Prediction of CO_2 footprint: A hybrid pore-scale simulation and analytical modeling

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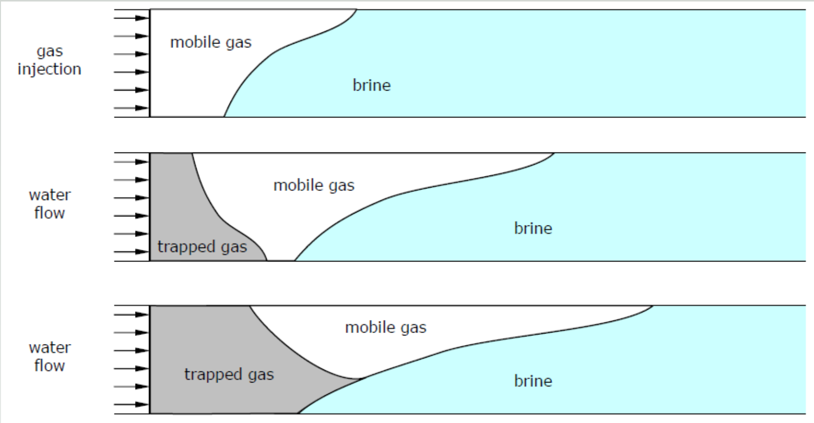
CO_2 plume stabilization

- Storage of carbon dioxide in geological formations is a promising tool for reducing global atmospheric CO_2 emissions.
- To evaluate the storage efficiency and assess leakage risks: An accurate understanding of the subsurface spreading and migration of the plume of mobile CO_2 during and after injection, including its shape, size and the extent.
- Our **objective**: how far will the CO_2 plume travel (that is, what is the footprint of the plume), and for how long does the CO_2 remain mobile?
- Our **approach**: Combining a large-scale analytical solution with embedded pore-scale simulations to capture sub-scale phenomena in predicting the CO_2 migration during injection and post-injection periods.
- Our study **benefits**: help us in risk assessment and capacity estimation at the basin scale.
- Out **outcome**: an analytical expression for prediction of ultimate footprint of CO_2 and time-scale required for its complete trapping.

Theoretical model for prediction of CO_2 plume shape



CO_2 injection into a horizontal saline aquifer.

We model:

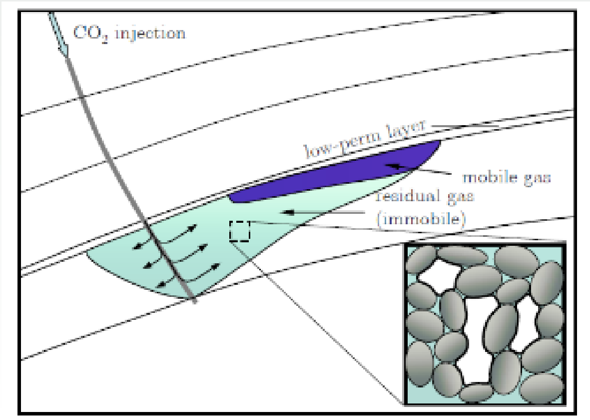
- **Injection period**: CO_2 is injection with a high flow rate, displacing brine (drainage), forming a gravity tongue.
- **Post-injection period**: CO_2 plume continues to migrate due to its buoyancy and the background hydraulic gradient (imbibition)
- CO_2 capillary trapping: at the tailing edge of the plume, CO_2 is trapped in residual form.
- Predicting the migration of CO_2 under **buoyancy** and **capillary trapping**

✓ **Assumptions in the model:**

- A sharp-interface approximation: the medium is either filled with CO_2 or brine.
- Horizontal and homogenous aquifer
- The dimension of aquifer is much larger horizontally than vertically (1D problem)
- Constant density and viscosities fro fluids

✓ **Distinctive features of the model:**

- Considering capillary trapping during post-injection period
- Considering the effect of regional groundwater flow in the evolution of the plume after injection stops.
- Considering the effect of plume shape at the end of injection on its migration during the post-injection (Accounting for the tongued shape of the plume at the end of injection)



Residual (capillary) trapping of CO_2.

