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Quantifying physical properties of Weyburn oil via molecular dynamics simulation

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HIGHLIGHTS

- Developed a generalized MD compositional model for the Weyburn CO_2-EOR process.
- Quantified CO_2 mixing under long term CO_2-EOR application.
- Captured the existence of fluid microstructures which impact CO_2 mixing processes.
- Captured CO_2-asphaltene interactions and gas exsolution as pressure declines.

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ABSTRACT

Weyburn and Bakken reservoirs represent two medium gravity tight oil reservoirs who are currently utilizing CO_2 injection as an EOR recovery process. To properly establish the CO_2 recovery potential, extensive data are required to characterize CO_2-oil mixing characteristics. Such data include compositional changes on oil density and oil viscosity as well as component diffusion coefficients. Additional effects of fluid-rock (sand and clay) interactions are also of importance especially due to the tight oil characteristics of such reservoirs.

The necessary laboratory data are currently not available to build a reliable field prediction model. Laboratory experiments are costly and time consuming and often show wide variability, especially for non-equilibrium properties for binary and ternary mixtures. This implies significant uncertainties in the previously employed Weyburn 7 component compositional model used for field simulations.

Here, we build a 15 component molecular dynamics (MD) model for the Weyburn oil and its mixing with CO_2 to quantify these essential equilibrium and non-equilibrium process parameters. Via MD simulation, we established these parameters for the Weyburn oil at two different field conditions. These property results can be used in future CO_2-EOR field simulation for Weyburn. A similar MD strategy can be used for other tight oil reservoirs (e.g. Bakken reservoir). This work establishes that MD simulation can be used as a cost-effective tool, along with laboratory experiments and field simulation, in an integrated approach to proper analysis of an EOR development strategy.

1. Introduction

The Weyburn field, one of the largest medium gravity crude oil fields in Canada, was discovered in 1955. The field covers approximately 180 km^2 in the southeastern corner of Saskatchewan and produces oil from the Midale beds of the Mississippian Charles formation [1]. The IEA GHG Weyburn CO_2 Monitoring and Storage Project was designed to study methods for monitoring CO_2 movement in the subsurface and to determine the security of storing CO_2 in depleting oil reservoirs for hundreds to thousands of years. Whittaker [2] provides an overall summary of the IEA GHG Weyburn CO_2 monitoring and storage project in context with geological characterization of the Weyburn field for geological storage of CO_2.

The Bakken reservoir represents a similar oil with extensive laboratory and field investigations [3,4]. The CO_2 EOR performance of this reservoir system also depends critically on its oil characteristics and how it mixes with CO_2. Researchers at the EERC and at the Texas A&M university was able to recover 60–95% of the hydrocarbon in rock samples from the middle, upper, and lower Bakken layers [5]. Further examples of tight oil reservoirs with varying

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compositional characteristics can be found in a review article by Olsen [6]. In all cases, expensive laboratory tests can be expected to constrain the development of these reservoirs, and MD analysis would provide a useful, cost-effective alternative to obtain the essential physical properties. This approach was discussed in detail in our first paper Uddin et al. [7].

Bao et al. [8] proposed an innovative approach for direct coupling of MD methods into reservoir simulation in order to analyze CO_2 mixing and sequestration in field modeling. However this is an extremely computer-intensive approach. Instead we propose a two-step decoupled approach, such that MD simulation is utilized to quantify physical properties that can be thereafter used directly in reservoir simulation models as with experimental results.

Numerous research groups have used molecular modeling methods (Monte Carlo MC and molecular dynamics MD) to generate equilibrium and non-equilibrium properties of reservoir oils and this continues to be an area of active research. Our previous paper Uddin et al. [7] has provided a restricted overview of some such activities. Additional interesting work includes molecular simulation of CO_2 solubility in octane [9], a Monte Carlo study of binary and ternary liquid–liquid equilibrium [10], as well as the use of united atom potentials to study vapor–liquid equilibrium of long-chain alkanes [11]. More specific to our current objective is the work of Ungerer and coworkers [12,13] to generate representative multi-component compositional models of gas condensate reservoirs.

The main objective of the present study is to illustrate the use of molecular dynamics (MD) as a tool for PVT generation and analysis, specifically for the Weyburn oil. As gas composition variation is characteristic of the Weyburn CO_2 monitoring and storage production method, there is a critical need to quantify varying lighter gas components interaction with the heaver ends, especially under conditions of high CO_2 loading. Additionally, a secondary objective is to illustrate MD as a tool for fluid microstructure prediction and micro-structure variations. Here we will use temperature variation as an easy probe to alter these micro-structure behaviors, although pressure variation such as that occurring with Weyburn production may induce similar micro-structure variations.

