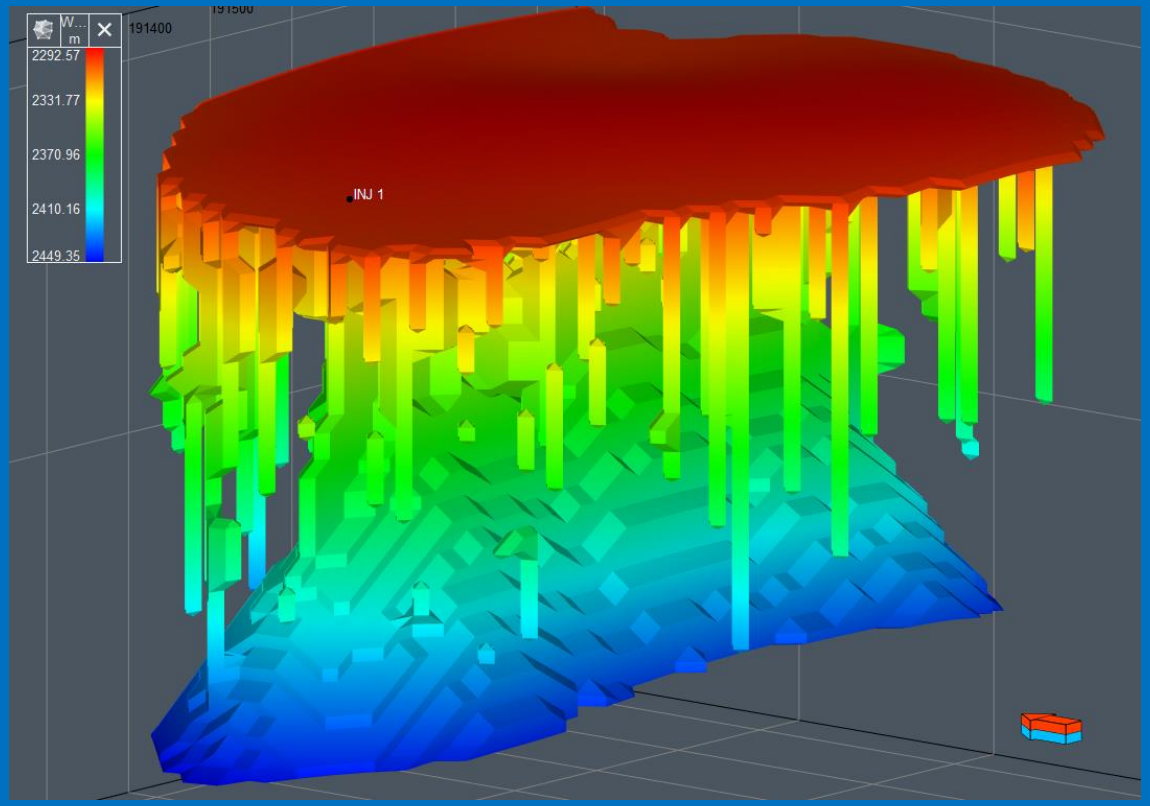
UNIVERSITY OF ABERDEEN

SIRG

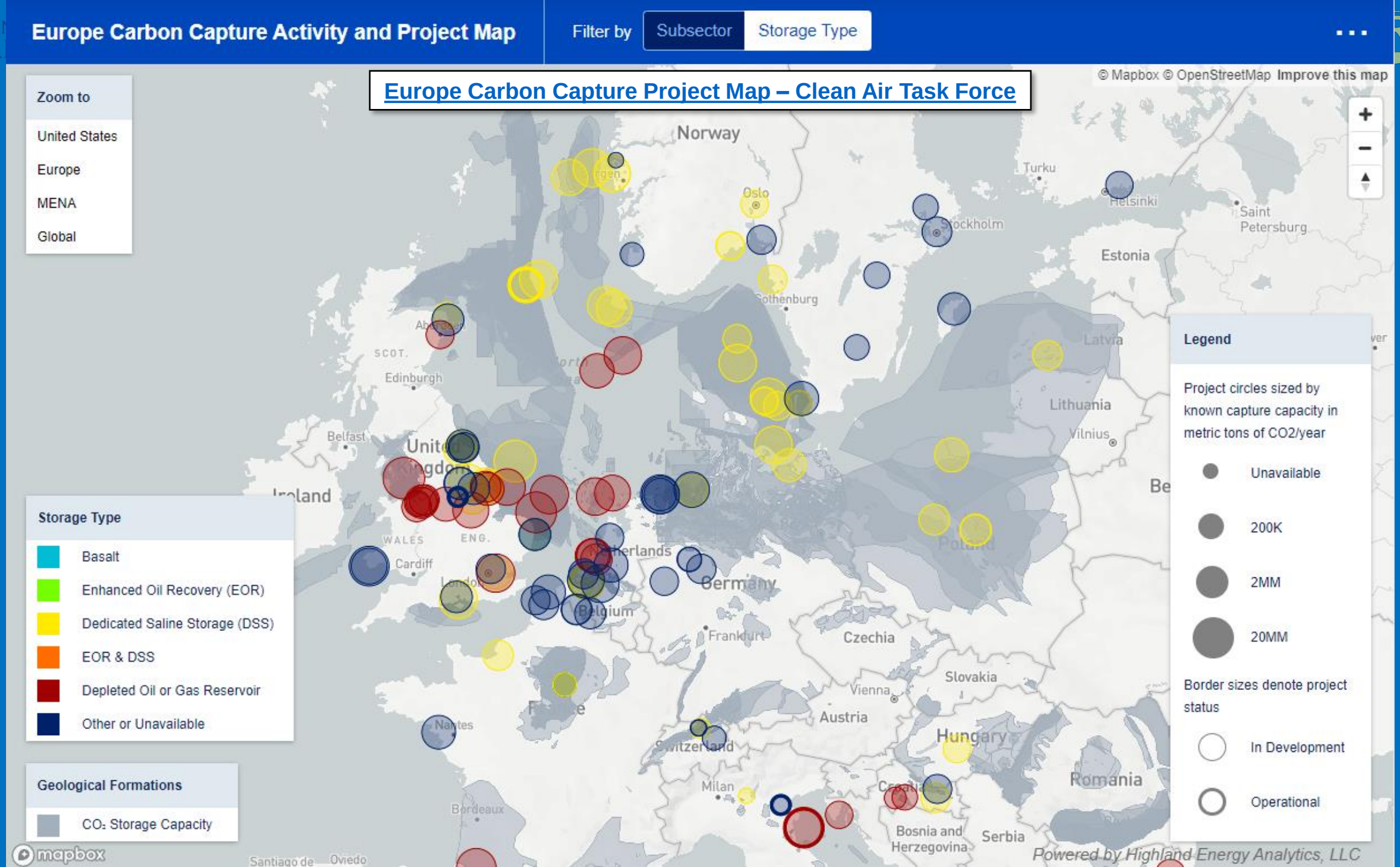
Modelling CO2 Flux Regimes Post-Injection – Diffusion, Convection and Gravity Slumping

