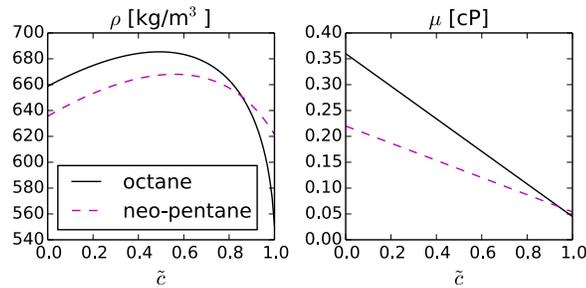


Figure 1: Density and viscosity for binary CO₂-hydrocarbon mixtures. Properties calculated for neo-pentane mixture at 100 bar and 310 K and for octane mixture at 200 bar and 353 K. Density model from Peng-Robinson.

Binary mixture	Temperature [K]	Pressure [bar]	Density* [kg/m ³]	Viscosity* [cP]	Max. density [kg/m ³]
Neo-pentane CO ₂	310	100	636 622	0.022 0.054	668
Octane CO ₂	353	200	658 554	0.036 0.045	685

Table 1: Binary CO₂-hydrocarbon mixture properties. *Values given for pure component.

Numerical simulation of convective mixing

Due to the non-monotonic phase behavior described above, an unstable density inversion will develop in the mixing zone, eventually leading to gravity-driven convection of CO₂ with oil under favorable conditions. This type of behavior has been well-studied for CO₂-brine systems, but where the density is monotonic. The *convect* simulator was developed that solves the non-dimensional flow and transport equations for a two-component single-phase mixture using a fully implicit solution method. We note that there is no assumption on the flow field (i.e. Boussinesq). All results are rescaled to dimensional units given the chosen fluid and rock properties.

Simulations were performed using CO₂ mixing with two single-component oils, neo-pentane and octane. Each simulation is initialized with one pure-component fluid overlying the other (miscible conditions). Two initial conditions are simulated—the first with CO₂ overlying the oil, and second with CO₂ under the oil. Late-time behavior for systems initialized with CO₂ on top (Fig. 2) show the downward migration of dense fingers. The fingers are approximately 10 cm wide for both oil systems. The onset time for octane is slower than neo-pentane, both are on the order of days. For systems initialized with CO₂ on bottom (Fig. 3), the convection is faster and more complex. Light fingers with high CO₂ concentration move upwards while dense fingers with maximum density move downwards. The dense fingers move faster than the light fingers. The light fingers eventually stop migrating upwards once the dense fingers reach the bottom. Flux lines show that density variations significantly impact the flow field.

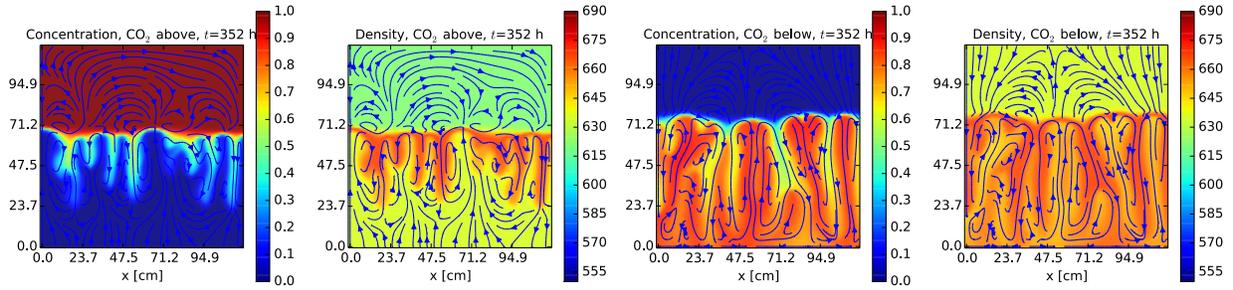


Figure 2: Concentration and density plots for CO₂-neo-pentane mixture. CO₂ initialization on top (left) and on bottom (right). Solution rescaled for permeability of 100 mD, diffusivity of 10⁻⁹ m²/s, porosity of 10 %.

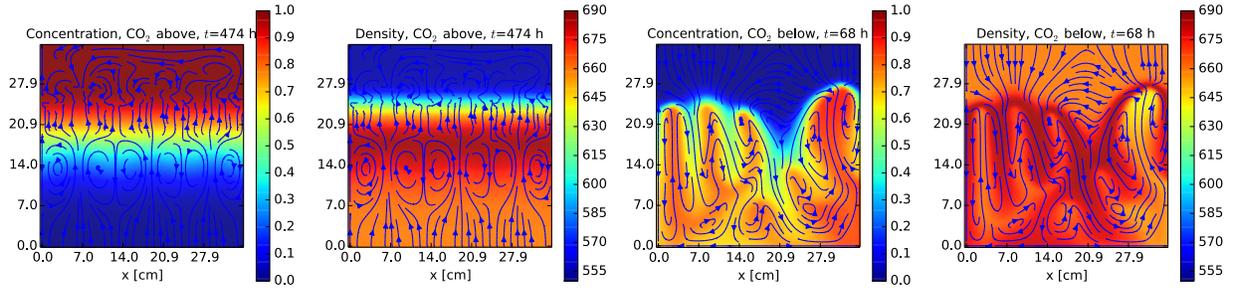


Figure 3: Concentration and density plots for CO₂-octane mixture. CO₂ initialization on top (left) and on bottom (right). Solution rescaled for permeability of 100 mD, diffusivity of 10⁻⁹ m²/s, porosity of 10 %.

Summary

The results of convective mixing simulations give important insight into the impact of non-monotonic density. The following implications of this study can be noted:

- CO₂ convection in oil begins much more rapidly, has smaller fingers and faster finger speed compared to convection in CO₂-brine systems.
- The behavior of CO₂ convection from below occurs in two directions and is significantly more unstable (faster onset time and finger speed). CO₂ is eventually stopped from upward migration if the initial layer is less than 60% of the oil layer.
- The two-way mixing behavior leads to non-negligible density variations that cannot be analyzed using linear stability theory (Boussinesq approximation is invalid).