2. Weyburn field development history

Development began shortly after discovery with the drilling of 675 wells on 32 ha (80 acre) spacing. Based on the fracture trend, the lines of wells are oriented NE-SW and NW-SE. After 8 years of primary production, water flooding was initiated in 1964 using inverted nine-spot patterns. In the 1980s, a number of infill wells were drilled, which reversed the trend of declining production, and in the 1990s a number of horizontal wells were drilled, which resulted again in significant incremental production. By 1999, there were 824 active wells in the field, of which 514 were vertical producers, 142 horizontal producers and 168 vertical water injectors [14]. Cumulative production was 52 million m^3, approximately 24% of the 220 million m^3 of original oil-in-place. By this time, production was declining rapidly, which led to plans for a tertiary recovery strategy, miscible CO_2 injection. This new phase of development for the field was planned to begin in the fall of 2000.

2.1. Field development strategy

CENOVUS, the current field operator, is carrying out its CO_2 flood in a number of well-defined stages over the next 25 years. There are major geological features in the Weyburn unit which determine fluid flow behavior. The Midale beds are capped by the tight Midale Evaporite, and can be divided into two major lithologic units: an upper marly and lower vuggy zone. The marly is a chalky dolomite with an average permeability of less than 10 mD and an average porosity of 26%. The vuggy zone is a highly fractured limestone with widely varying porosity and permeability, but typically lower porosity and higher permeability than the marly. The dominant NE-SW fracture trend in the vuggy produces higher permeability in that direction, and was a significant factor considered in development of the field. This can be considered as an example tight oil system.

Primary production was carried out from 1956 to 1964 in this pattern. Water injection into the central wells began in June 1964 and this secondary recovery period lasted until September 2000, when the tertiary recovery period began. CO_2 injection commenced in September 2000 with injection into the three central row wells and continues to date.

2.2. Pattern 1 reservoir simulation study

Numerical simulations for the CO_2 miscible flooding strategies were conducted at Alberta Innovates – Technology Futures (AITF) under Phase I of the IEA GHG Weyburn CO_2 monitoring and storage project. These single pattern simulations are the building blocks to carry out simulations of the entire 75-pattern CO_2 flooding and storage project. AITF conducted relatively fine-grid simulations for the some single patterns and a coarse-grid simulations for 75-pattern representing the entire planned CO_2-EOR area.

Uddin et al. [15] extracted a simulation grid for pattern 1 together with a half pattern buffer from the larger patterns simulation grid. Production history matches and predictions were conducted applying a 7 component composition model. The overall phases of the simulation study were as follows:

Initial state: homogeneous p & composition; p = 14.5 MPa.
1956–1964: primary depletion; p = 6.72 MPa at end.
1964–2000: water flood; p = 21.11 MPa at end.
2000–2010: CO_2 injection; p = 21.16 MPa at end.

The simulation study ended in 2010. History matched gas, water and oil productions were attempted with good oil and water matches. Gas production history was found to be quite inadequate. It is probable that the gas exsolution process was not fully captured. During CO_2-EOR phase, diffusion and dispersion model was required to capture the CO_2 spatial distribution and production characteristics.

For our present MD study, we wish to contrast the average conditions existing at the start of field production plus that at the end of CO_2 injection. For the former, we assume a uniform pressure of 14.5 MPa and a homogeneous oil composition. For the latter, we will use the simulation predictions of Uddin et al. [15]. Fig. 1 shows the pattern-wide variation of pressure and oil density at the end of ten years CO_2 EOR injection at the top of the Marly layer (i.e. zone of highest gas concentration). Fig. 2 shows the corresponding CO_2 and C1N2 mol fractions in the oil phase at the same time point. This information was used to estimate a typical average reservoir pressure of 21.16 MPa and the oil phase composition listed in Table 1, as discussed below.

2.3. Oil composition – PVT data

A compositional model for Weyburn oil has been developed [16] in IEA GHG Weyburn Project Task 5.3. This is a seven-component model, one of the components being CO_2. It was developed based on oil samples collected from the reservoir, with PVT model parameters tuned to match oil density, viscosity, gas oil ratio (GOR), saturation pressure and minimum miscibility pressure (*MMP*). Details of the model and its development are given in a separate report [17]. The Peng–Robinson equation of state has been used for the PVT model development. Default parameters supplied by the EOS model were used, with point checks against