Effect of Heterogeneity and Geochemical Reactions on Dissolution-Induced Aqueous Phase Convection in the Long-Term Storage of CO_2 in Saline Formations

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Introduction

- **We need to predict the spatial distribution and phase partitioning of the CO_2 in the long-term (100-1000's years).**

- **Dissolved CO_2 increases the density of formation water and can induce slow convection in the aqueous phase**

- **Convection significantly accelerates the overall dissolution process.**

- **Previous work estimated the time of onset of convection, but ignored heterogeneity and possible chemical interactions.**

Challenges

- **Field-scale simulation requires upscaling of convective processes to coarse grids.**

- **Can the effect of heterogeneity on convection within a grid block be represented just by effective permeabilities?**

- **How strong is the coupling between convection and geochemistry? Will either consumption of CO_2 or permeability alteration change the rate of convection?**

Flow model

- 2D vertical cross-section, 25 m x 25 m.
- Porosity 20%, Permeability 10^{-13} m^2 (≈ 100 mD), k_v/k_h=0.5
- Top boundary condtion of constant dissolved CO_2
- pressure 20 MPa, temperature 90 C
- Small random perturbation (5%) added to permeability field.

Heterogeneity model

- A Markov chain Monte Carlo method (MCMC) is used to create a random distribution of thin horizontal shales, represented as ellipsoids of width w and thickness t, with shale volume fraction F_s.
- The effective vertical permeability k_v^{eff} of the whole domain is approximately given by

$$k_v^{eff} = k_v (1- F_s)/(1+ w F_s/(2 t))^2$$

(Begg and King, 1982). Accurate values for k_v^{eff} and k_h^{eff} are obtained by single phase flow simulations.

- The shale width w is varied, adjusting F_s and k_h so that k_v^{eff}, k_h^{eff} and k_v/k_h are constant.

Cases of heterogeneity

- Fix the coarse-scale permeabilities, while varying the fine-scale distribution of shales.

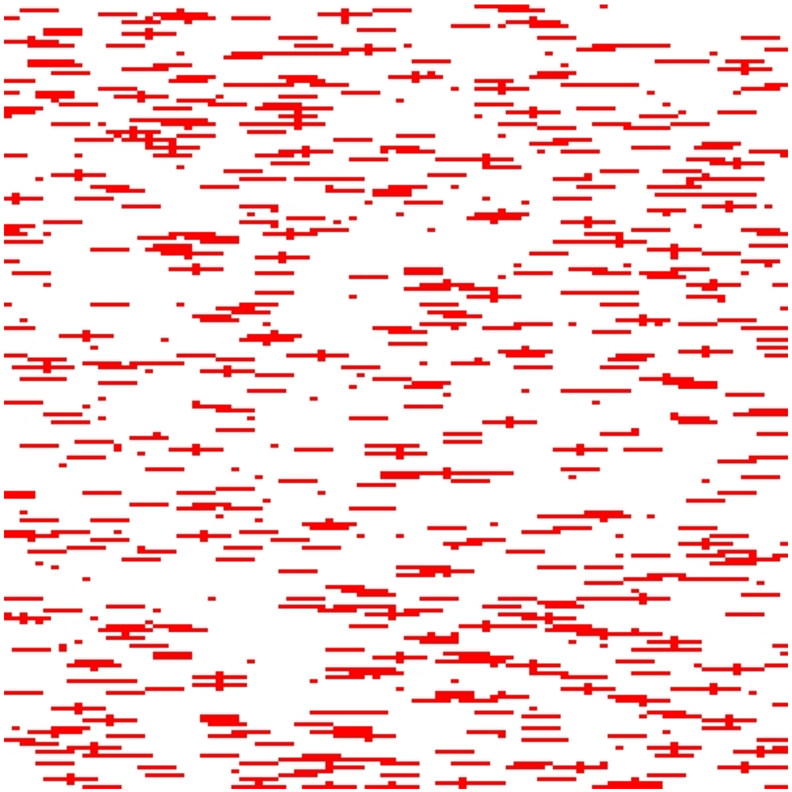
- In all cases, $t = 0.125$ m, $k_v/k_h = 0.5$, $k_h^{eff} = 8.53 \times 10^{-14}\ m^2$, and $k_v^{eff} = 1.67 \times 10^{-14}\ m^2$