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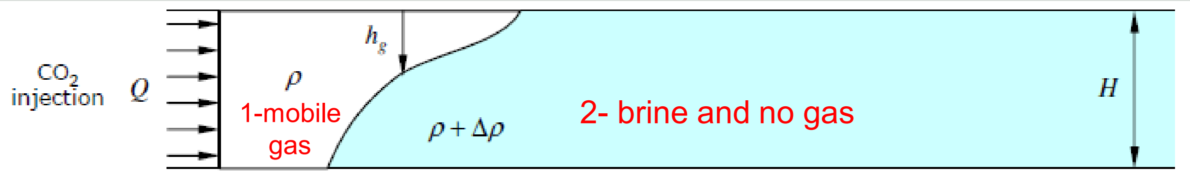
Mathematical model

- **Injection period:**

  - Two separate regions:

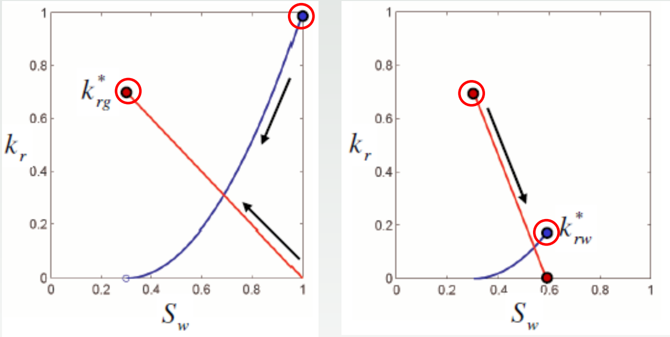
(1) Mobile gas (S_g) and connate (immobile) brine (S_{wc})
(2) Fully-saturated mobile brine and no gas (CO_2)



- Horizontal volumetric flux of ach fluid is calculated by the extension of Darcy's law for multiphase flow:

Relative permeability

$$u_g = \begin{cases} -K\dfrac{k_{rg}^*}{\mu_g}\left(\partial_x p_l - \rho g \partial_x h_g\right) & if\ 0 < z < h_g \\ 0 & if\ \ h_g < z < H \end{cases} \qquad u_w = \begin{cases} 0 & if\ 0 < z < h_g \\ -K\dfrac{1}{\mu_w}\left(\partial_x p_l - (\rho + \Delta\rho) g \partial_x h_g\right) & if\ \ h_g < z < H \end{cases}$$



Relative permeability curves

- Mass balance for the CO_2 phase results in the governing equations for the plume thickness during injection:

$$\emptyset(1 - S_{wc})\partial_t h_g + \partial_x\left(f_g Q - K\Delta\rho g H \bar{\gamma}_g (1 - f_g)\partial_x h_g\right) = 0, \qquad f_g = \frac{\bar{\gamma}_g}{\bar{\gamma}_g + \bar{\gamma}_w}, \qquad \bar{\gamma}_g = \frac{k_{rg}^*}{\mu_g}\frac{h_g}{H}, \qquad \bar{\gamma}_w = \frac{1}{\mu_w}\frac{H - h_g}{H}.$$

$\emptyset$: Porosity
K: Permeability
Swc: Connate water saturation
fg: gas fractional flow

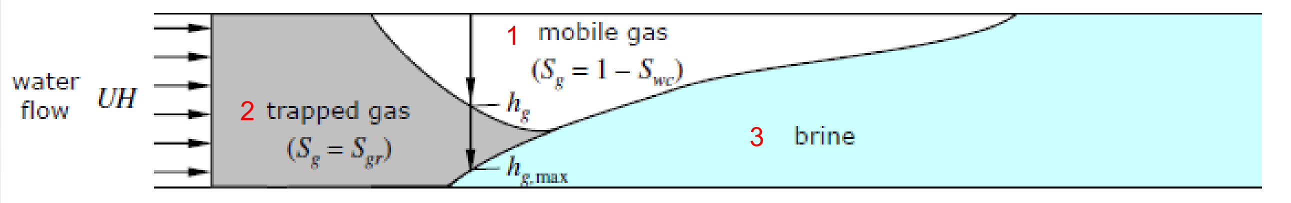
Mathematical model

- **Post-injection period:**

- The "initial condition" for this period is the shape of the plume at the end of injection.

