STREAMLINE BASED SIMULATION OF CO_2 INJECTION IN SALINE AQUIFERS

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ABSTRACT

Design and implementation of CO_2 sequestration projects in saline aquifers require, in part, a solid understanding of the key physical mechanisms that determine distribution of the injected CO_2 within the target aquifer. This understanding then forms the basis for model formulation and development of simulation techniques appropriate for resolving the essential physics. In addition, a significant level of uncertainty exists as to the spatial distribution of rock properties. This, in turn, calls for development of simulation tools that are accurate and computationally efficient enough that repeated simulations can be performed to assess uncertainties in predicted movement of the injected CO_2.

In this paper we address the question of how to simulate accurately and efficiently the injection phase of CO_2 storage in saline aquifers at field scale. In these flow settings, we seek to resolve the permeability heterogeneity of a given aquifer as well as to represent adequately the interplay of gravity, capillary and viscous forces.

We demonstrate that compositional streamline simulation is an accurate and efficient method for predicting the movement of CO_2 in aquifers during the injection period. We describe how to handle the compositional effects (solubility of CO_2 in brine) in a very efficient manner based on look-up tables and explicit calculation of phase distributions and compositions, followed by evaluation of transport properties. The streamline approach is compared to conventional finite difference simulation tools.

1. INTRODUCTION

Considerable effort has been devoted to the development of reservoir simulation tools for the oil industry, and high quality simulators are available that handle effectively many of the flow problems appropriate to oil and gas reservoirs. One area where simulator development is continuing, however, is in the simulation of processes in which components transfer between the phases present in the porous medium. Injection of CO_2 into saline aquifers involves such component transfers, as the injected CO_2 dissolves in any undisplaced brine. An overview of available technology for simulation of CO_2 flows in aquifers, including contributions from the groundwater community as well as the oil and gas community, is reported by Harris *et al.* (2005). These methods are all based on Eulerian finite difference/volume/element methods.

Up to this point, no investigation of the efficiency of compositional streamline simulation (a Lagrangian approach) has been reported for CO_2 injection in saline aquifers. A large literature describes the development and application of streamline simulation to prediction of flow in three-dimensional heterogeneous reservoirs. See the papers of King and Datta-Gupta (1998) and Crane *et al.* (2000) for many references to the full range of work on streamlines.

The use of compositional streamline simulation for gas injection processes was demonstrated by Thiele and coworkers (Thiele *et al.*, 1995 and 1997). Jessen and Orr (2002) showed how to combine the streamline approach with multicomponent analytical solutions for three-dimensional gas displacement problems, and Seto *et al.* (2003) applied that approach to the simulation of a gas condensate recovery process. Several investigators have shown that effects of gravity can be represented by operator splitting (e.g. Crane *et al.*, 2000; Jessen and Orr, 2004). Thus, there is considerable evidence that compositional streamline methods can be applied to describe the interaction of compositional effects associated with component transfers and dissolution that occur in CO_2 sequestration processes.

We begin by describing how to improve the computational efficiency of streamline simulation when applied to CO_2/brine systems. Then we report a comparison of streamline simulations with equivalent black-oil formulations to assess the efficiency and accuracy of existing technology relative to that of compositional streamline simulation. The comparison of the streamline approach with a black-oil finite volume approach was chosen due to the simplicity and efficiency of the black-oil models over finite volume compositional models. Finally, we discuss the limitations of the streamline approach.

2. COMPOSITIONAL EFFECTS

For given temperature, pressure and salinity, the solubility of CO_2 in the aquifer and the amount of water vapor that is present in a CO_2-rich gas phase in equilibrium with CO_2 saturated brine can be predicted by a standard equation of state, e.g. Peng-Robinson, using a non-symmetric binary interaction coefficient matrix (Yan *et al.* (2004), Kumar *et al.* (2005)). The densities and viscosities of the equilibrated phases can also be predicted quite accurately using an appropriate set of temperature dependent volume translation parameters.

