Supplementary file

Three-dimensional simulation of geologic carbon dioxide sequestration using MRST

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Validation of implementation: Phase composition and PVT output

Figs. S1-S5 provide the validation of our implementation. The different validation data are listed in the figure captions and legends, and, whenever possible, plotted alongside the results of our implementation. Figs. S1-S3, in particular, validate the calculations to obtain the gas-oil solution ratio (R_s), brine formation-volume factor (B_b), and phase dynamic viscosities (μ), while Figs. S4 and S5 provide comparisons to experimental data on density and viscosity of the CO_2 and aqueous phase, respectively.
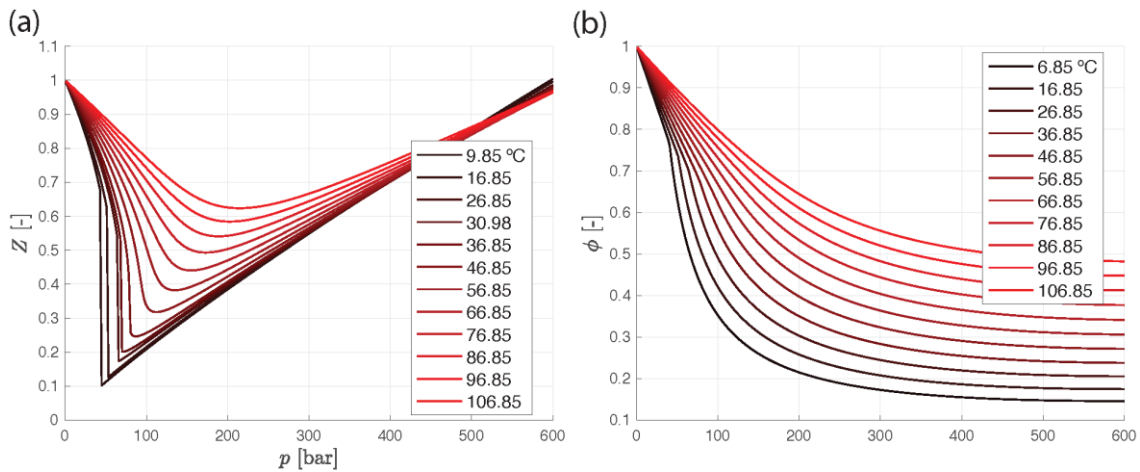

Fig. S1. Predicted CO_2 coefficients: (a) Compressibility factor (Z), cf. Fig. 8 in Spycher et al. (2003), and (b) fugacity coefficient (ϕ), cf. Fig. 9 in Spycher et al. (2003).

As noted in the main text, we compute the CO_2 density from Redlich and Kwong (1949). In Figs. S4(a) and S4(b), the results based on the Redlich-Kwong EoS are slightly off compared with some of the experimental data that were published later. Our implementation uses Fenghour et al. (1998)'s model to calculate the CO_2 viscosity, but, similar to Hassanzadeh et al. (2008), we neglect the critical enhancement term. This has negligible effects at reservoir temperature (typically at or above 40 ℃ for CO_2 storage), but leads to slight inaccuracies at lower temperatures, as shown in Figs. S4(c) and S4(d).