- Three separate regions:

  (1) Mobile gas (S_g) and connate water ($S_w = S_{wc}$)
  (2) Mobile water and trapped gas (S_{gr})
  (3) Mobile water and no gas ($S_w = 1$)



U: Groundwater flowrate

- Application of Darcy's law to the sharp-interface model (Gas and water Darcy's velocities):

$$u_g = \begin{cases} -K\frac{k_{rg}^*}{\mu_g}(\partial_x p_l - \rho g \partial_x h_g) & if\ 0 < z < h_g \\ 0 & if\ h_g < z < h_{g,max} \\ 0 & if\ h_{g,max} < z < H \end{cases}$$

$$u_w = \begin{cases} 0 & if\ 0 < z < h_g \\ -K\frac{k_{rw}^*}{\mu_w}(\partial_x p_l - (\rho + \Delta\rho) g \partial_x h_g) & if\ h_g < z < h_{g,max} \\ -K\frac{1}{\mu_w}(\partial_x p_l - (\rho + \Delta\rho) g \partial_x h_g) & if\ h_{g,max} < z < H \end{cases}$$

- Mass balance for the CO_2 phase: The governing equation for the plume thickness during the post-injection period:

$$\partial_t(\emptyset(1 - S_{wc})h_g) + \partial_t(\emptyset S_{gr}(h_{g,max} - h_g)) + \partial_x(Q_g) = 0$$

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Solution to the model: Injection period

- Make assumption to simplify the model (mobility ratio (M) <<1): Hyperbolic model

- **Plume evolution equation** during injection (dimensionless form):

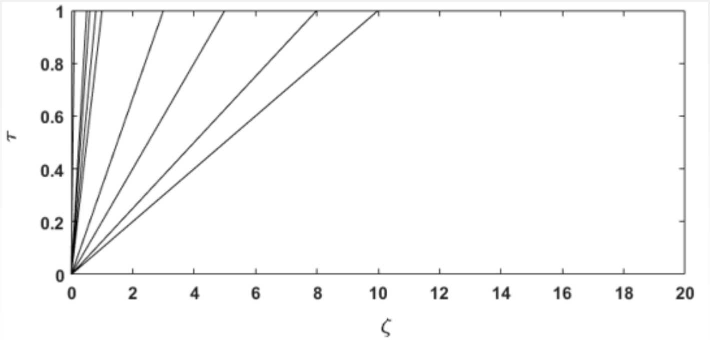
$$(1 - S_{wc})\partial_\tau h + \partial_\xi f = 0\,,\qquad f(h) = \frac{h}{h + M(1-h)},\qquad M = \frac{1/\mu_w}{k^*_{rg}/\mu_g} = mobility\ ratio$$

μw: Viscosity of water
μg: Viscosity of gas
k^*_{rg}=end-point relative permeability

- Dimensionless variables: $h = \frac{h_g}{H},\quad \tau = \frac{t}{T},\quad \xi = \frac{x}{L}.$

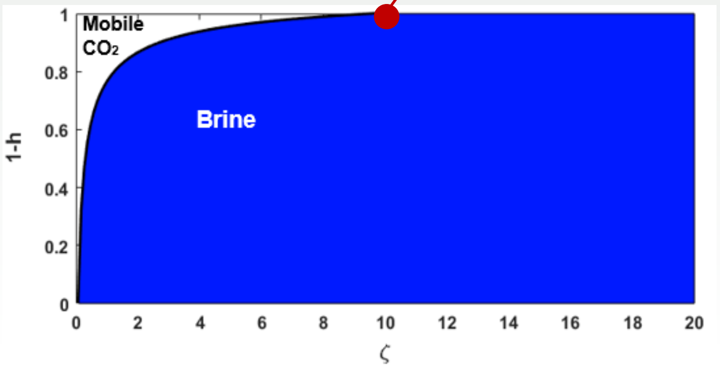
T: Injection time
$L = \frac{QT}{H\emptyset}$

- This is the Riemann problem with solution of **rarefaction wave**.
- Solution to this problem determines the **drainage front** in the injection period.

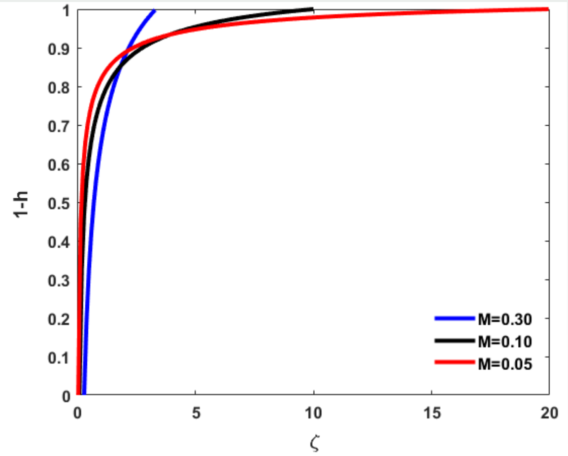


Diverging rarefaction wave on ξ-τ plane.