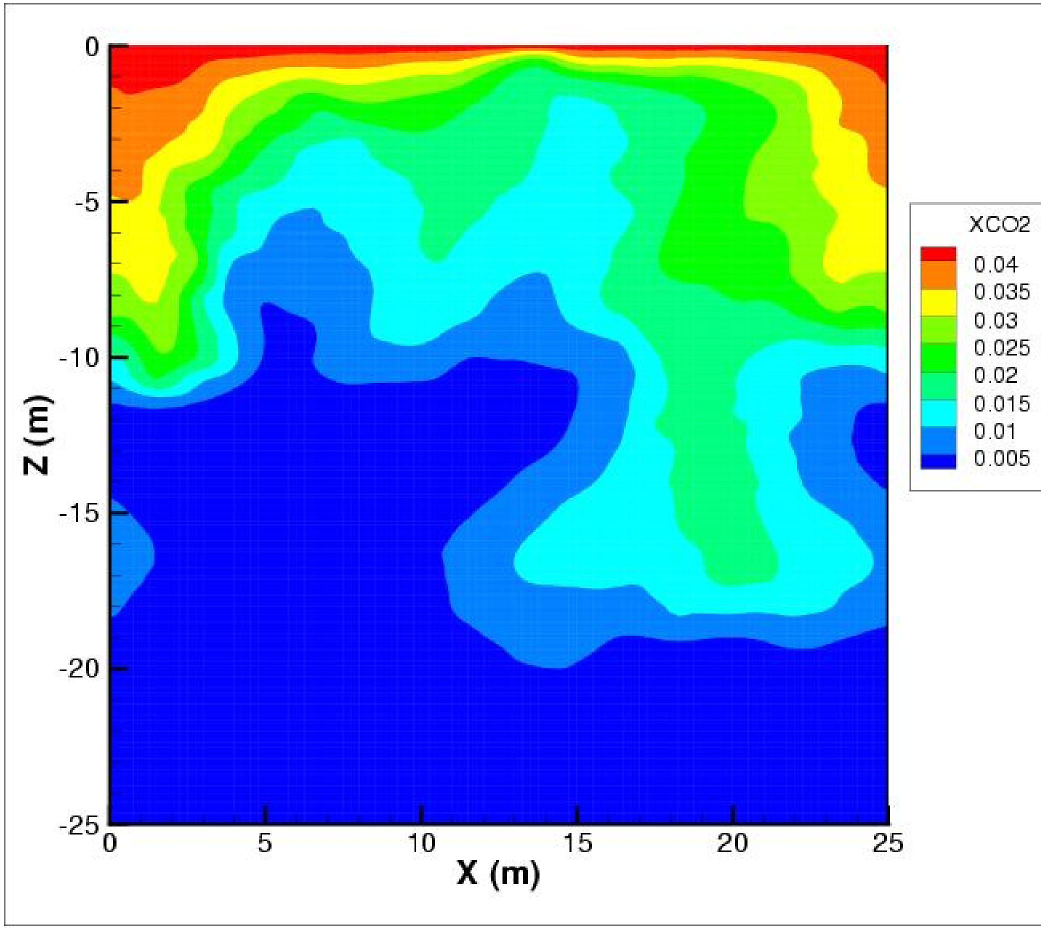
  – Case 1: $w = 1.5$ m. $F_s = 0.153$, $k_h = 1.17 \times 10^{-13}\ m^2$

