

Introduction

CO₂ solubility trapping is an important CO₂ trapping mechanism in long-term CO₂ sequestration (CCS) in deep aquifers. An accurate representation of the capillary pressure is crucial in modeling CO₂ solubility trapping.

Usually, a P_c curve is either S-shaped (e.g., van Genuchten model) or convex (e.g., Brooks-Corey model). Their entry-pressure representations are different.

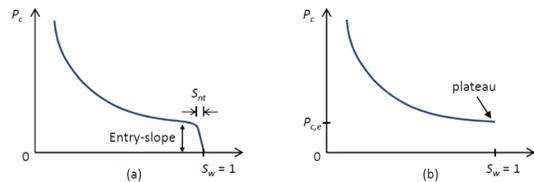


Figure 1: Capillary entry-pressure representations: (a) van-Genuchten-type (VG-type) representation; (b) Brooks-Corey-type (BC-type) representation.

Here, we show that the entry-pressure representation can greatly affect the rate of CO₂ solubility trapping, even when the S_{nt} is very small.

Why is this important?

- (1) The impact on simulation result can be huge.
- (2) Most CCS simulations employ one of the two P_c models.
- (3) The VG model is almost exclusively used in the simulations performed by TOUGH2.

Simulation Model

2D vertical cross-section (x and z directions) of the benchmark model of Dahle et al. (2009)^[1]

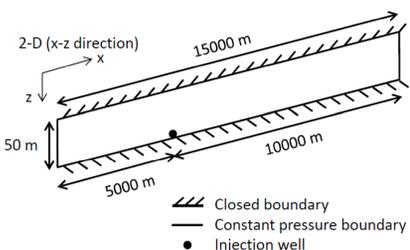


Figure 2: Sketch of the aquifer model.

Table 1: Properties of the aquifer model.

Name	Value
Grid number	$N_x = 150, N_y = 1, N_z = 40$
Gridblock size	$d_x = d_y = 100 \text{ m}, d_z = 1.25 \text{ m}$
Permeability	$k_x = k_y = k_z = 100 \text{ md}$
Porosity	$\phi = 0.15$
Dip	1 %
Depth at the well	3025 m
Temperature	84.4 °C
Salinity	0

$$k_{rw} = (S_w^*)^4, k_m = 0.4[1 - (\hat{S}_w)^2](1 - \hat{S}_w)^2, \quad (1a)$$

$$S_w^* = (S_w - S_{wi}) / (1 - S_{wi}), S_{wi} = 0.2, \quad (1b)$$

$$\hat{S}_w = (S_w - S_{wi}) / (1 - S_{wi} - S_{nc}), S_{nc} = 0. \quad (1c)$$

$$P_c = P_{c,e} (S_w^*)^{-0.5}, P_{c,e} = 0.2 \text{ bar}. \quad (2)$$

Simulation Results – Base Case

Injection rate: 9000 metric ton / year; Injection time: 20 years.
Simulator: Stanford General Purpose Research Simulator (GPRS)
Fully Implicit Method.
Base case: Modify Eqn (2) into VG-type, $S_{nt} = 0.005$.

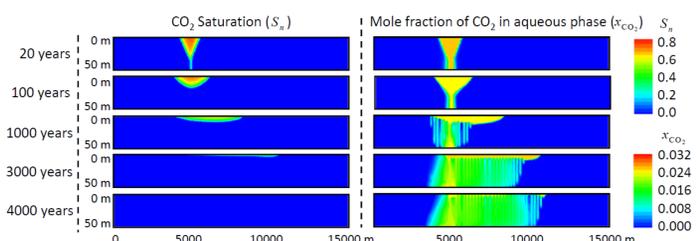


Figure 3: Base case simulation results. Hysteresis is not modeled for simplicity.

Entry-Pressure Representations

Keeping all other parameters unchanged, simulations are performed using different representations of the capillary entry pressure.

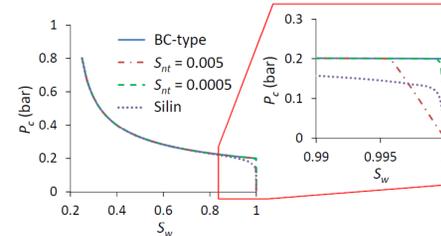


Figure 4: Different representations of the capillary entry pressure.

All four curves in Figure 4 are similar, except for the small difference near $S_w = 1$. However, these apparently small differences in the P_c curves lead to very large differences in the long-term predictions.

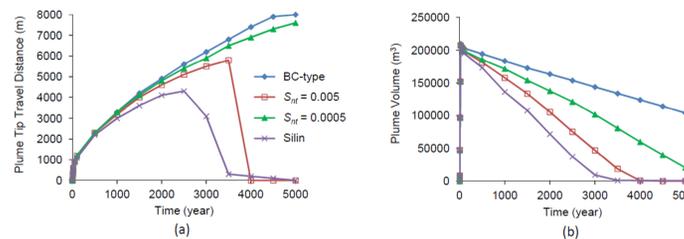


Figure 5: The sensitivity of simulation results to different entry-pressure representations.

Note that when dissolution is not modeled, the entry-pressure representation almost has no impact on simulation results.

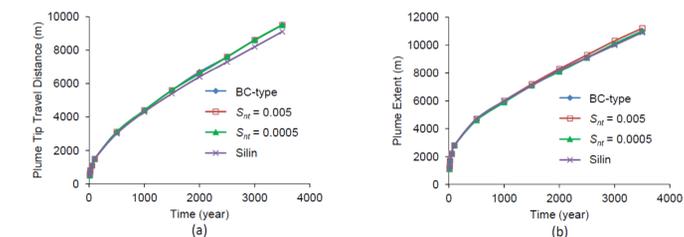


Figure 6: Simulation results when dissolution is not modeled.