Understanding dissolution flux regimes, convective instability, and their implications for simulation modelling & CCS/GCS project design



CO2 Dissolution not just as a safeguard, but as a strategy

sean.kelly@abdn.ac.uk


Europe Carbon Capture Activity and Project Map
Filter by
Subsector
Storage Type
Europe Carbon Capture Project Map – Clean Air Task Force
© Mapbox © OpenStreetMap Improve this map
Zoom to
United States
Europe
MENA
Global
Legend
Project circles sized by known capture capacity in metric tons of CO2/year
Unavailable
200K
2MM
20MM
Border sizes denote project status
In Development
Operational
Storage Type
Basalt
Enhanced Oil Recovery (EOR)
Dedicated Saline Storage (DSS)
EOR & DSS
Depleted Oil or Gas Reservoir
Other or Unavailable
Geological Formations
CO₂ Storage Capacity
Norway
Oslo
Stockholm
Helsinki
Turku
Saint Petersburg
Estonia
Latvia
Lithuania
Vilnius
Gothenburg
Edinburgh
Belfast
Ireland
Cardiff
Germany
Belgium
Netherlands
Frankfurt
Czechia
Slovakia
Vienna
Austria
Hungary
Romania
Switzerland
Milan
Bosnia and Herzegovina
Serbia
Nantes
Bordeaux
Powered by Highland Energy Analytics, LLC

2024-2034 CCS Projects in UK and EU Scenarios

Scenario	Total CO2 Storage (2024–2034, *Mt*)	Investment (10 Years) *£ Billion*
Planned Projects Only	346	£24-£30
"Worst-Case"	450–550	£32–53
Low-Range	750–800	£55–65
Mid-Range	800–950	£75-£100
High-Range	950–1,050	£103-£125

SCCS (2024) and other sources – Scenarios ranges based on key uncertainties related to cost, CO2 price, capacity, deliverability etc

CO2 Transport Processes

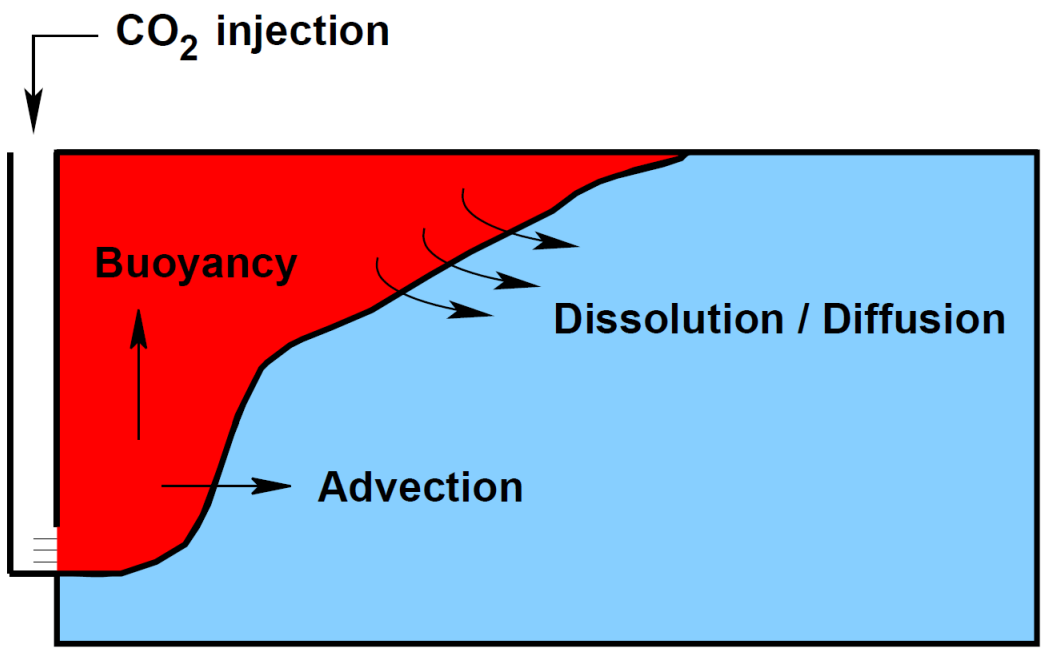


Figure 3.14: Relevant transport processes of CO_2.

Advection & Buoyancy

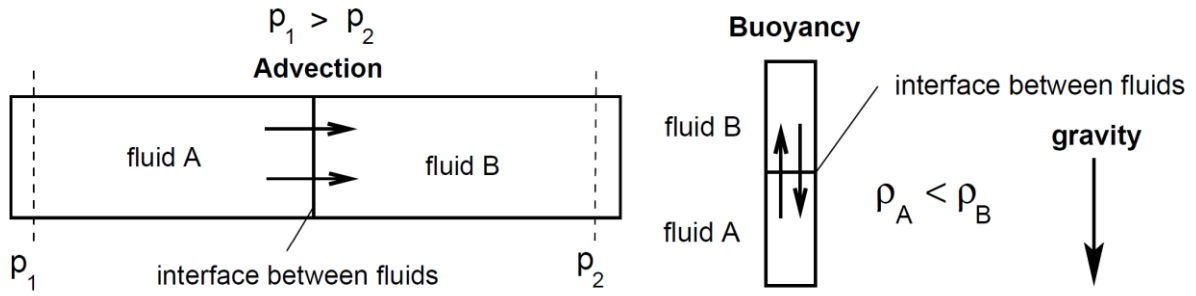


Figure 2.8: Advection and buoyancy in multi-phase flow. Advection is caused by pressure gradients. In this example, fluids A and B are displaced from left to right. Density differences cause buoyancy flow. Here, fluid A flows upwards, because it has a lower density than fluid B.