  – Case 2: $w = 2.5$ m. $F_s = 0.1$, $k_h = 1.0 \times 10^{-13}\ m^2$

  – Case 3: Homogeneous permeability $k_v = k_v^{eff}$ and $k_h = k_h^{eff}$

Case 1 (w = 1.5 m) after 200 years





Shale distribution

Dissolved CO_2

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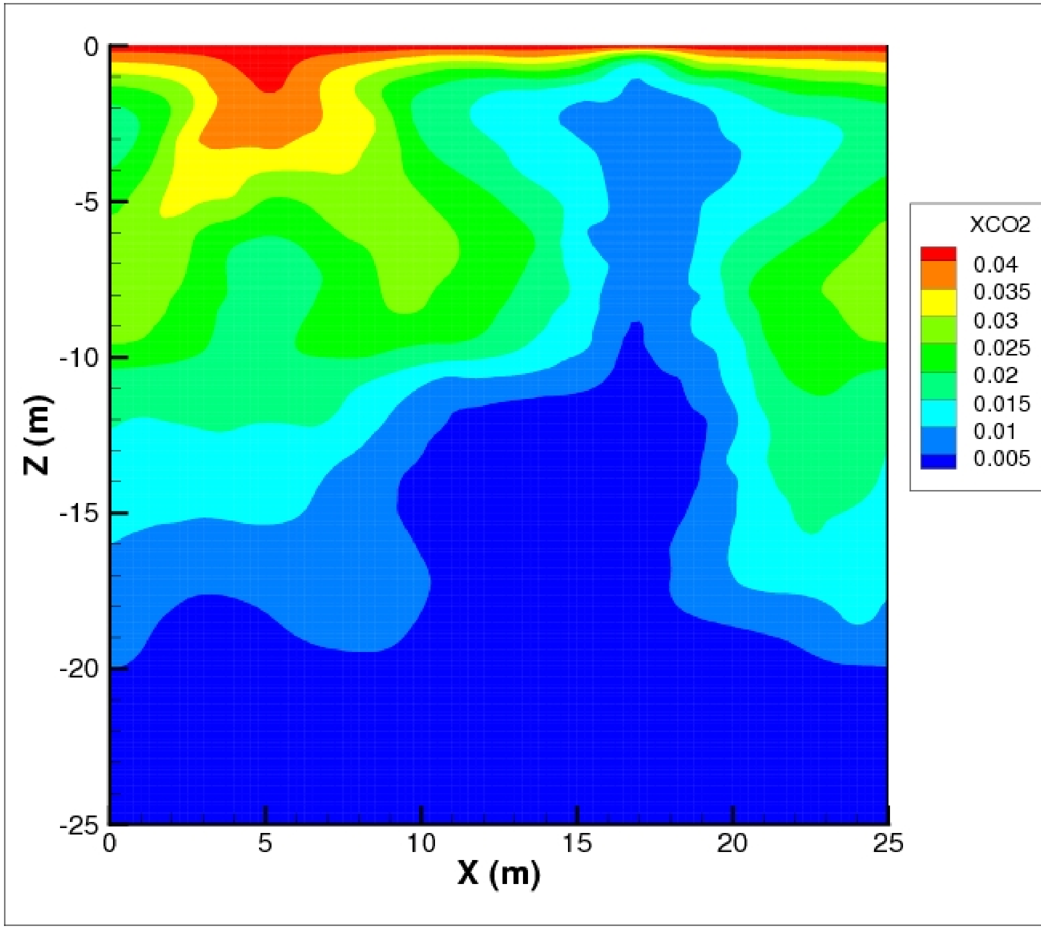
Case 2 (w = 2.5 m) after 200 years

Shale distribution



Dissolved CO_2

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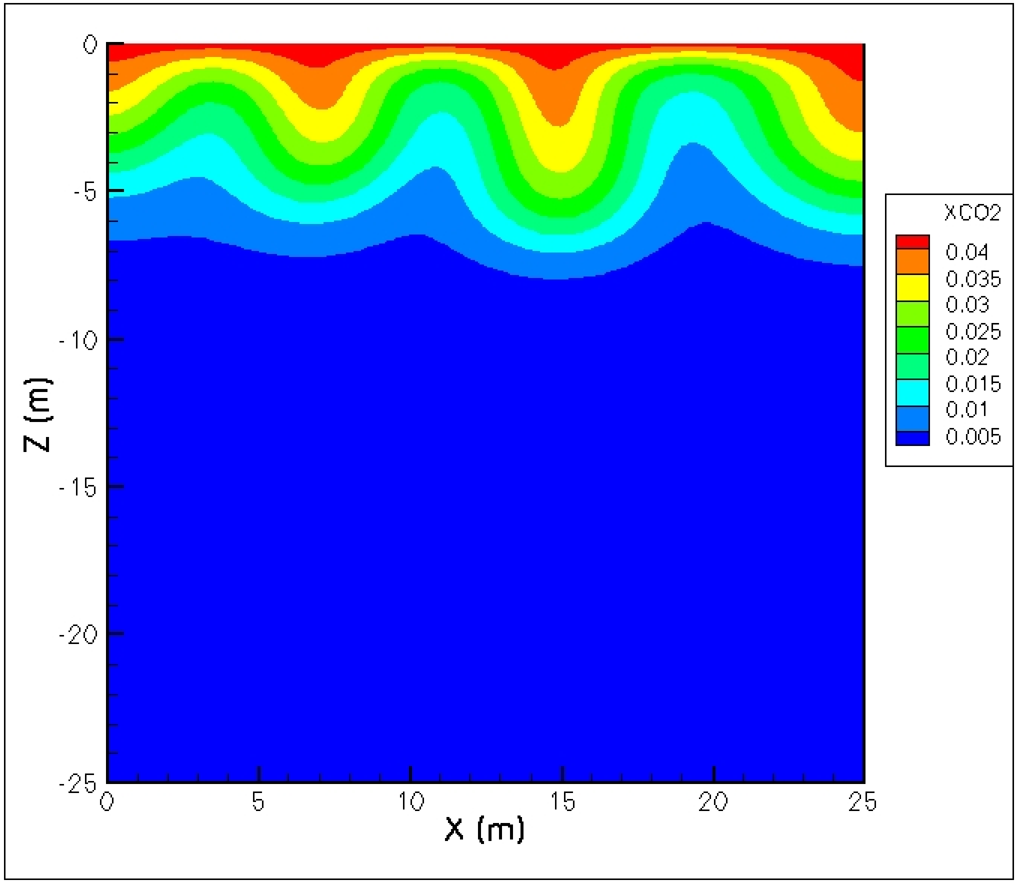
Case 3 (homogenous) after 200 years