(ξ_{inj},τ =1) , ξ_{inj}= $\frac{1}{(1-S_{wc})M}$



CO_2 drainage front at the end of injection period (τ =1) for M=0.1 Swc=0.4.



Effect of mobility ratio (M) on the shape of CO_2 plume at the end of injection.

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Solution to the model: Early post-injection period

- **Plume evolution equation** during post-injection (τ >1) :

$$R\partial_\tau h + \partial_\xi f = 0\,,$$

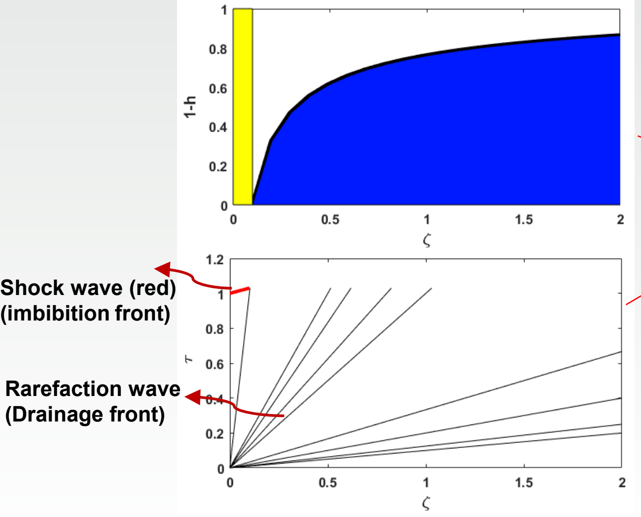
$$R = \begin{cases} 1 - S_{wc} & if\ \partial_\tau h > 0\ (drainage) \\ 1 - S_{wc} - S_{gr} & if\ \partial_\tau h < 0\ (imbibition) \end{cases}$$

$$f = \begin{cases} \dfrac{h}{h + M(1-h)} & if\ \partial_\tau h > 0\ (drainage) \\ \dfrac{h}{h + k_{rw}^{*} M(h_{max} - h) + M(1 - h_{max})} & if\ \partial_\tau h < 0\ (imbibition) \end{cases}$$

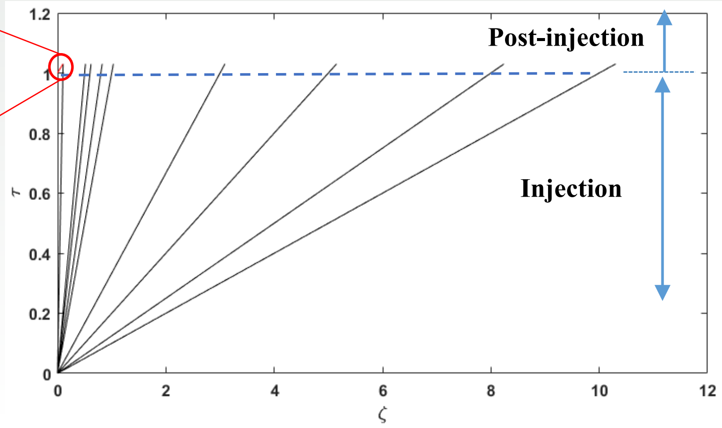
- The solution to the drainage front continues to be a divergent **rarefaction wave**.
- The solution to the imbibition front is a **shock wave**.

