Comparison of Two CO_2 EOS Algorithms: Minor Contrasts in State Properties may Translate to Significant Contrasts in Predicted Migration Histories

Weon Shik Han, Brian McPherson, Michael Raines, Anthonius Sulaiman
New Mexico Institue of Mining and Technology, Kinder Morgan CO_2 company

Abstract

Two different EOS algorithms were assembled and compared - one is a Modified Redlich-Kwong (MRKEOS) and the other is Span and Wagner's (SWEOS). In general, results of state properties for the two algorithms were consistent, except for solubility of CO_2 in groundwater/brine; the MRKEOS underestimates solubility of CO_2 in water when compared to experimental data. However, the primary purpose of this study was not just comparison of the state properties calculated by each EOS, but rather how any differences in predicted state properties propagate into contrasts in flow and transport of CO_2 and, ultimately, in contrasting predictions of CO_2 migration and fate.

Problem statement

Diverse numerical codes such as TOUGH2, TOUGHREACT, PHREEQC, NUFT, CHRUNCH, chemTOUGH and GEM-GHG have been applied to research related to CO_2 sequestration (Johnson, 2001; Pruess and Garcia, 2002; Doughty and Pruess, 2004; Nghiem et al., 2004; Gaus et al., 2005; Knauss et al., 2005; White et al., 2005). Certain numerical codes include lookup tables representing thermophysical properties. In other studies, less accurate EOSs were used to the overcome excessive computational time requirements.

As described, many EOSs have been developed and applied to simulation of CO_2 sequestration. However, no previous research focused on how individual EOSs might impact the migration of Co_2.

- Water: IFC (1967), IAPWS -IF (1997), Saul and Wagner (1987), Hill(1990), Wagner and Prub (2002)
- CO_2 : Ideal gas law (1834), Van der Waals (1873), Virial equation, Redlich-Kwong (1949), Soave, (1972), Peng-Robinson (1976), Span and Wager (1996)
- Mixture : Anderson et al (1992), Duan et al., (1996)
- Solubility : Diamond and Akinfiev (2003), Duan and Sun (2003), Spycher et al. (2003), Sorenson et al. (2003), Spycher and Pruess, (2005)

Assembly of EOSs

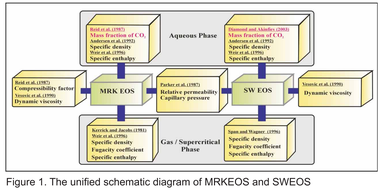


Figure 1. The unified schematic diagram of MRKEOS and SWEOS

The MRKEOS employs modification of the van der Waals equations, while the SWEOS utilizes an empirical representation of the fundamental equation of Helmholtz energy. Both EOSs algorithms were assembled for calculating thermophysical properties, including density, fugacity, enthalpy, viscosity, and solubility of CO_2 in gaseous and supercritical phases, and mixtures or solutions of CO_2 in water as functions of pressure and temperature.

Interrelationship of thermophysical propeoties

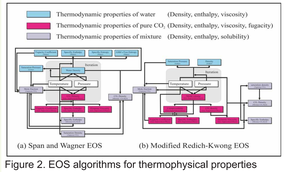


Figure 2. EOS algorithms for thermophysical properties

Figure 2 describes the interrelation between thermophysical properties within the integrated EOS algorithms. The gray box shows the location where the primary variables are switched into pressure and temperature. The arrows indicate the direction of the input parameters for the subsequent calculation of thermophysical properties.

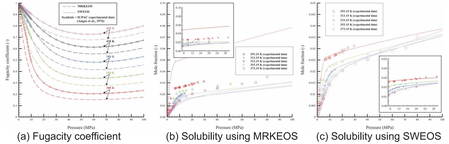


Figure 3. Thermophysical properties of pure CO_2 with experimental data

It should be emphasized that all thermophysical properties are interrelated within the integrated EOSs. As a result, the lower predicted fugacity coefficients from MRKEOS clearly affect the calculated values of mole fractions even though the solubility algorithm is correct in MRKEOS.

Errors generated by fugacity coefficient discrepancy affect subsequent calculations. The calculation of solubility requires fugacity coefficient as an input parameter (see Figure 2). The discrepancy is illustrated in the solubility plots (Figure 3). The discrepancy of solubility originates from underestimation of fugacity coefficients.