Dissolved CO_2

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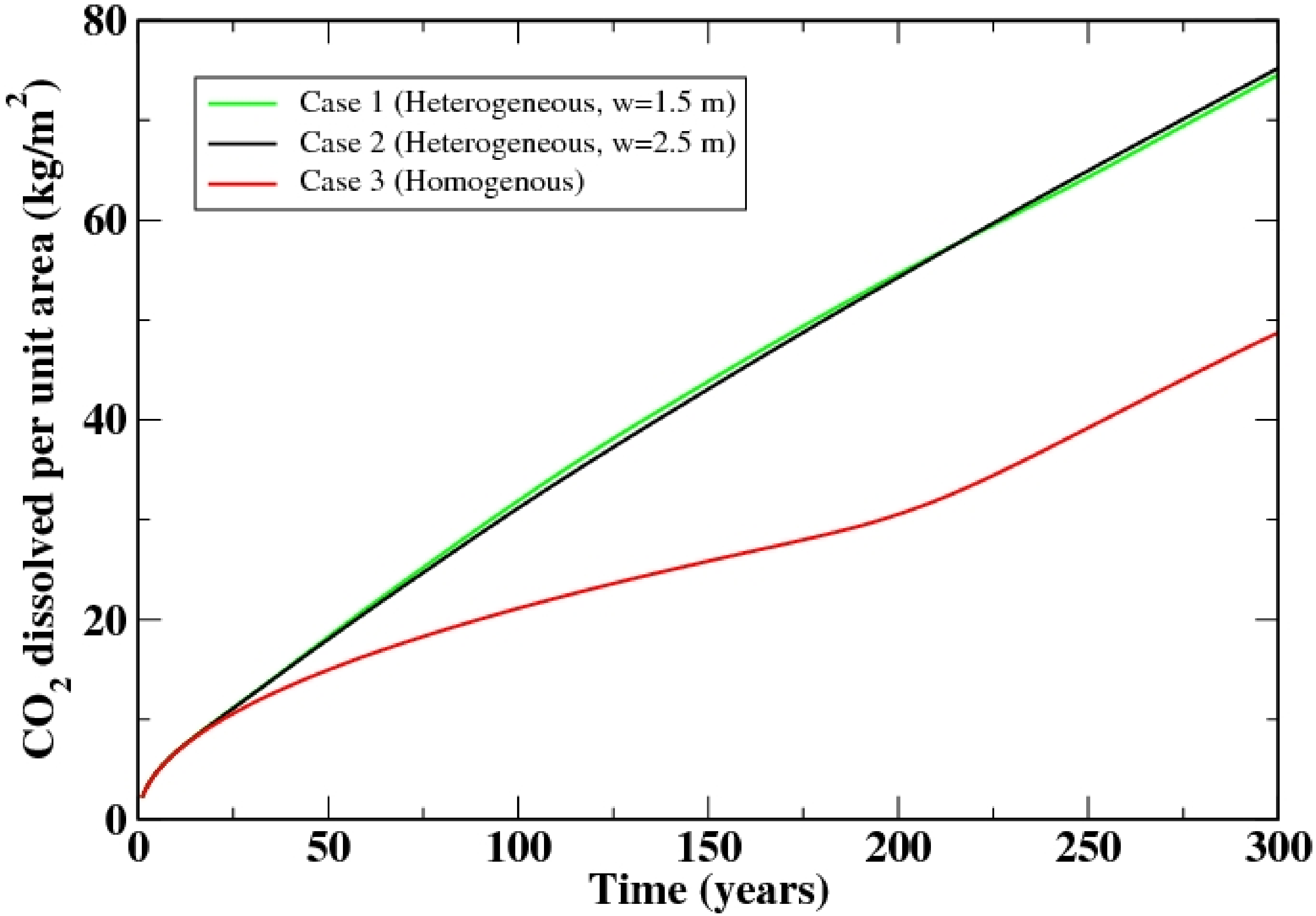


Each curve is an average over 10-20 realizations of permeability

Analysis of effects of heterogeneity

- Convection is established more rapidly in the heterogeneous cases (1 and 2) than in the homogeneous case (3).