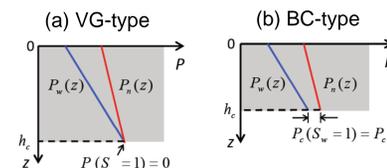
Causes of the Sensitivity

Gravity-capillary equilibrium:

$$P_w(z) = P_w|_{z=h_c} - r_w g (h_c - z), \quad (3a)$$

$$P_n(z) = P_n|_{z=h_c} - r_n g (h_c - z), \quad (3b)$$

$$P_c(z) = P_n(z) - P_w(z), \quad (3c)$$



Simulation: 1D vertical column of 50 m. Each gridblock is 1 cm in size. Initially, $S_n = 0.8$ at the top 0.8 m, below is 0. The simulated CO₂ saturation distribution under equilibrium match analytical solutions exactly.

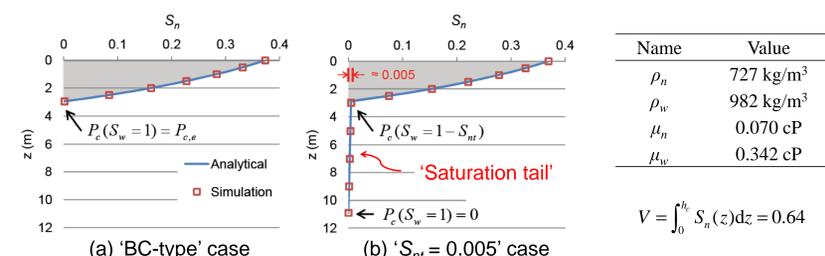


Figure 7: CO₂ saturation distribution under gravity-capillary-equilibrium (no dissolution).

The VG-type representation creates a 'saturation tail' under the major body of the CO₂ plume. This is **not a numerical artifact** – it is corroborated by analytical solutions. The 'tail' has almost no impact when dissolution is not modeled (e.g., Fig 6).

$$\text{Length of the 'saturation tail': } h_c^{VG} - h_c^{BC} \approx [P_c^{VG}|_{S_w=1} - P_c^{BC}|_{S_w=1}] / [(r_w - r_n)g], \quad (4)$$

When dissolution is modeled, the 'tail' can quickly dissolve, refill, and dissolve again. The cycle repeats, facilitating CO₂ dissolution.

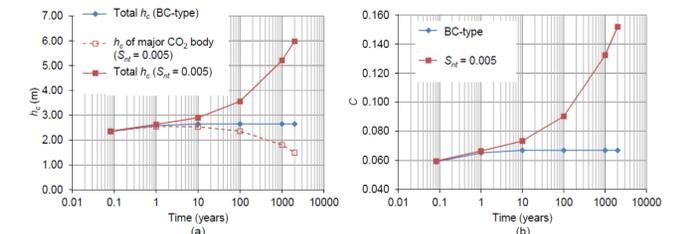


Figure 8: Development of the transition zone (dissolution is modeled). $C = \int_0^{h_c} x_{CO_2}(z) dz$

Characteristic time for the development of the transition zone [2]:

Important factors: $k_z, \Delta r, I = k_r / m, S_{nc}$ in Eqn (1c)

Density-driven convection is an important process in CO₂ solubility trapping [3,4]. We show that the VG-type representation facilitates the convection process.

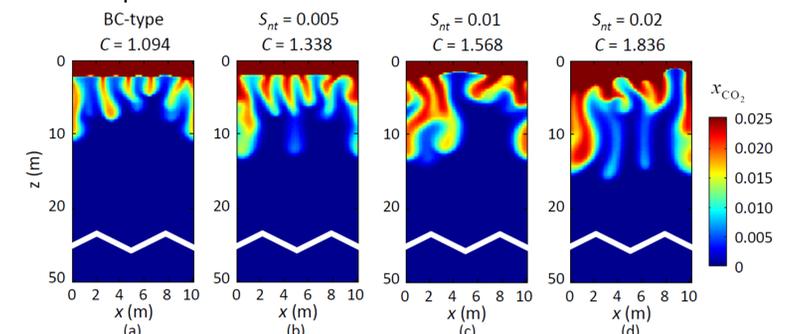


Figure 9: Influence of entry-pressure representation on density-driven convection.

Conclusions

- (1) VG-type capillary entry-pressure representation can accelerate CO₂ solubility trapping significantly, compared with the BC-type.
- (2) Simulation results are sensitive to the slope of the VG-type curve around the entry-pressure region.
- (3) Recognizing this problem is important to long-term CCS simulation.
- (4) We recommend using BC-type P_c model for its conservative estimates of CO₂ solubility trapping.

References

- [1] Dahle, H.K., et al. A Model-Oriented Benchmark Problem for CO₂ Storage, 2009; http://org.uib.no/cipr/Workshop/2009/CO2/benchmark_definition.pdf
- [2] Nordbotten, J. M. and H.K. Dahle, Impact of the Capillary Fringe in Vertically Integrated Models for CO₂ Storage, *Water Resour. Res.*, 47(2), W02537, 2011.
- [3] Ennis-King, J. and L. Paterson, Role of Convective Mixing in the Long-Term Storage of Carbon Dioxide in Deep Saline Formations, *SPE J.*, 10(3): 349-356, 2005
- [4] Riaz, A., et al., Onset of Convection in a Gravitationally Unstable Diffusive Boundary Layer in Porous Media, *J. Fluid Mech.*, 548, 87-111, 2006.

Acknowledgements

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