Dissolution

Dissolution of CO_2 in water: CO_2 dissolves in water, forming carbonic acid (H_2CO_3), hydrogen carbonate (HCO_3^-), and carbonate (CO_3^{2-}) in accordance with the reaction equation

$$\begin{aligned} CO_2 + H_2O &\rightarrow H_2CO_3, \\ H_2CO_3 + H_2O &\rightarrow HCO_3^- + H^+ + H_2O, \\ HCO_3^- + H_2O &\rightarrow CO_3^{2-} + H^+ + H_2O. \end{aligned} \quad (3.2)$$

Diffusion

Diffusion is the equilibration of differences in density or velocity of molecules due to Brownian molecular movement (e.g. MESCHEDE (2004) [73]). Thus, diffusive fluxes are driven by concentration gradients or temperature gradients. In contrast to advection and buoyan--- diffusion is independent of orientation, i.e. it behaves the same in all spatial directions. A

Bielinski 2007

CO2 Dissolution Flux

1. Why dissolution flux matters ?
2. What controls it (Ra)?
3. What flux regimes exist ?
4. How flux evolves over time ?

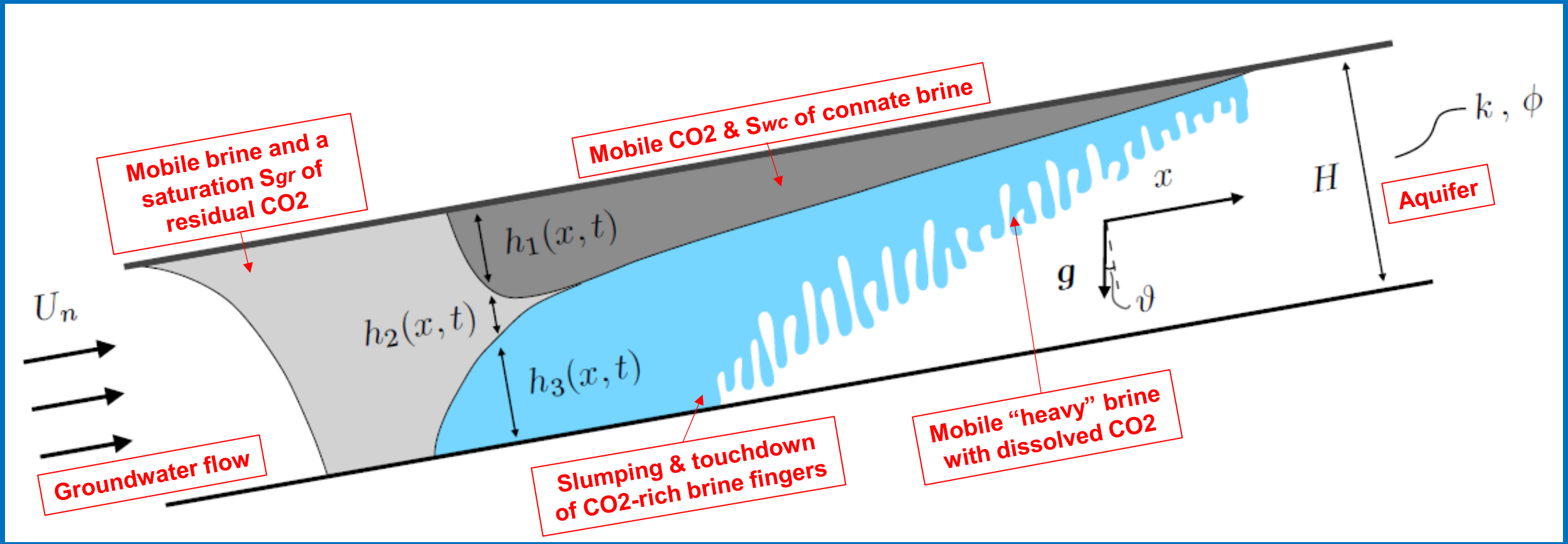
Sleipner
- **Total injected CO_2 (as of ~2024):** ~21–22 Mt
- **Dissolved mass (13% first ~13 years injection): ≈ 1.8 Mt CO_2**

Analytical Modelling

Reservoir Simulation

CCS/GCS Design

Post-Injection Migration Processes



MacMinn et al. 2011

Fundamentals of CO_2 Dissolution in the Subsurface

Convective Mixing:

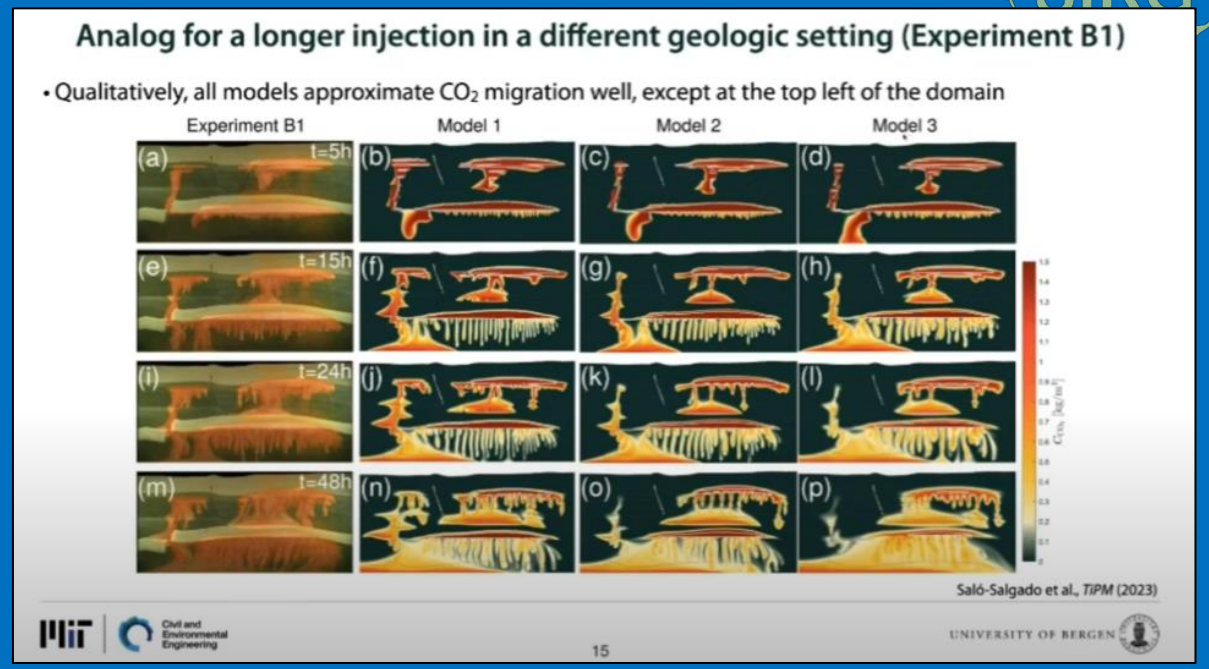
Dense, CO_2-rich brine sinks, initiating convection that enhances mass transfer.