Given that the system in question is a binary system with only one independent phase mole fraction ($x_2 = 1\text{-}x_1$), very efficient calculation of the phase behavior in compositional simulation can be performed using a K-factor lookup table generated prior to performing the streamline calculation. During the initialization of a given injection calculation, temperature, salinity and expected pressure range are estimated and a one dimensional table (pressure as independent variable) is generated for the equilibrium K-factors, phase densities and viscosities. During the actual simulation, mole fractions of vapor and phase compositions can be calculated explicitly given the pressure (K-factors) and an overall composition ($\underline{z}$) from

$$\beta = -\frac{(z_1\alpha_1 + z_2\alpha_2)}{\alpha_2\alpha_1}, \quad \alpha_i = z_i(K_i - 1) \tag{1}$$

and

$$x_1 = \frac{z_1}{1 - \beta + \beta K_1}, \qquad y_1 = K_1 x_1 \tag{2}$$

Eq. (1) is used to test if an overall composition is in the two-phase region at a given pressure. For values of β between 0 and 1, equilibrium phase compositions are evaluated from Eq. (2) whereas the corresponding phase densities and viscosities are evaluated from look-up tables using an appropriate interpolation scheme. For single phase mixtures ($\beta<0$ or $\beta>1$), density

and viscosity is evaluated directly the equation of state. Fig. 1 shows the variation of equilibrium K-factors as a function of pressure for the CO_2-brine system at 298K.

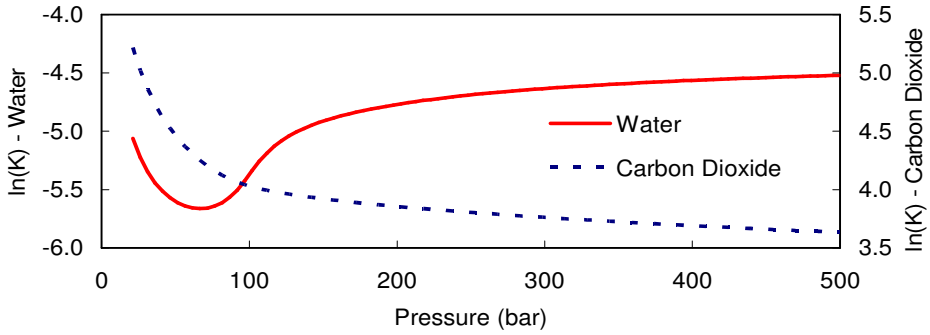

FIGURE 1: Equilibrium K-factors for CO_2 – Brine (250000 ppm) at 298K.

The CPU time for performing 10^6 equilibrium calculations at random pressures between 1 and 500 bar and random feed compositions, was found to be an order of magnitude less for the look-up table approach than that of a general state of the art flash algorithm.

3. CALCULATION EXAMPLES

The lookup-table approach described above has been implemented in the compositional streamline simulator CSLS (Gerritsen *et al.* 2005) and tested for a range of displacement calculations. To compare the compositional streamline approach with a commercial black-oil simulator, an equivalent black-oil representation of the phase behavior was generated by simulating a differential depletion experiment (DDE) with the thermodynamic module of CSLS. Throughout the comparison, the temperature of the aquifer in question is assumed to be constant at 323K. The black-oil properties at this temperature along with relative permeability functions used in the reported calculation examples are shown in Fig. 2. In a black-oil formulation, the solubility of CO_2 in the brine is modeled by a solution gas-water ratio (R_S)

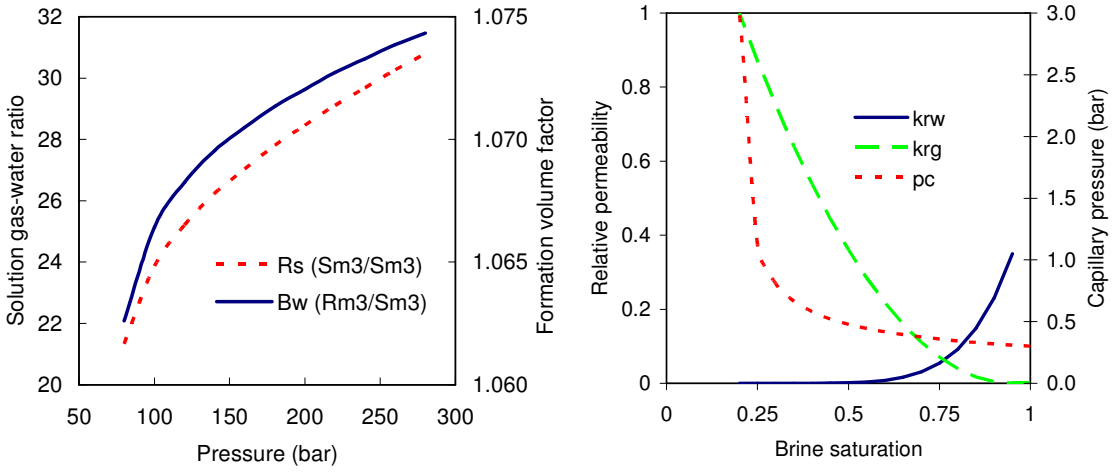

FIGURE 2: Black oil properties (a) and saturation functions (b) used in calculation examples.