$$\tau_c = \frac{\Gamma}{\Gamma - M} \quad \textbf{Collision time}$$

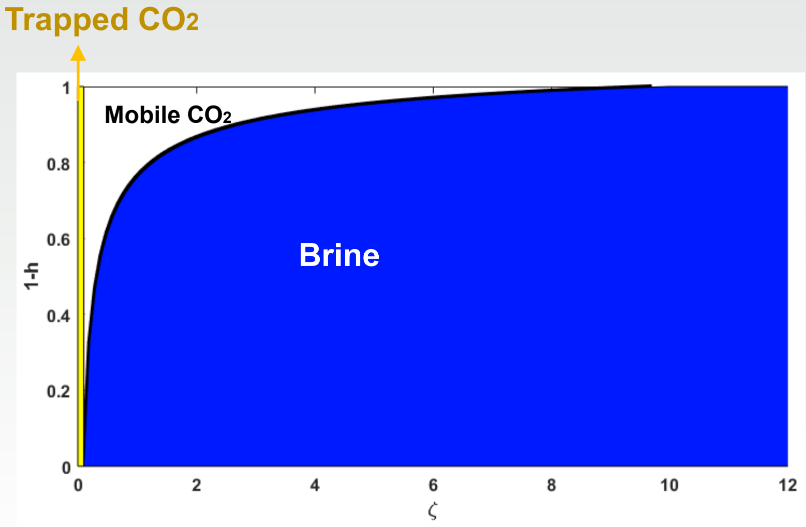
$$\Gamma = \frac{1}{1 - S_{wc} - S_{gr}} \quad \textbf{Capillary trapping coefficient}$$



Collision of the imbibition shock with the slowest ray of the drainage rarefaction.



Diverging rarefaction and shock waves on ξ-τ plane. M=0.1, Swc=0.4, Sgr=0.3.



Profile of the mobile CO_2 plume (white) and trapped CO_2 (yellow) when the drainage front detaches from the bottom of the aquifer.

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Solution to the model: Late post-injection period

- **Late post-injection period (sweep stage):**
- Once the mobile plume detaches from the bottom of the aquifer.
- The solution comprises the continuous **interaction of a progressively faster shock with a rarefaction wave**.

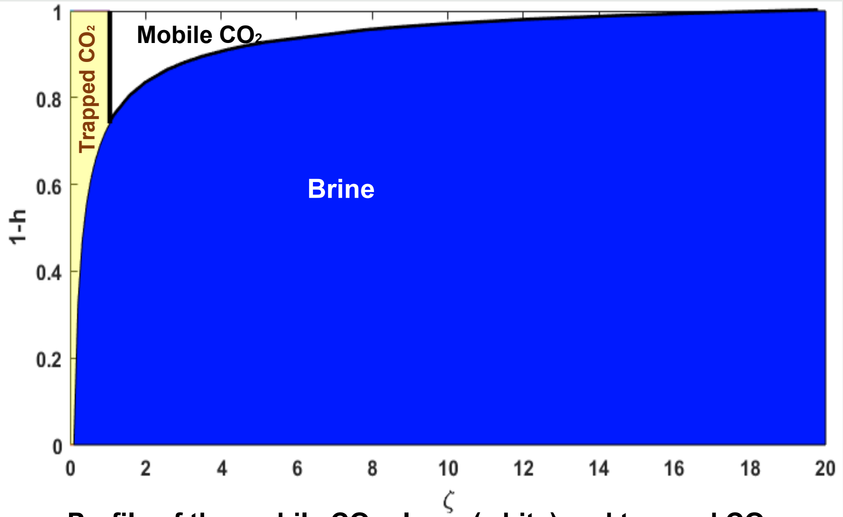
$$\tau(h_m) = \Gamma(\Gamma - M)\left(\frac{M + (1 - M)h_m}{M(\Gamma - 1) + (1 - M)\Gamma h_m}\right)^2, \quad \tau_c < \tau < \tau_{max}$$

Capillary trapping coefficient (Γ)

Mobility ratio (M)