Formation of carbonic acid (H_2CO_3) as CO_2 dissolves in brine.

- Density increase due to dissolved CO_2 is slight (0.1-1%) but sufficient to drive convection.
- CO_2-saturated brine is denser → sinks under gravity
- Promotes convective fingering and slumping
- Enhances dissolution by renewing contact with fresh brine

Result:

- Plume becomes increasingly stabilized, improving storage security.
- Dissolution reduces the buoyancy of CO_2, minimizing leakage risk.
- Combined effect significantly reduces mobile CO_2 and leakage risk over time.
- Dissolution trapping reduces mobile-phase CO_2, enhancing seal integrity



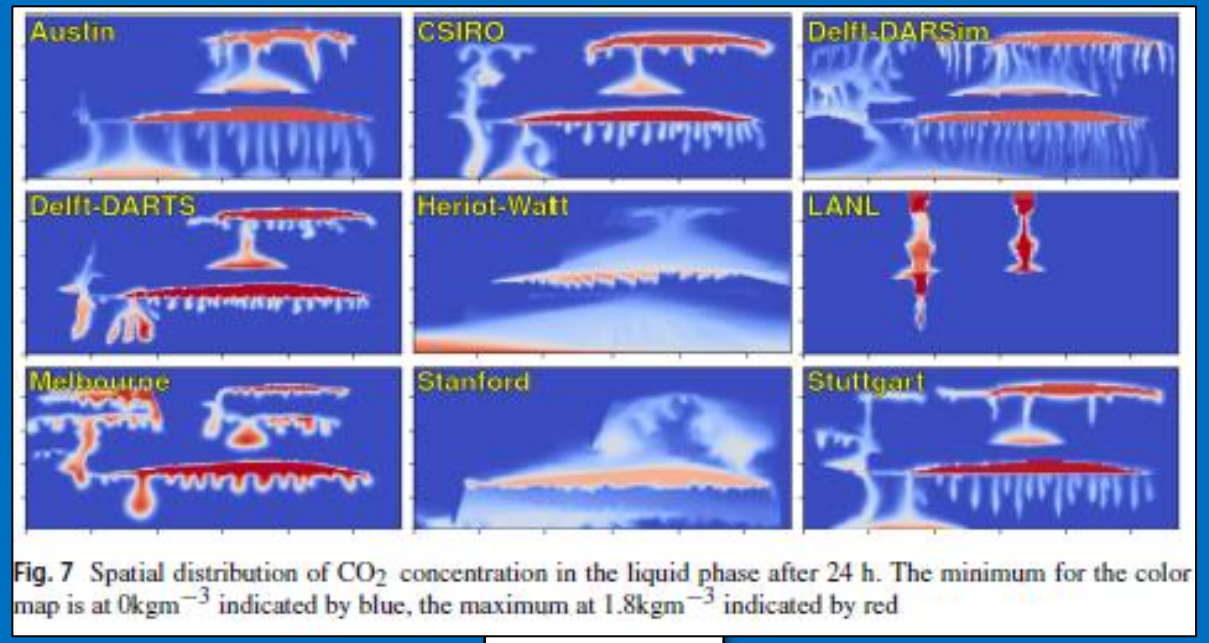


Fig. 7 Spatial distribution of CO_2 concentration in the liquid phase after 24 h. The minimum for the color map is at $0 kgm^{-3}$ indicated by blue, the maximum at $1.8 kgm^{-3}$ indicated by red