The density of pure water and sodium chloride brines is computed using the correlation provided by Rowe Jr and Chou (1970). We then use the correlation by Garcia (2001) to compute the density of aqueous solutions with dissolved CO_2. The experimental results provided by Yan et al. (2011) demonstrate that this correlation approximates adequately the density of aqueous solutions of CO_2 (Fig. S5(a)). Finally, we compute the viscosity of aqueous solutions using the model by Islam and Carlson (2012). Comparing Fig. S5(b) to their Fig. 7 shows negligible differences for the $H_2O + CO_2$ (saturated) and $H_2O + NaCl$ (1m) $+ CO_2$ (saturated) lines. These differences can be explained by slight discrepancies in the mass fraction of CO_2 at saturation.
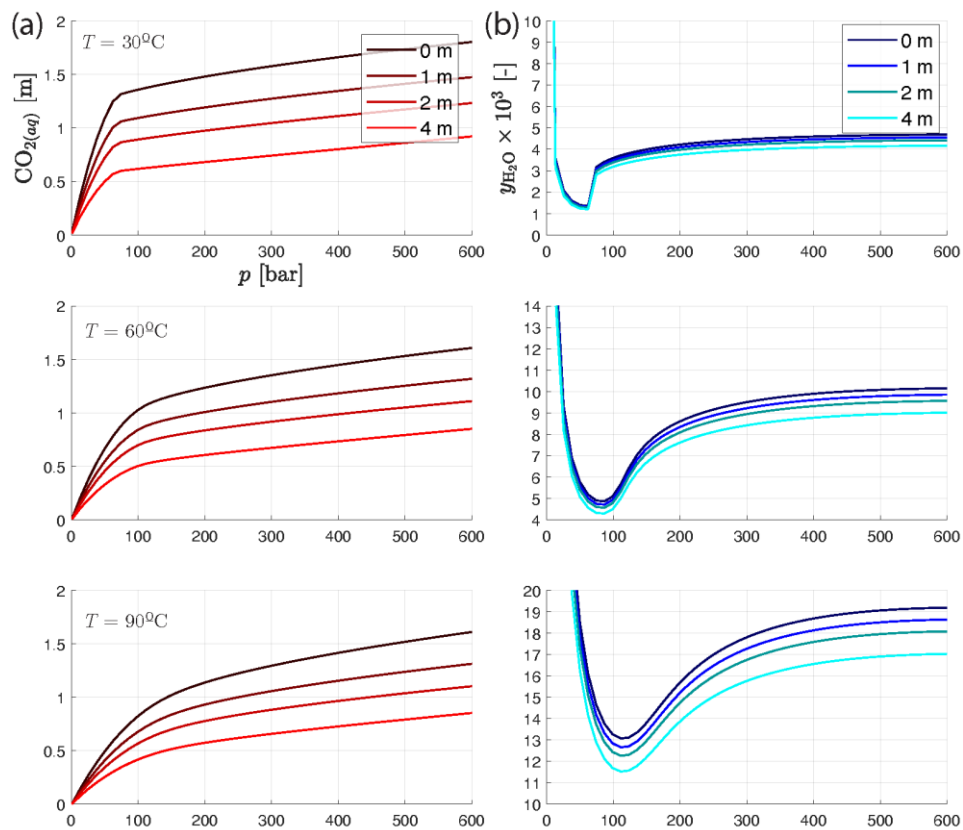

Fig. S2. Predicted mutual solubilities at 30, 60, and 90 °C for 0-4 molal sodium chloride brines. Solubilities are expressed as: (a) Molality of CO_2 in the aqueous phase, and (b) 1000 × the mole fraction of H_2O in the gaseous phase. Cf. Fig. 2 in Spycher and Pruess (2005).
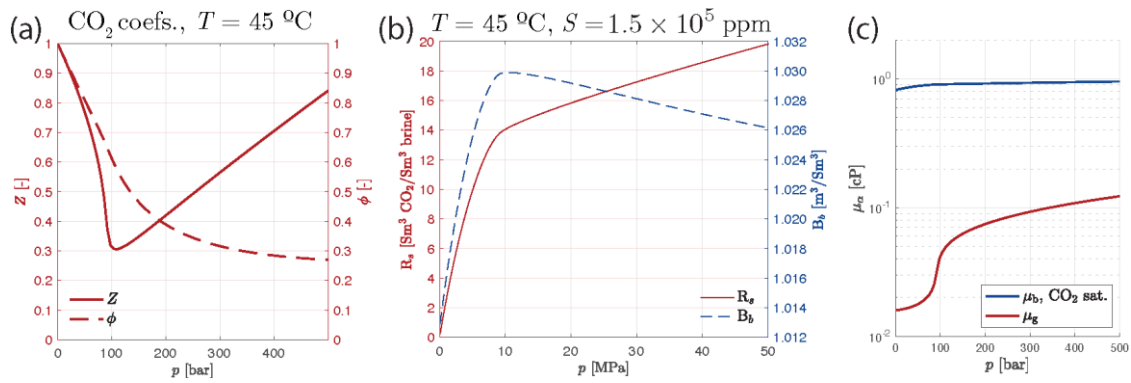
Fig. S3. Comparison to results by Hassanzadeh et al. (2008): (a) Gas compressibility factor and fugacity coefficient (cf. their Fig. 5c), (b) gas-oil solution ratio (R_s) and brine formation volume factor (B_b; cf. their Fig. 5a) and (c) dynamic viscosities (μ) neglecting water vaporization (cf. their Figs. 5(b), 5(d)). There are minor differences in brine viscosity with respect to their Fig. 5b, because they neglect the effect of dissolved CO_2.
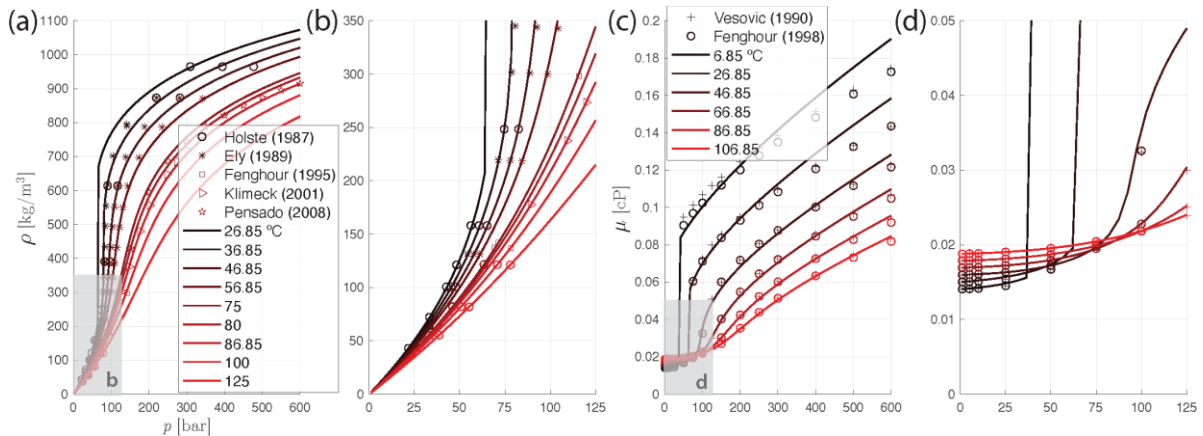