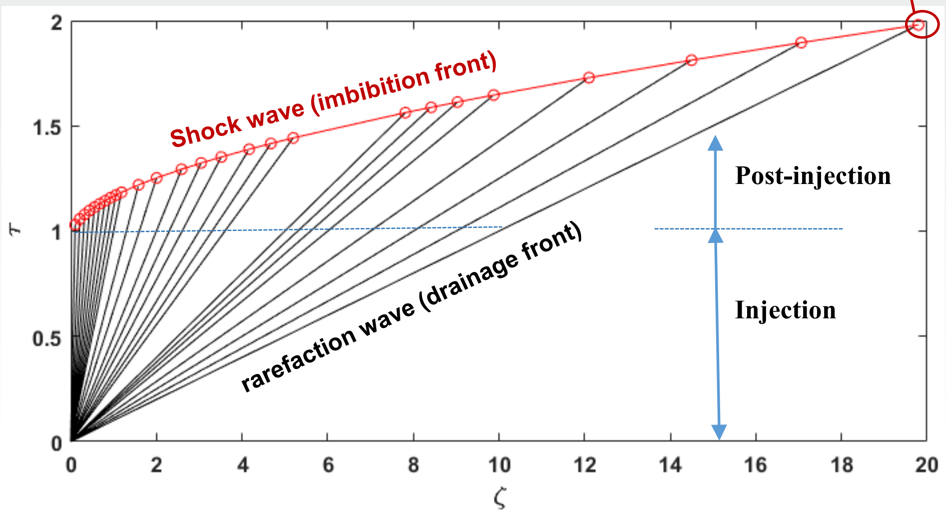
$\tau_{max} = \frac{\Gamma(\Gamma - M)}{(\Gamma - 1)^2}$: Time scale for complete trapping

$\xi_{max} = \frac{\Gamma(\Gamma - M)}{(\Gamma - 1)^2}\frac{M}{1 - S_{wc}}$: Maximum migration distance of CO_2 plume (ultimate footprint of CO_2)



Profile of the mobile CO_2 plume (white) and trapped CO_2 (yellow) at some intermediate time ($\tau_c < \tau < \tau_{max}$).

(ξ_{max}, τ_{max})



Complete solution on (ξ-τ)-space until the entire CO_2 plume has been immobilized in residual form.

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Footprint of the CO_2 plume and trapping efficiency factor

- The mobility ratio (M) and the capillary trapping coefficient (Γ) emerge as the key parameters in the assessment of CO_2 storage in saline aquifers.
- Larger values of Γ result in more effective trapping of the CO_2 plume; it increases with increasing residual gas saturation.
- The ultimate footprint of the plume is proportional to the mobility ratio.
- The maximum migration distance is also strongly dependent on the shape of the plume at the end of the injection period.

➢ **Storage efficiency factor due to capillary trapping:**

- **Efficiency factor:** the ratio of the volume of CO_2 injected and the pore volume of the aquifer ($V_{CO2} = E_{capil}V_{pore}$)

$$\boldsymbol{E_{capil}} = \frac{\mathbf{2}}{\boldsymbol{\xi_{inj}} + \boldsymbol{\xi_{max}}} = \mathbf{2}(\mathbf{1} - \boldsymbol{S_{wc}})\boldsymbol{M}\frac{\Gamma^{\mathbf{2}}}{\Gamma^{\mathbf{2}} + (\mathbf{2} - \Gamma)(\mathbf{1} - \boldsymbol{M}(\mathbf{1} - \Gamma))}$$

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Calculation for a case scenario

- **Aquifer properties:** $k = 100\, md = 10^{-13} m^2,\ \ \emptyset = 0.2,\ \ H = 100\, m$
- **Injection conditions**: P=100 bar ,T=40°C $\rho \approx 400\, kgm^{-3},\ \Delta\rho \approx 600\, kgm^{-3},\ \mu_g \approx 0.05 \times 10^{-3} kg/ms,\ \mu_w \approx 0.8 \times 10^{-3} kg/ms$
- **Rock-fluid properties**: $S_{wc} = 0.4,\ S_{gr} = 0.3$ and $k^*_{rg} = 0.6$ $\Gamma = 0.3\ ,\ \ M \approx 0.1$
- **A sequestration project**: 100 megatons of CO_2 injection per year, for a period of T=50 years
- Injection at 100 wells, with interval spacing of 1km $Q = 1250\, m^2/yr\ ,\ \ Q/H = 12.5\, m/ry$
- **Background groundwater flow**: $U = 0.1\, m/yr$

- The expected footprint of the plume and time scale for complete trapping (in dimensionless quantities):

$$\boldsymbol{\xi}_{max} = 95\ \ ,\ \boldsymbol{\tau}_{max} = 5.7$$

- Dimensional values:

$$x_{max} = \frac{QT}{H\emptyset}\xi_{max} \approx 300\, km\ \ ,\qquad t_{max} = T\left(1 + \frac{Q}{UH}\right)(\tau_{max} - 1) \approx 30{,}000\, years$$

- **Capillary trapping efficiency factor**: $E_{capil} \approx 1.8\%$ (1-4% by suggested by the DOE Regional Carbon Sequestration Partnerships)