Comparison between MRKEOS and SWEOS

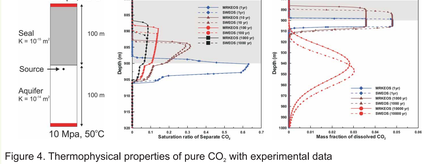


Figure 4. Thermophysical properties of pure CO_2 with experimental data

(1) Mass fractions of dissolved CO_2 from SWEOS are greater than MRKEOS. (Effect of solubility discrepancies)

(2) The rate of gravitational segregation from SWEOS is greater than that from MRKEOS. (Effect of mixture density)

(3) Gravitational segregation is going to be dominant after all separate phase CO_2 is dissolved.(Effect of relative permeability)

The mass fraction from both MRKEOS and SWEOS was respectively 0.038 and 0.050 at this simulation condition. Although the difference (0.050-0.038=0.012) of mass fraction between MRKEOS and SWEOS is small, the actual mass contrast in CO_2 between MRKEOS and SWEOS is huge (see Figure. 5)

(1) The value of maximum difference was 259 tons at 2000 yr. The 259 tons is 12% of the total injected CO_2 (2160 tons).

(2) All mass of separate CO_2 converted into dissolved CO_2 after 4000 yr by SWEOS. However, MRKEOS required 6000 yr to store CO_2 as a complete dissolved phase.

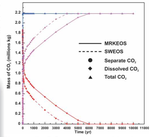


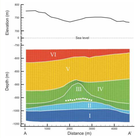
Figure 5. CO_2 mass partitioning between MRKEOS and SWEOS

Case study: EOSs comparison

Figure 6. Location of SACROC

The SACROC Unit is the oldest CO_2 Enhanced Oil Recovery (EOR) operation in the United States, with CO_2 injection since 1972 years.

CO_2 injection: about 13.5 million tons CO_2/yr
CO_2 recycling: about 7 million tons CO_2/yr
Net storage of about 6.5 million tons CO_2/yr
Total accumulation: more than 55 million tons CO_2.



- Model size: 4685 m x 274.5 m
- Six stratigraphic features
- Upper and bottom boundaries: Dirichlet boundary
- Lateral boundaries: No flow
- 13 CO_2 injection wells : 60 thousands tons of CO_2 during 30 years.

Unit	Formation	Kx (m^2)	Porosity
I	Lower Strawn	10^{-14}	0.20
II	Upper Strawn	10^{-15}	0.20
III	Cisco&Canyon	10^{-14}	0.25
IV	Wolfcamp SH	10^{-17}	0.15
V	Wolfcamp SS&SH	10^{-16}	0.20
VI	Wolfcamp LS	10^{-14}	0.25

Figure 7. SACROC unit of the Horseshoe atoll, in western TX

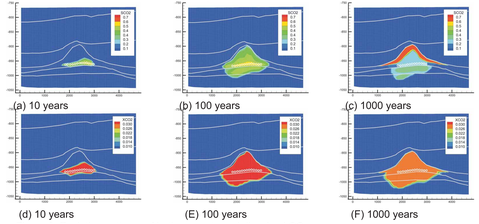


Figure 8. Evolution patterns of both separate and dissolved CO_2

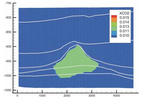


Figure 9. Discrepancy of dissolved CO_2 between MRKEOS and SWEOS at 1000 years

The Wolfcamp shale acts as seal unit at 1000 years simulation (Figure 8). Most of separate CO_2 has accumulated just below the seal and shows the highest saturation ratio.

Figure 9 is a comparison between MRKEOS and SWEOS at 1000 years

Brine EOS sensitivity analyses

Adams and Bachu (2002) recognized the importance of brine state properties and provided critical reviews about the currently available density and viscosity algorithms of brine. However, most of previous research conducted mainly compared EOSs with experimental data and did not consider the detail aspect of how the individual EOS algorithms might affect the transport of sequestered CO_2. Therefore, sensitivity analyses were conducted to investigate how brine density, viscosity, and CO_2 solubility may affect the transport of separate CO_2 at various concentrations.

Algorithms of density, viscosity, and solubility within SWEOS were replaced algorithms representing brine (Figure 2)

Density: Batzel and Wang (1992)
Viscosity: Palliser and Mckibbin (1998)
Solubiliy: Duan and Sun (2003)

Density and solubility EOS is critical. However, viscosity EOS is apparently not critical to CO_2 migration.