Fluidflower

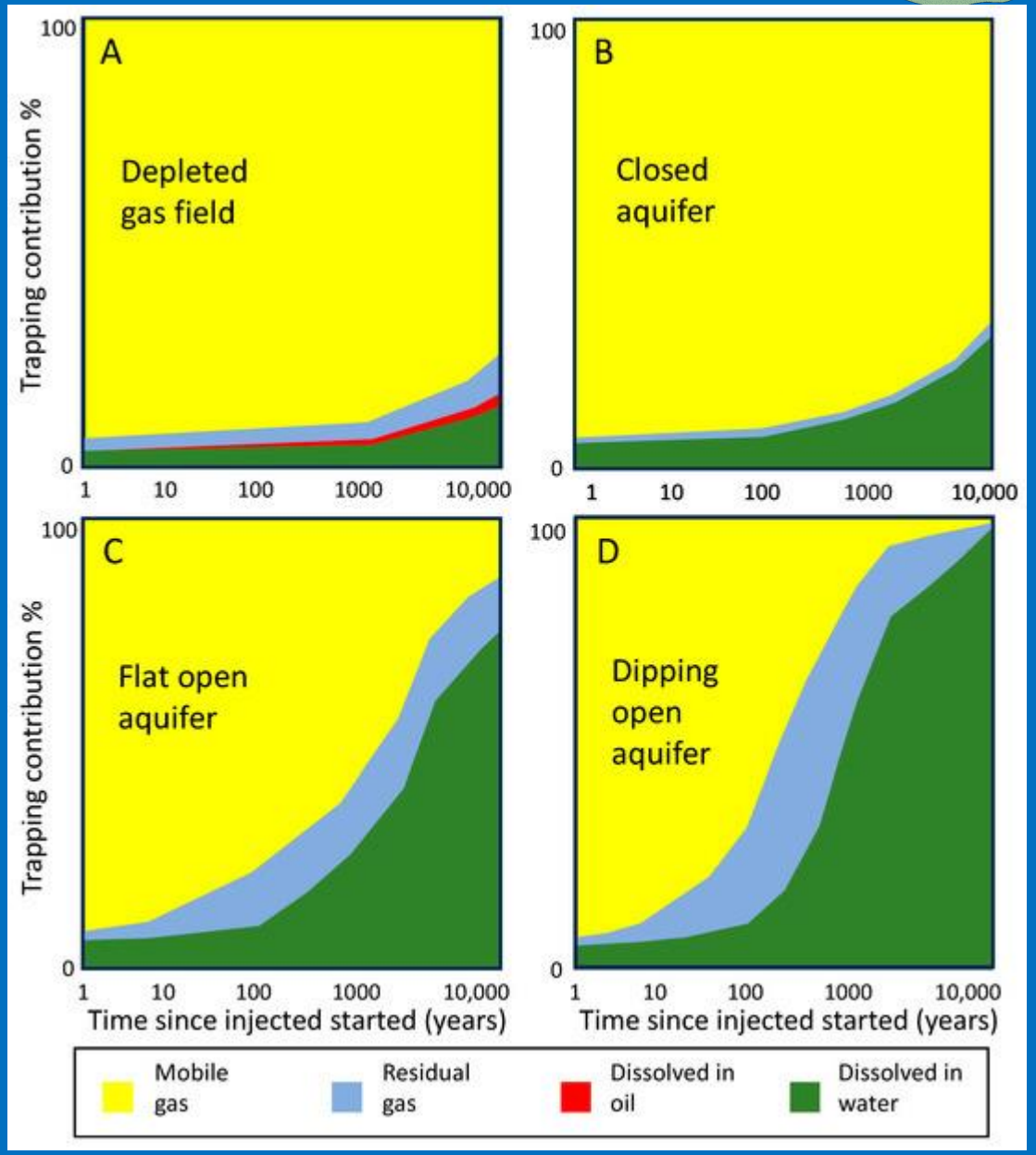
Dissolution Trapping

Introduction

Carbon capture and storage (CCS) relies on several trapping mechanisms. Among them, **dissolution trapping** plays a crucial long-term role by reducing buoyancy and immobilizing CO_2 in formation brine.

However:

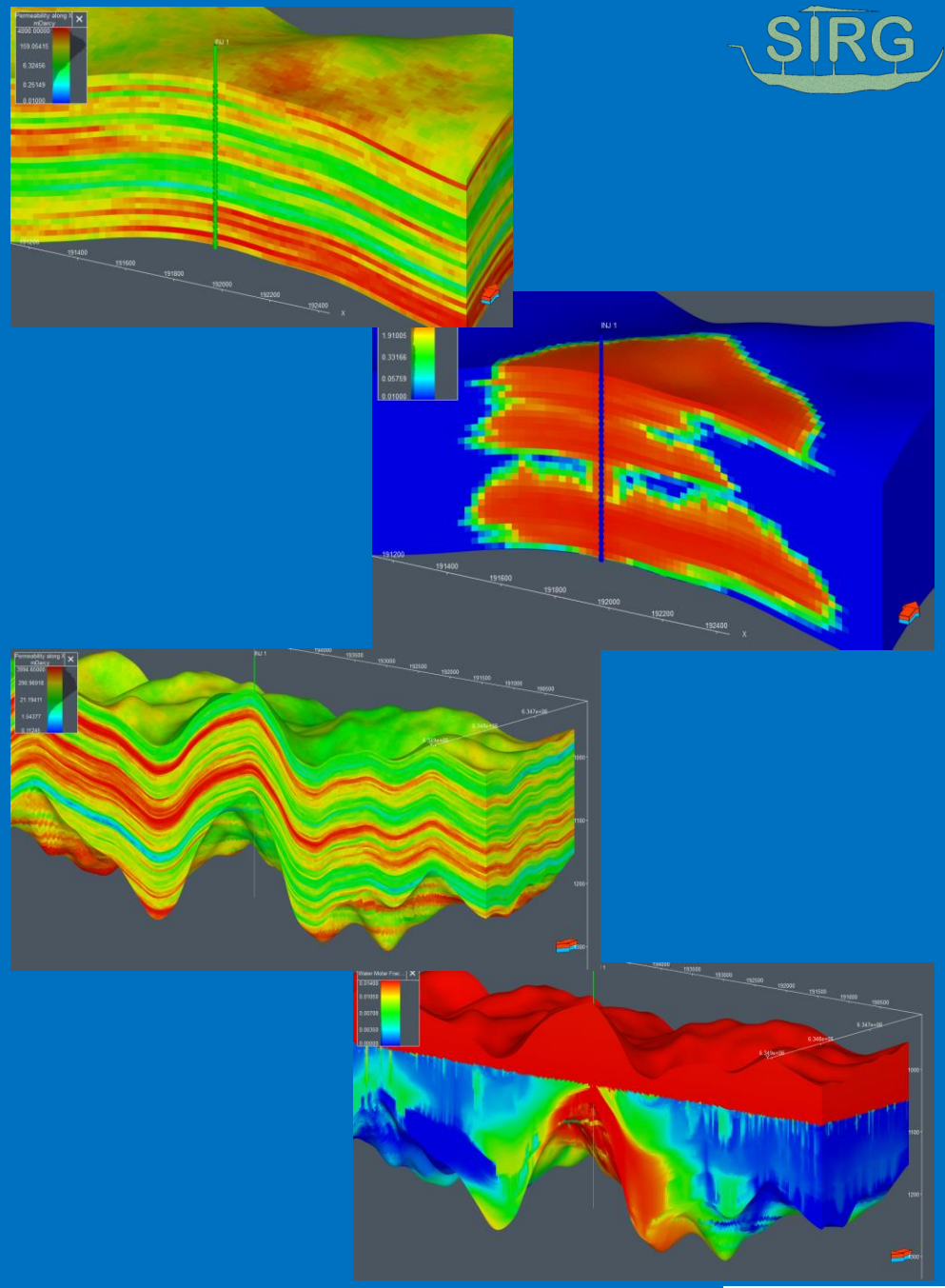
- It is often underrepresented in simulations
- It plays out over **long timescales**
- It is influenced by complex geological and thermophysical factors
- This presentation focuses on **how and why dissolution occurs**, **what controls it**, and how to design better CCS projects to leverage it.