Initial calculations were performed for a one-dimensional (1D) domain to gauge the impact of capillary forces on the displacement behavior. The saturation profile predicted by the streamline calculation (CSLS) is compared in Fig. 3 with fully implicit (FIM) black-oil calculations, with and without inclusion of effects of capillary pressure.

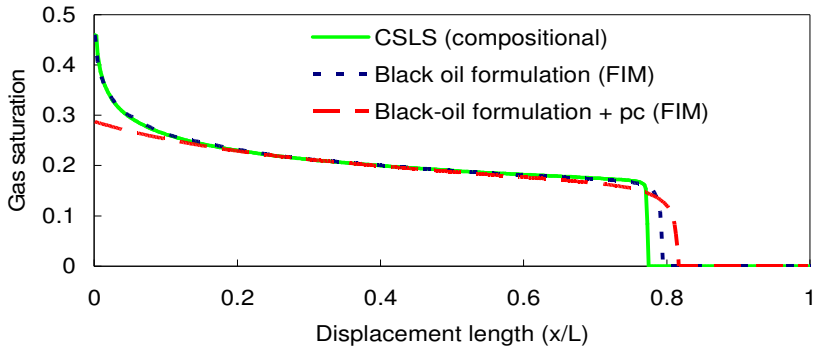

FIGURE 3: 1D displacement calculations using CSLS and FIM: Impact of capillarity.

Fig. 3 suggests that capillarity plays a more significant role near the injection point than around the leading edge of the displacement. In this drainage process capillarity opposes a reduction in the brine saturation towards the residual near the injection boundary. The overall effect of capillarity on the displacement characteristics, however, is seen to be minor. Additional considerations about the impact of capillarity in 3D displacements are given in the discussion section.

To illustrate the efficiency of compositional streamline simulation, two three-dimensional (3D) models were investigated:

- Model A; a 1250m by 1250m by 100m section of a heterogeneous aquifer was represented by a 50x50x10 computational grid (25000 active cells).
- Model b; a 4500m by 4500m by 160m section of a heterogeneous aquifer was represented by a 180x180x16 computational grid (518400 active cells).

The permeability variation within the computational domain of Model B is shown in Fig. 4.

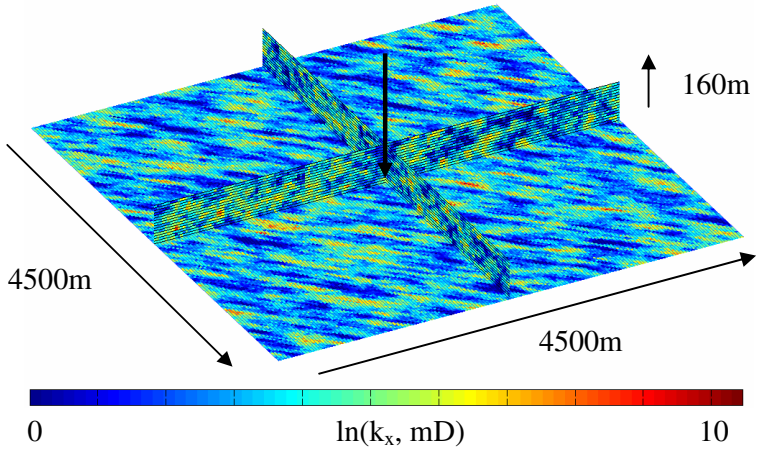

FIGURE 4: Permeability heterogeneity of Model B

The average permeability of Model B is 100mD, and the average porosity is 0.3. The initial pressure at the top of the aquifer is 90 bars, and CO_2 is injected at 150 bars in the center of the domain for 10 years corresponding to approximately 2.5% of the aquifer pore volume. Production wells were placed at the outer edges of the model and operated at a fixed bottom-hole pressure of 90 bar to mimic a constant pressure boundary condition. Fig. 5 compares the saturation distribution at the end of the injection period for the two simulation approaches. The two approaches are seen to be in good agreement.