- The average vertical spacing between shales may be larger than the length scale at which fingers begin. Locally the fingers experience a vertical permeability closer to the fine scale value of k_v rather than the 'global' value of k_v^{eff}.

- In the homogeneous case, the vertical permeability at all length scales is k_v^{eff} and the finger instability is slower to begin.

Local shale distribution

- The largest vertical spacing between shales is approximately

$$-\ln(p)\ t/F_s \text{ for small } p$$

where p is the probability of exceeding that spacing, t is the shale thickness and F_s is the volume fraction of shale.

- In the heterogeneous cases shown here (1 and 2), this spacing is several metres for p=0.05, which exceeds the initial scale on which fingering begins for these permeabilities.

Upscaling of heterogeneity in convection

- For a homogeneous domain with effective permeabilities, the onset of convection is much later than in the two heterogeneous cases.

- However the rate of plume growth at longer times is similar, since then the plume motion depends on k_v^{eff} and k_h^{eff}.

- Upscaling of convection must take account of the scale-dependence of permeability
  - fine-scale vertical permeability controls finger initiation
  - coarse-scale vertical permeability controls plume growth.

Coupling reactions to convective flow

- The driving force in convection is the increase in fluid density due to dissolved CO_2. If reactions consume CO_2, then this driving force lessens.

- Net precipitation of minerals will reduce porosity and permeability, and inhibit convection.

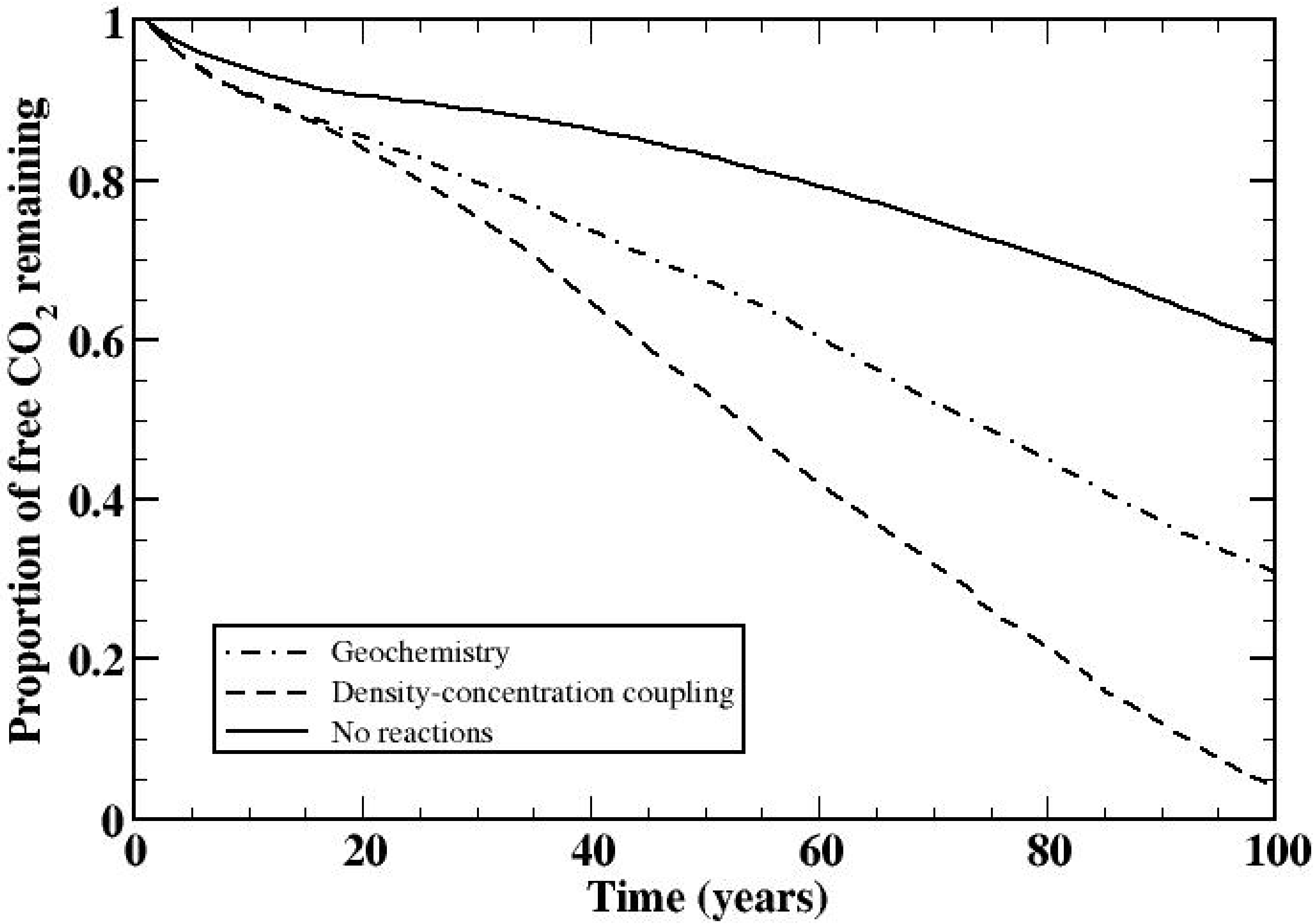
- Geochemical reactions also change the aqueous concentrations of ionic species, and this could either favor or oppose convection. This further coupling can be included using the approach of Monnin (1994).