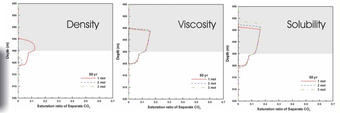


Figure 9. Sensitivity analysis of separate CO_2 along various concentration at 50 years

Case study: Prediction of CO_2 migration at SACROC, TX

Geologic framework from Geophysical data

A geologic model has been built for quantifying naturally occurring porosity and permeability distribution at Northern Platform in SACROC by the Texas Bureau of Economic Geology. This model was based on analyzing the results of three dimensional seismic surveys and data from four hundred wells. This geologic model consists of the Pennsylvanian group, Cisco and Canyon, which are the most oil producing formations in Northern Platform. The approximate size of model is 4000 m wide and 10,000 m long.

Upscaling of porosity and permeability

Upscaling is a technique that reduces the number of elements by increasing the size of elements. Although the geologic model characterizes the natural heterogeneity in Northern Platform, the application to multiphase flow is still constrained due to the enormous number of elements.

Upscaling of porosity is relatively easy compared to that of permeability. However, permeability generally shows directional variability. We obtained upscaling algorithms developed through equivalent resistor network model (King, 1989)

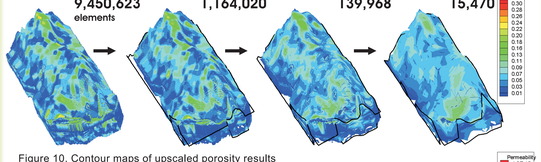


Figure 10. Contour maps of upscaled porosity results

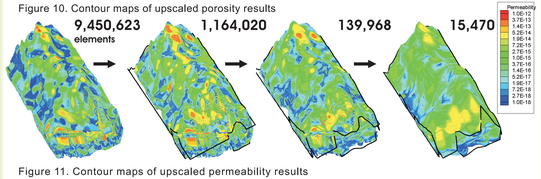


Figure 11. Contour maps of upscaled permeability results

History matching analysis

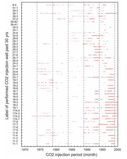


Figure 12. History of CO_2 injection activity past 30 years and location of CO_2 injection

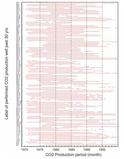


Figure 13. History of CO_2 Production activity past 30 years and location of CO_2 production well

3,048,845,748kg (13 millions tons) of CO_2 has been injected at 51 wells during past 30 years
6,104,258,074kg (6 millions tons) of CO_2 has been produced at 119 wells during past 30 years
6,944,587,674 kg (7 millions tons) of CO_2 currently accumulated at North platform in SACROC.

Top boundary: No flow
- Bottom boundary: No flow
- Eastern and western boundaries: Constant
- Salinity: 159,000 mg/l (Vest et al., 1970)

- 40 CO_2 injection wells: 0.13 millions tons from 1970 to 2000
- 55 CO_2 production wells: 0.65 millions tons from 1970 to 2000
- Total simulation: 100 years from 1970 to 2070

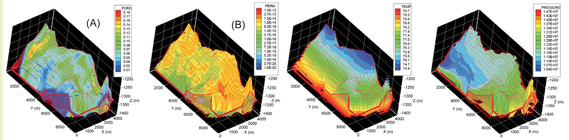


Figure 14. Initial condition after 10,000 year (a) porosity, (b) permeability (m^2), (c) temperature (°C), (d) pressure (Pa)

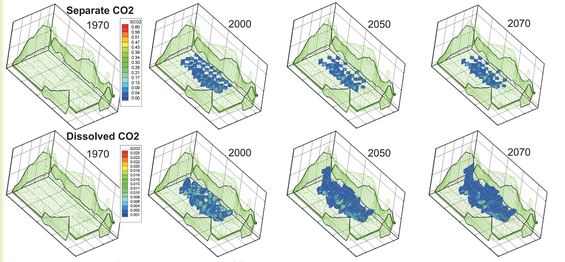
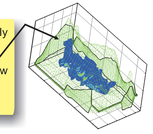


Figure 15. Prediction of separate and dissolved CO_2 distribution

Current model is developed based on
(1) Realistic geometry of Cisco and Canyon formation
(2) Realistic porosity and permeability field
(3) Reasonable estimated source histories

(1) Separate CO_2 more widely distributed at western flank
(2)Existence of preferential flow pathway at northern part of reef