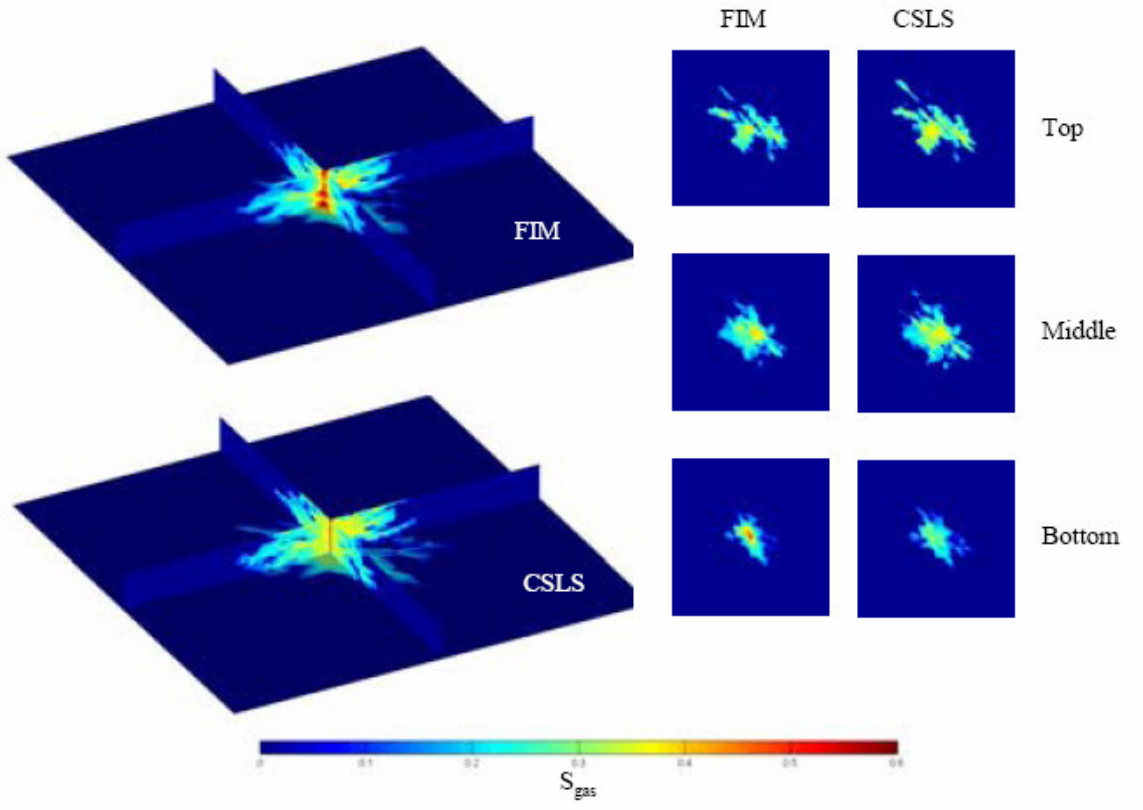

FIGURE 5: Distribution of CO_2 saturations after 10 years

In this setting, the flow of the injected CO_2 is strongly affected by gravity and permeability heterogeneity. The injected CO_2 rises to the top of the formation where the flow of the plume is then restricted to high permeability zones.

The CPU time for the streamline simulation was 21 min, whereas the time for running the equivalent black-oil simulation was 232 min. The modest computation time clearly demonstrates the potential of compositional streamline simulation to allow for uncertainty assessment through multiple realizations of the model parameters in a reasonable time frame. An equivalent compositional finite difference calculation is not currently feasible due to the global time step restriction in IMPES models or the more diffusive nature of fully implicit (FIM) that may render the displacement calculations less accurate. These example computations demonstrate, therefore, that high resolution, three-dimensional, field-scale streamline simulations can be performed with quite reasonable computation times. A summary of CPU requirements for the flow settings investigated is given in Table 1.