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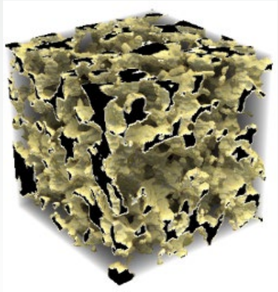
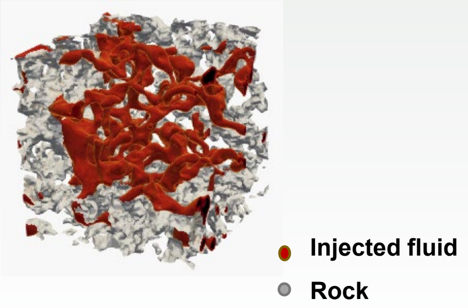
Integrating the model with pore-scale simulations

- The mobility ratio (M) and the capillary trapping coefficient (Γ) emerge as the key parameters in the assessment of the ultimate extent of CO_2 plume.
- The mobility ratio (M) and the capillary trapping coefficient (Γ) depend on the residual saturation and end-point relative permeability.
- These parameters depend on the rock heterogeneity, fluid-rock properties such as wettability and viscosity of fluids.
- Integrating the model with pore-scale simulations to account for the effect of pore-scale properties.

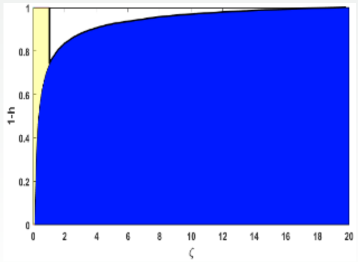
Image of 3D rock sample → Direct pore-scale simulation of CO_2/ brine drainage and imbibition → (S_{wc}, S_{gr}, k^*_{rg}) → Apply the calculated parameters to the analytical model



Digitized rock sample of Tuscaloosa sandstone (from micro-CT image stack)



Using our in-house simulator (LBM)



Estimating the ultimate footprint of CO_2

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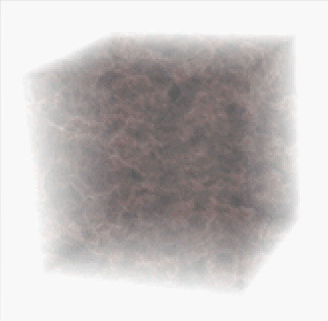
Integrating the model with pore-scale simulations

$\tau_{max} = 76.58$ Time scale for complete trapping
$\xi_{max} = 7.66$ Maximum migration distance of CO_2 plume (ultimate footprint of CO_2)