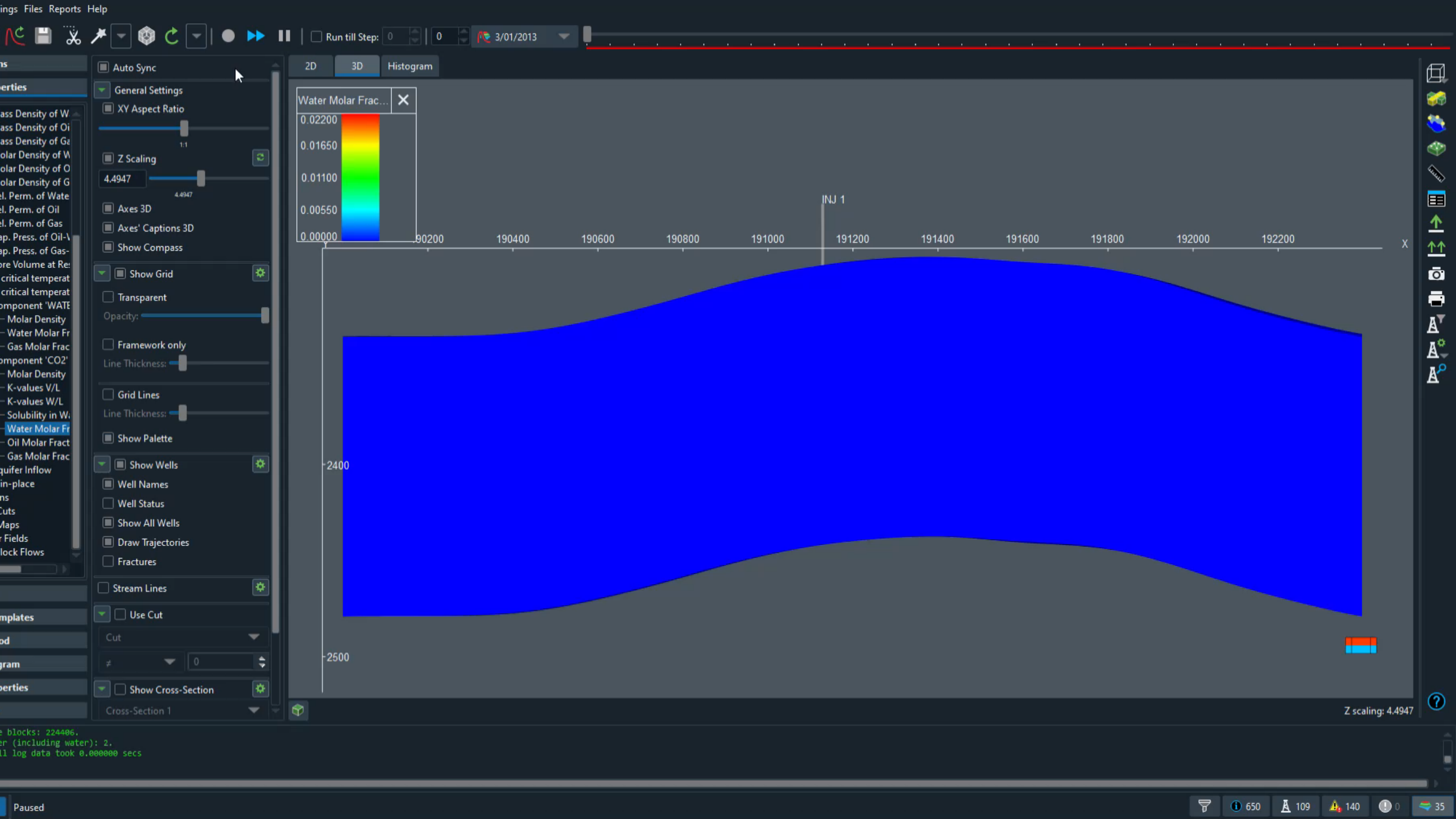


Worden 2024

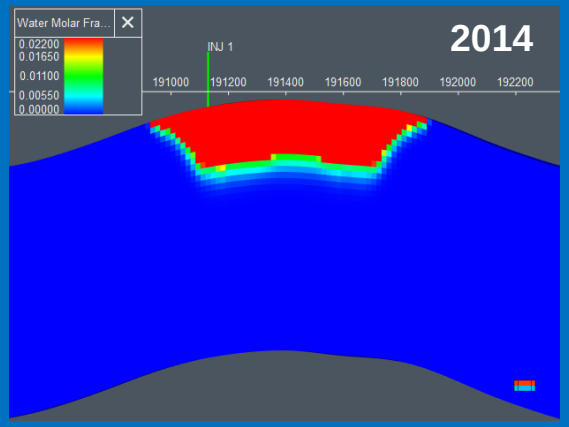
Controls on CO_2 Dissolution

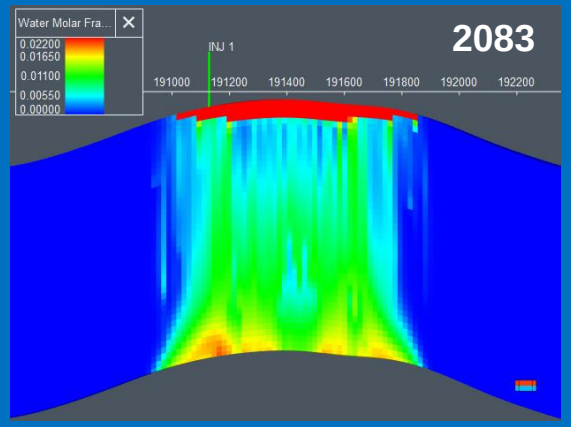
Parameter	Effect on Dissolution
Permeability	Promotes fingering and convective mixing Higher k promotes convection onset
Porosity	Governs brine volume available to dissolve CO_2
Brine Salinity	Reduces solubility and Δρ (density contrast)
Interface Area	Larger interface = higher dissolution flux
Heterogeneity	Alters plume paths; may suppress or focus mixing
Temperature/Pressure	High P = ↑ solubility; high T = ↓ solubility
Wettability	Affects CO_2 trapping and brine distribution Water-wet rocks promote brine dominance and dissolution contact efficiency