Geochemical model

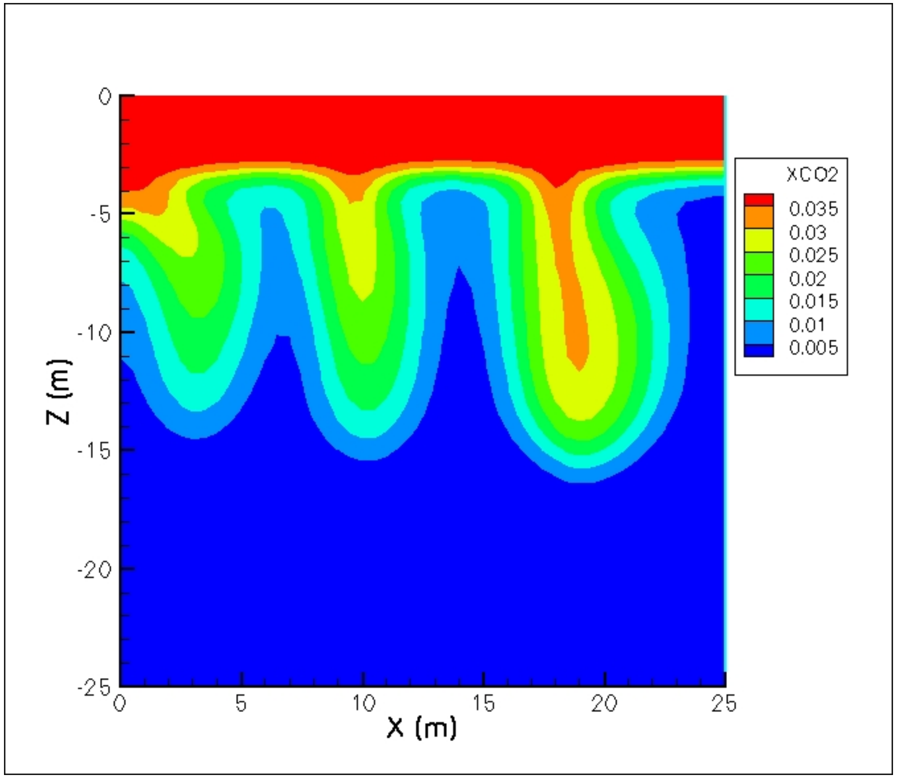
- A published geochemical model chosen for numerical simulation:

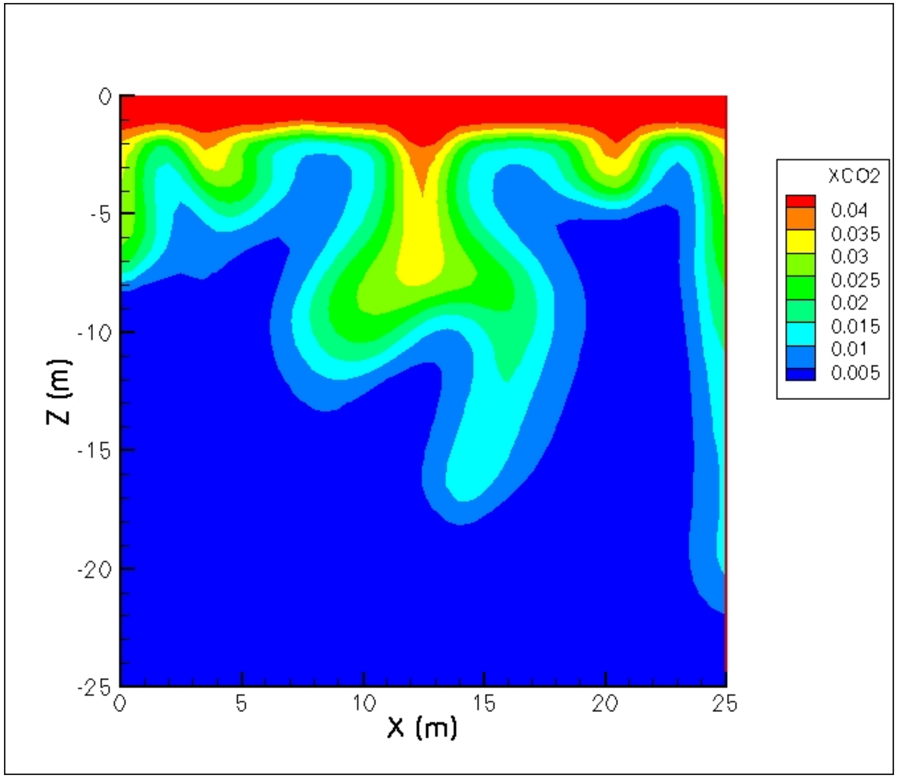
  Siliclastic mineralogy based on US Gulf coast
  (Xu, Apps, Pruess 2003):
  - net precipitation
  - permeability increase
  - dissolution of oligoclase and chlorite
  - precipitation of Na-smectite, calcite, dawsonite, quartz and kaolinite.