TABLE 1: Comparison of CPU requirements for 3D calculations: 2.8GHz

Model	N_{cells}	CSLS	FD-FIM	Ratio
A	25000	0.7 min	6 min	9
B	518400	21 min	232 min	11

Speed-up factors for 3D displacement calculations were found to be in the range of an order of magnitude. Additional increase in the speed-up factors is expected for larger computational domains where the pressure solves become increasingly CPU-time consuming. In the comparison presented, no effort was put towards optimization of the time-step control parameters of the FIM scheme that was run with the default parameter set. We emphasize, also, that the compositional streamline simulator used in this work is a research code that has not yet been fully optimized.

4. DISCUSSION

We have demonstrated that the proposed streamline formulation is significantly less CPU intensive than existing methods for the flow settings typically encountered during the injection phase of CO_2 sequestration in saline aquifers. For larger scale problems with more than 500K active grid cells, the run times for the proposed formulation are more than an order of magnitude lower than those for conventional numerical approaches.

Effects of capillarity are not included in the streamline approach but can be included in conventional approaches. To gauge the impact of capillarity on CO_2 plume development, black-oil simulations of Model A were performed including and excluding capillary pressure. Standard Leverett J-scaling was used to represent capillarity in the heterogeneous permeability field. The average permeability of the computational domain of Model A is 90mD with an average porosity is 0.3. CO_2 was injected at a constant rate of 2000 Rm^3/day for a period of 3 years corresponding to ~5% of the pore volume. The results of the three simulations are compared in Fig. 6, which shows the CO_2 distribution (gas saturation) within the computational domain at the end of the injection period.

Differences between the three simulations are quite small, which suggests that gravity and viscous forces dominate the displacement process. This, in turn, suggests that capillarity may be neglected, as in compositional streamline simulation, for a range of sequestration projects. Capillary forces resist invasion of non-wetting phase (CO_2) in low permeability zones. This, in turn, acts to reduce the amount that locations of streamlines will change as the simulation progresses. Reduced movement of streamlines during the injection period works in favor of the accuracy of the streamline approach, where streamlines are updated only periodically to account for effects of mobility changes and gravity segregation. However, a more detailed study is required to fully understand and map out the limitations of the streamline approach for this type of displacements. An initial investigation of the limitations of streamline methods, covering a full range of capillary to viscous forces, is reported for displacements in layered 2D systems by Sam-Olibale (2002).

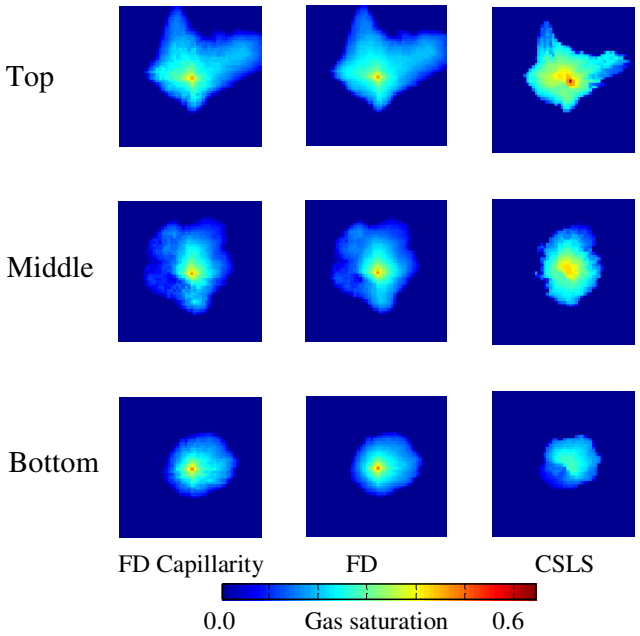

FIGURE 6: Effects of capillarity on CO_2 plume

For post-injection time scales, where gravity-driven flows, diffusion of dissolved CO_2, residual trapping of CO_2 due to flow reversal and CO_2 saturation reduction as a result of additional dissolution, and geochemical reactions become important mechanisms determining the long term fate of injected CO_2, computational methods other than the streamline approach will be more appropriate.

5. CONCLUSIONS

Based on the results presented we conclude that:

- Compositional streamline simulation is an efficient and accurate technique for predicting the injection phase of CO_2 injection in saline aquifers.
- CPU requirements for the streamline approach are an order of magnitude less than fully implicit black-oil modeling. The speed-up factor is expected to increase with increasing size of aquifer model.
- Compositional streamline simulation is efficient enough to allow its use in uncertainty assessment frameworks in which a large number of realizations must be run within a reasonable timeframe.

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