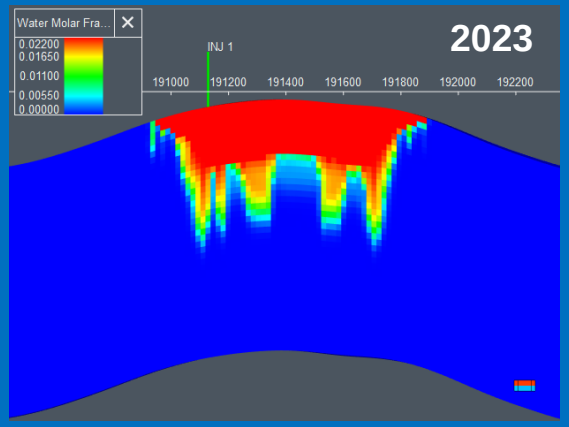


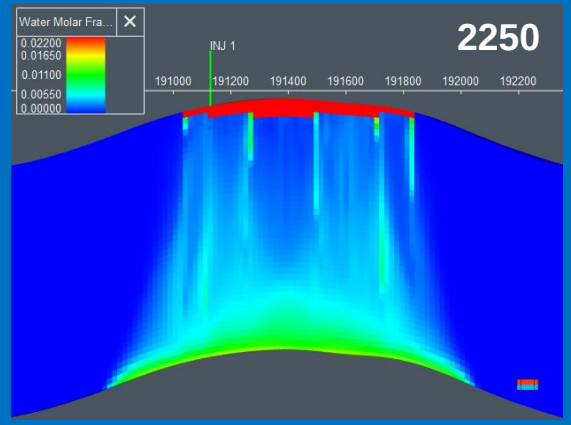

ings Files Reports Help
Run till Step:
3/01/2013
Auto Sync
General Settings
XY Aspect Ratio
1:1
Z Scaling
4.4947
Axes 3D
Axes' Captions 3D
Show Compass
Show Grid
Transparent
Opacity:
Framework only
Line Thickness:
Grid Lines
Line Thickness:
Show Palette
Show Wells
Well Names
Well Status
Show All Wells
Draw Trajectories
Fractures
Stream Lines
Use Cut
Cut
Show Cross-Section
Cross-Section 1
2D
3D
Histogram
Water Molar Frac...
0.02200
0.01650
0.01100
0.00550
0.00000
INJ 1
190200
190400
190600
190800
191000
191200
191400
191600
191800
192000
192200
X
2400
2500
Z scaling: 4.4947
Paused