Dissolution of CO_2 in Gulf Coast case



Effect of coupling ion concentration to density





Base case

Coupled density

Effect of coupling ion concentration to density

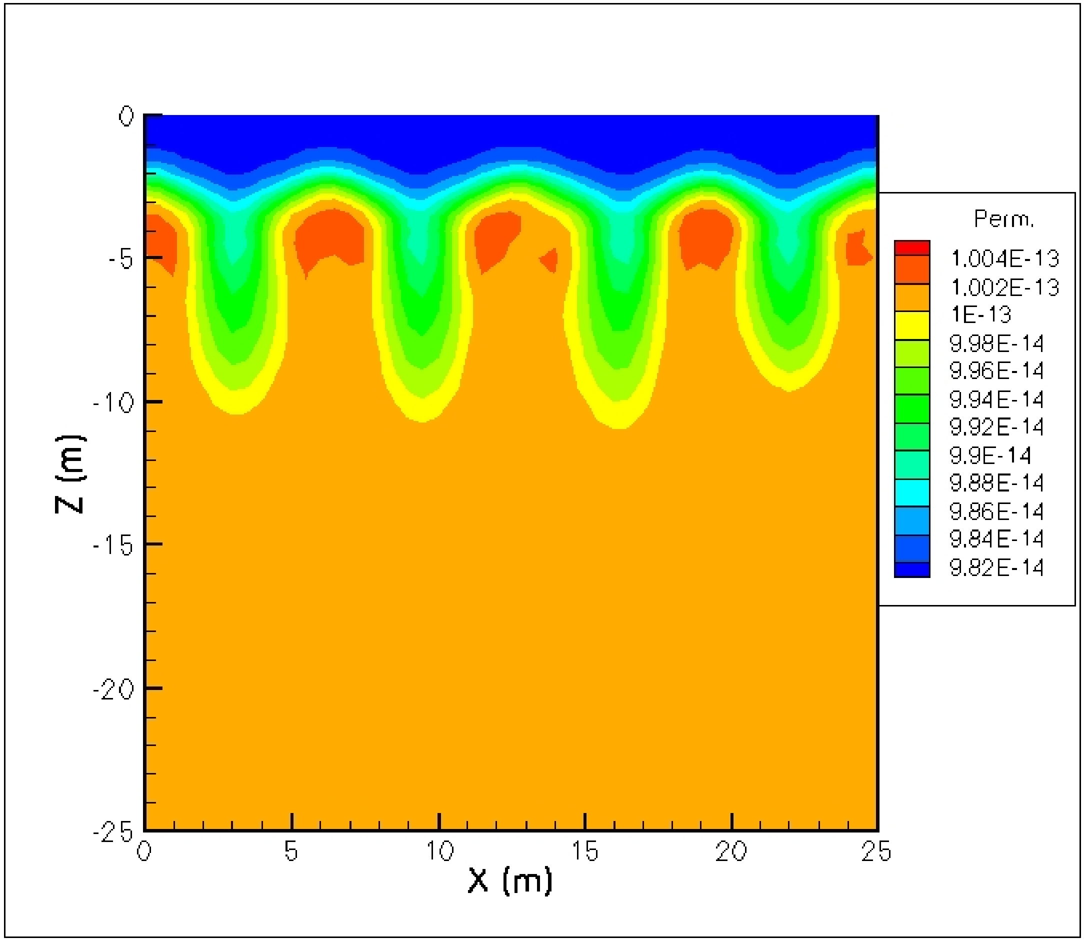
Coupling of density to ion concentrations:

- **appears to alter the plume structure, and feedback favors the development of fewer but larger plumes.**

- **significantly increases the rate of dissolution of CO_2**

More realizations are needed to confirm the effects on plume structure.