water-wet

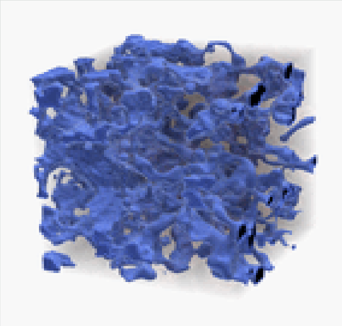
Saturated with brine

scCO2 Drainage

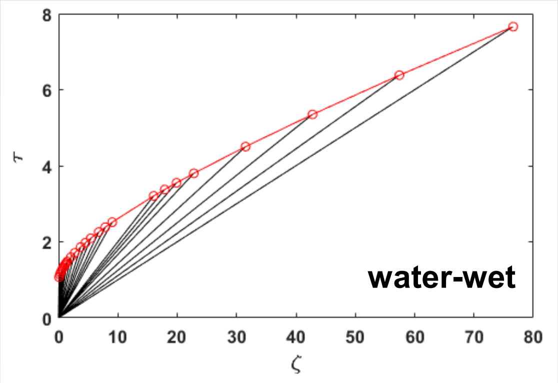


Injection period- S_{wc}

Brine Imbibition



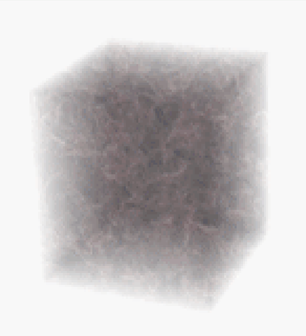
Post-injection period- S_{gr}



mixed-wet

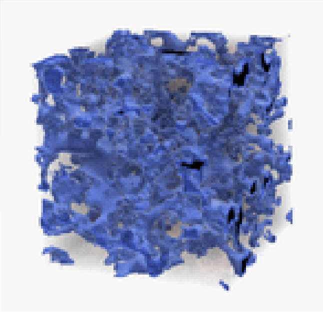
Saturated with brine

scCO2 Drainage



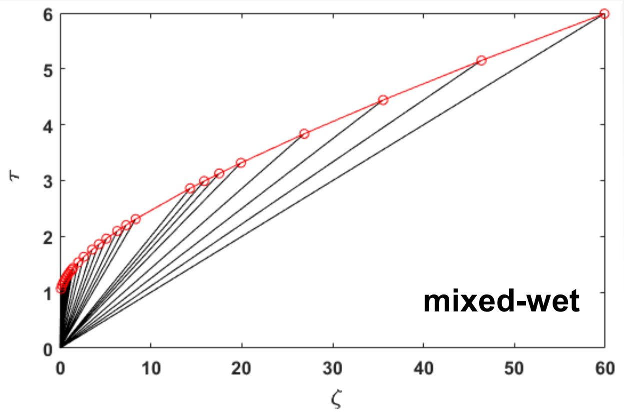
Injection period- S_{wc}

Brine Imbibition



Post-injection period- S_{gr}

$\tau_{max} = 59.89$
$\xi_{max} = 5.98$



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Key takeaways

- We developed a model of CO_2 migration in saline aquifers, that accounts for gravity override and capillary trapping.

- The main outcome of the model is an algebraic expression that can be used to evaluate quickly the ultimate footprint of CO_2 and the time scale required for its complete trapping.

- The model reflects dependencies on the mobility ratio and the capillary trapping coefficient, which depend on the pore-scale properties such as wettability.

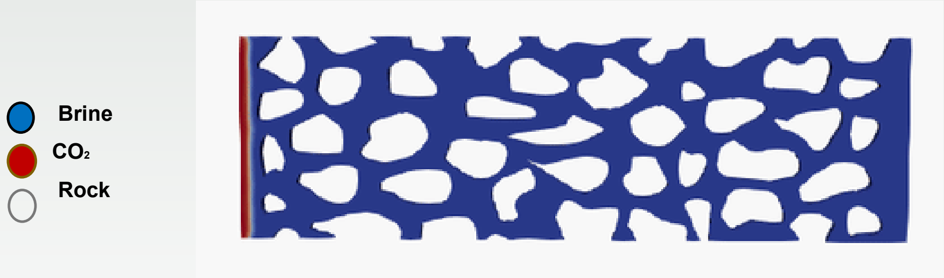
- Integration of the model with the pore-scale simulation provides the link between sub-scale properties and prediction of CO_2 migration.

Prospective directions

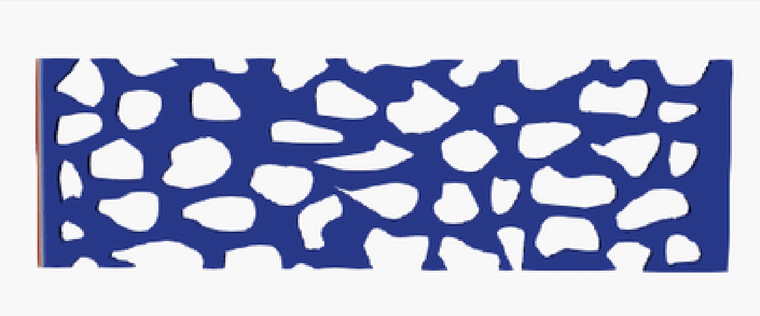
- **Prediction of CO_2 migration in a dipping aquifer**: some aquifers might be weakly slopped

- **Accounting for dissolution trapping in the model:**

  CO_2 from the buoyant plume dissolves into the ambient brine. Solubility can greatly slow the speed at which the plume advances



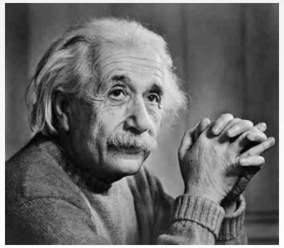
Evolution of CO_2 concentration during drainage in a 2D porous medium.



Evolution of CO_2/brine phase distribution during drainage in a 2D porous medium.

Thank you!

Questions?



- “A model should be as simple as possible, but no simpler.”
- Albert Einstein (c. 1940)

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