Fig. S4. CO_2 properties: (a)-(b) Density compared to experimental measurements by Holste et al. (1987), Ely et al. (1989), Fenghour et al. (1995), Klimeck et al. (2001), and Pensado et al. (2008); and (c)-(d) viscosity compared to tabulated data by Vesovic et al. (1990) and Fenghour et al. (1998).
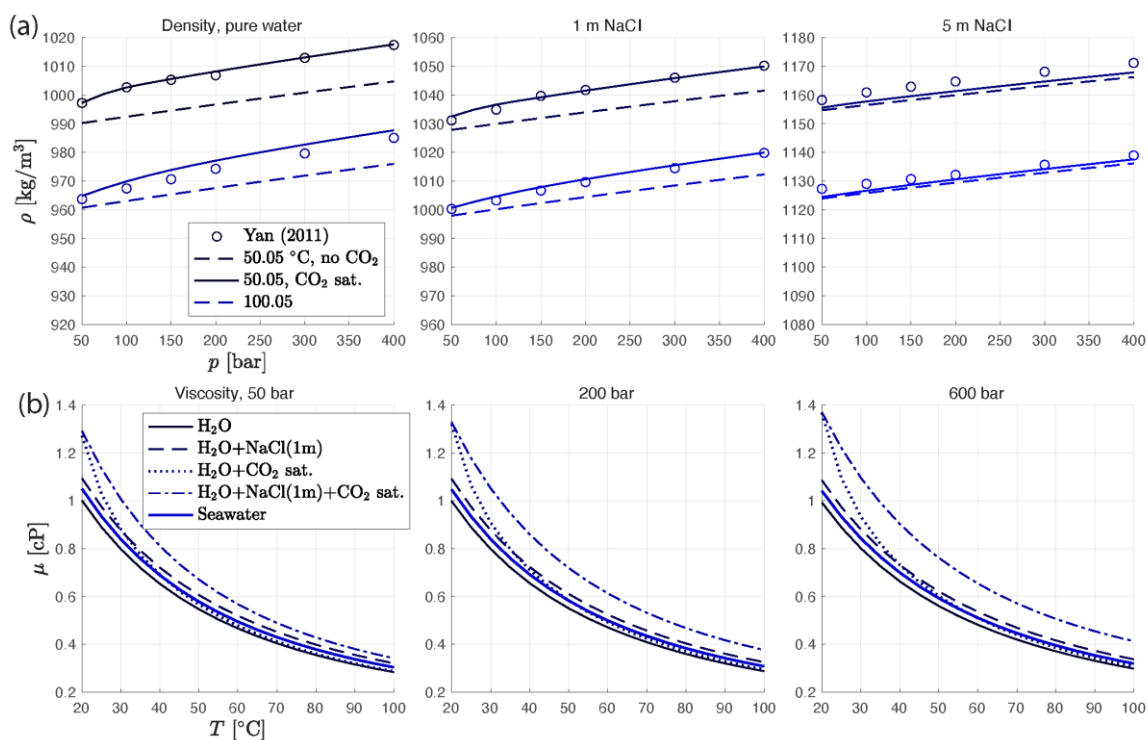
Fig. S5. Pure water, brine, and CO_2-saturated aqueous phase properties: (a) Density as a function of P at $T = 323.2$, 373.2 K compared to experimental measurements by Yan et al. (2011) (see their Figs. 14, 15 and 16), and (b) viscosity as a function of T, shown at $P = 50$, 200 and 600 bar (cf. Fig. 7 in Islam and Carlson (2012)).

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