Effect of permeability changes



Base case

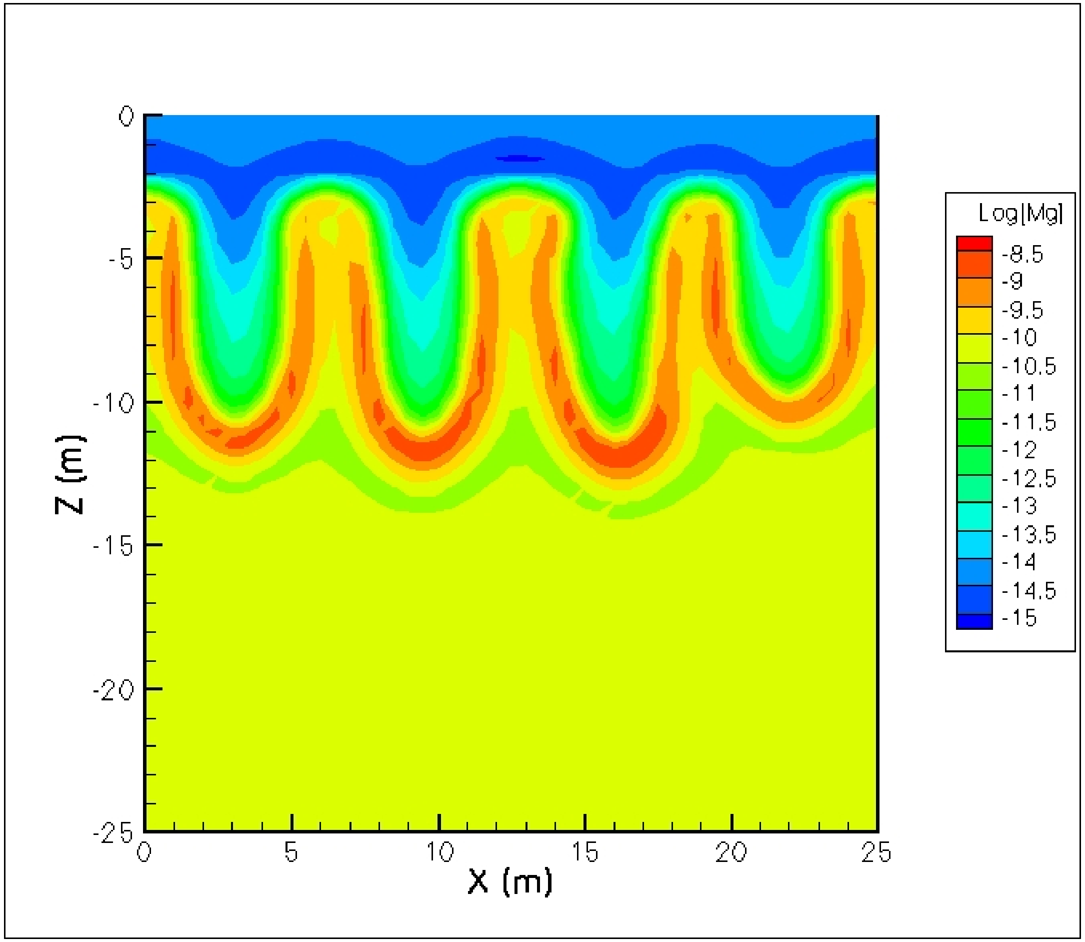
Effect of permeability changes

• The alteration in permeability is only slight (2%) due to the assumption of a cubic dependence on porosity.

• Since reactions are slow, the largest changes occur in the gas phase region at the top, where exposure to CO_2 is longest.

• There is a slight enhancement of permeability between the fingers due to the upflow there.

Effect of flow on geochemistry



Coupled density

Effect of coupling reactions to flow

- In this example, concentration of Mg^{2+} is enhanced by two orders of magnitude in a thin band at the front of the advancing plumes.

- Such "rind" patterns are common features in reactive transport.

- In convection, geochemistry is strongly driven by the flow pattern (i.e. transport of dissolved CO_2).

- Back-coupling of geochemistry to flow via permeability is weak.

Conclusions

- Heterogeneity has a strong influence on convection.
- Upscaling by using only the coarse-scale vertical permeability does not accurately capture all the important effects.
- The onset of convection depends more on fine-scale permeability, while the long-term plume development depends on coarse-scale permeability.
- Geochemical reactions can accelerate the consumption of CO_2 in convection, and this can be further enhanced by the coupling of ion concentrations to fluid density.
- The coupling of reactions to flow through permeability changes was weak in the example considered.

References

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