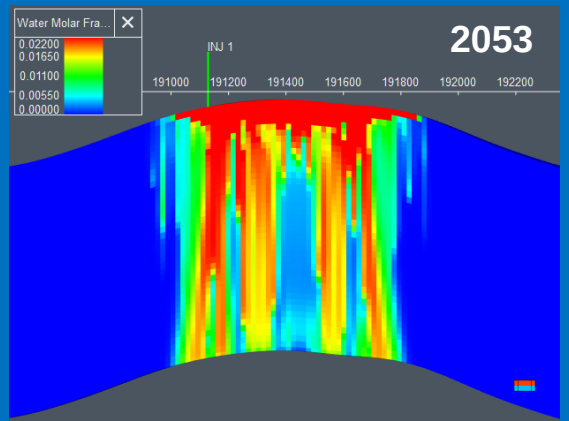
Test Model – CO2 Water Molar Fraction

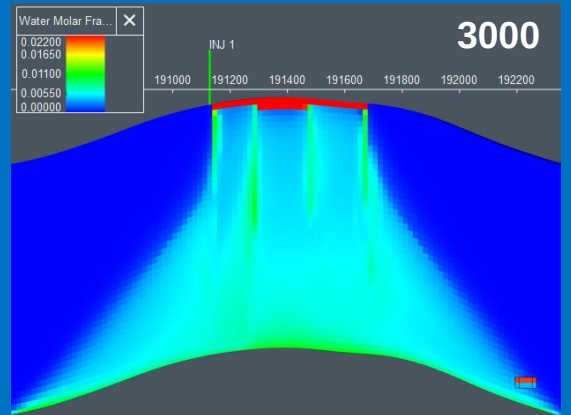


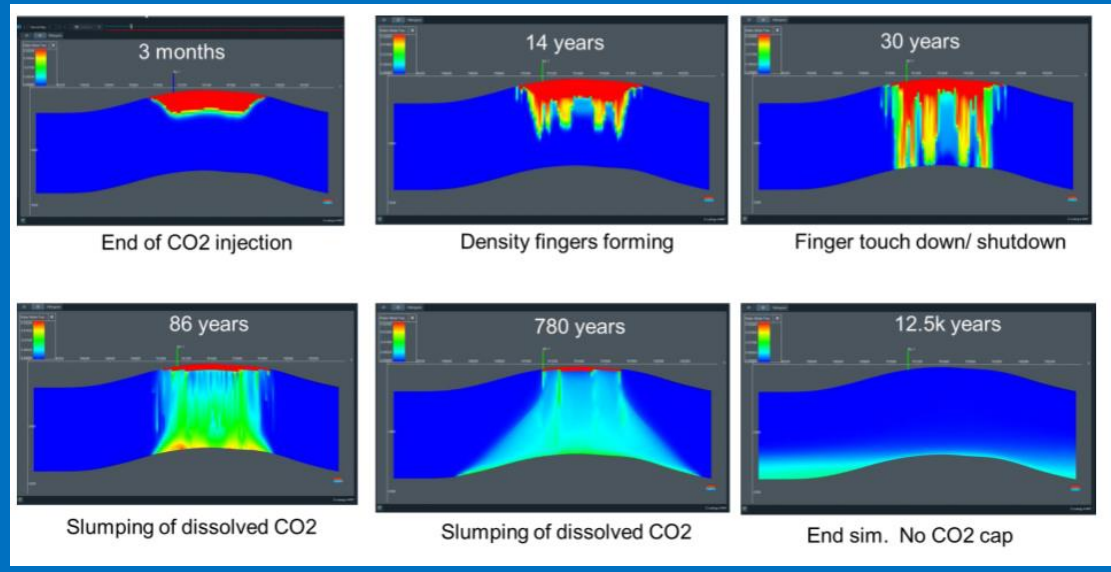




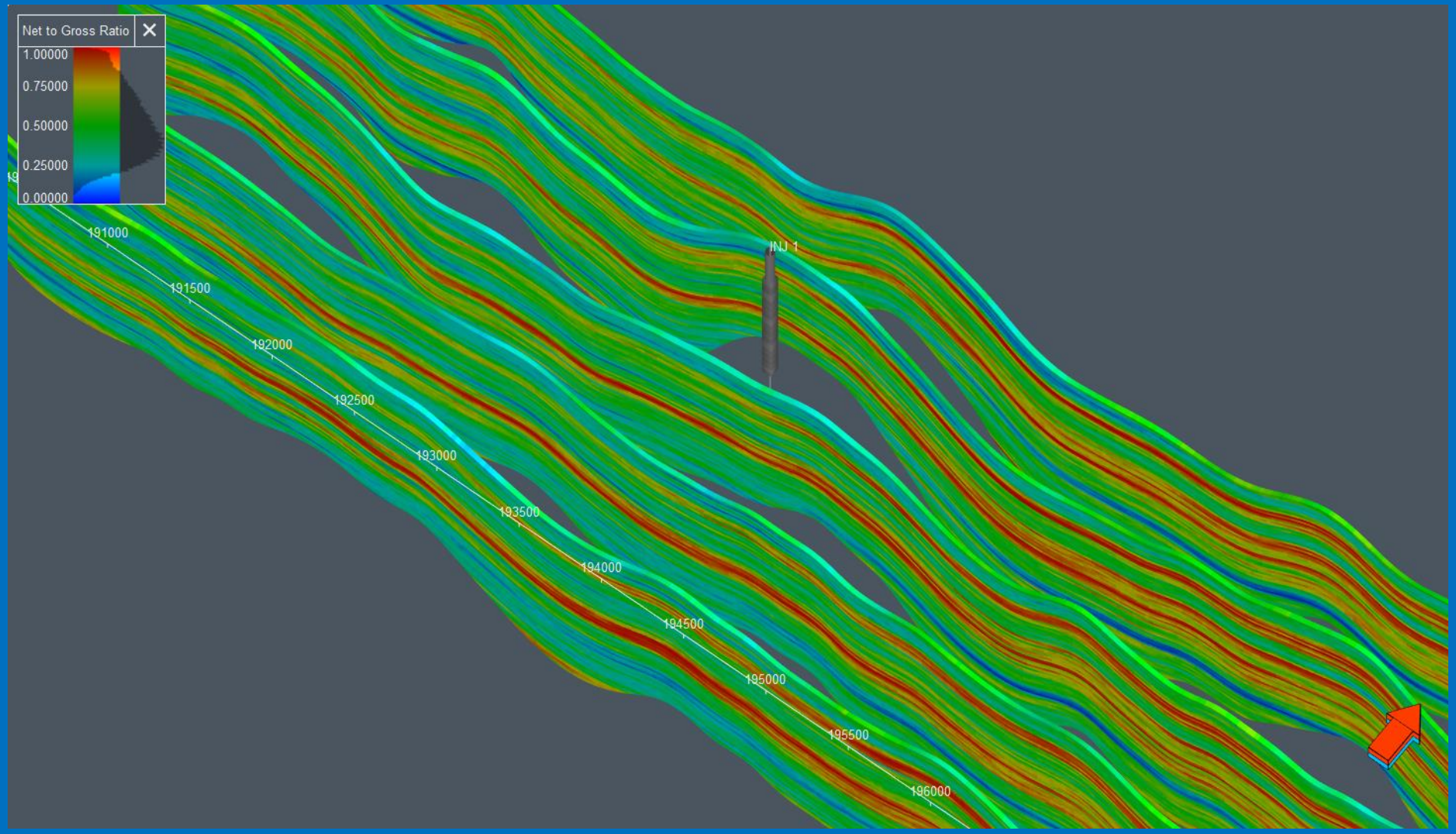


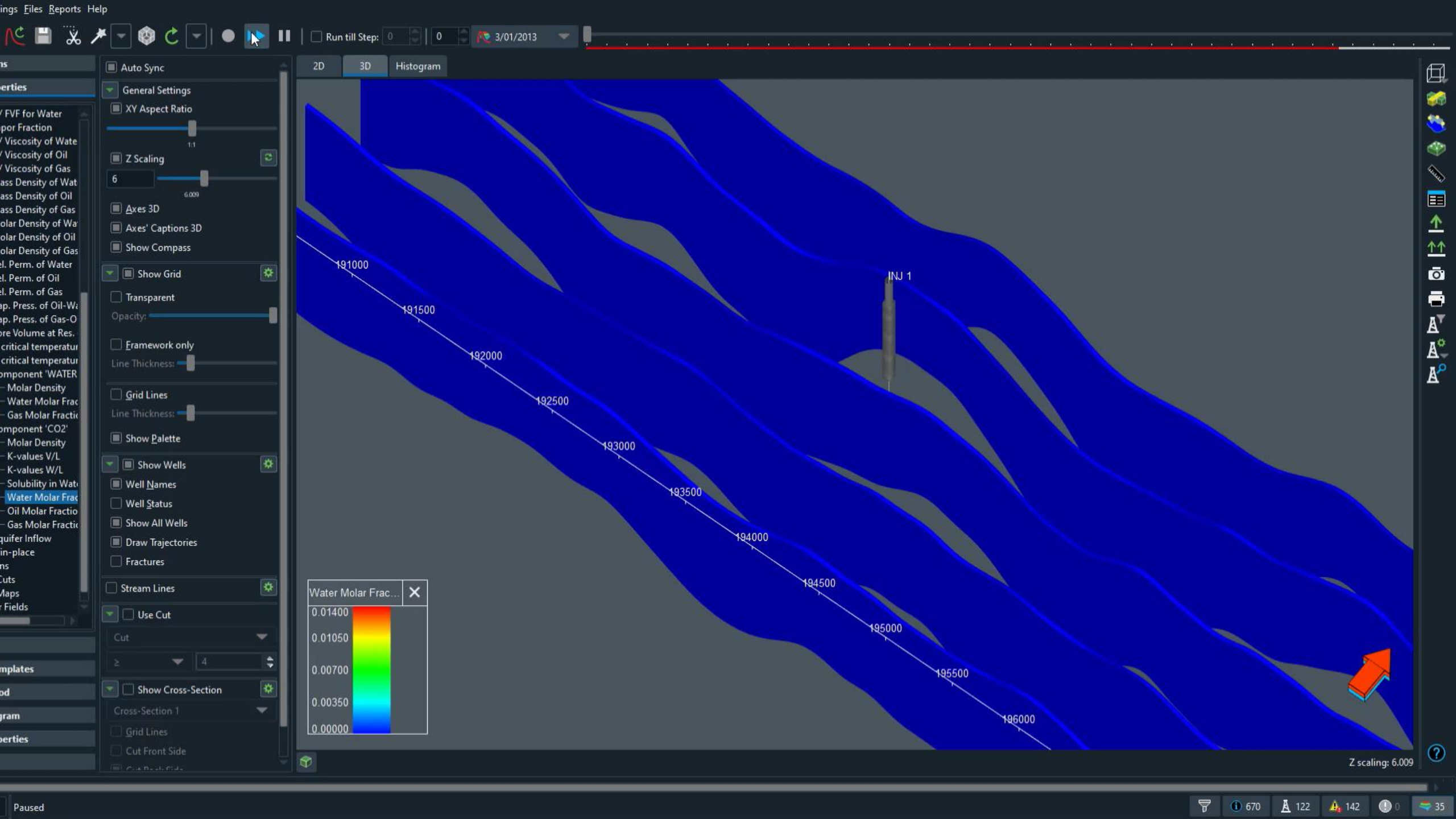


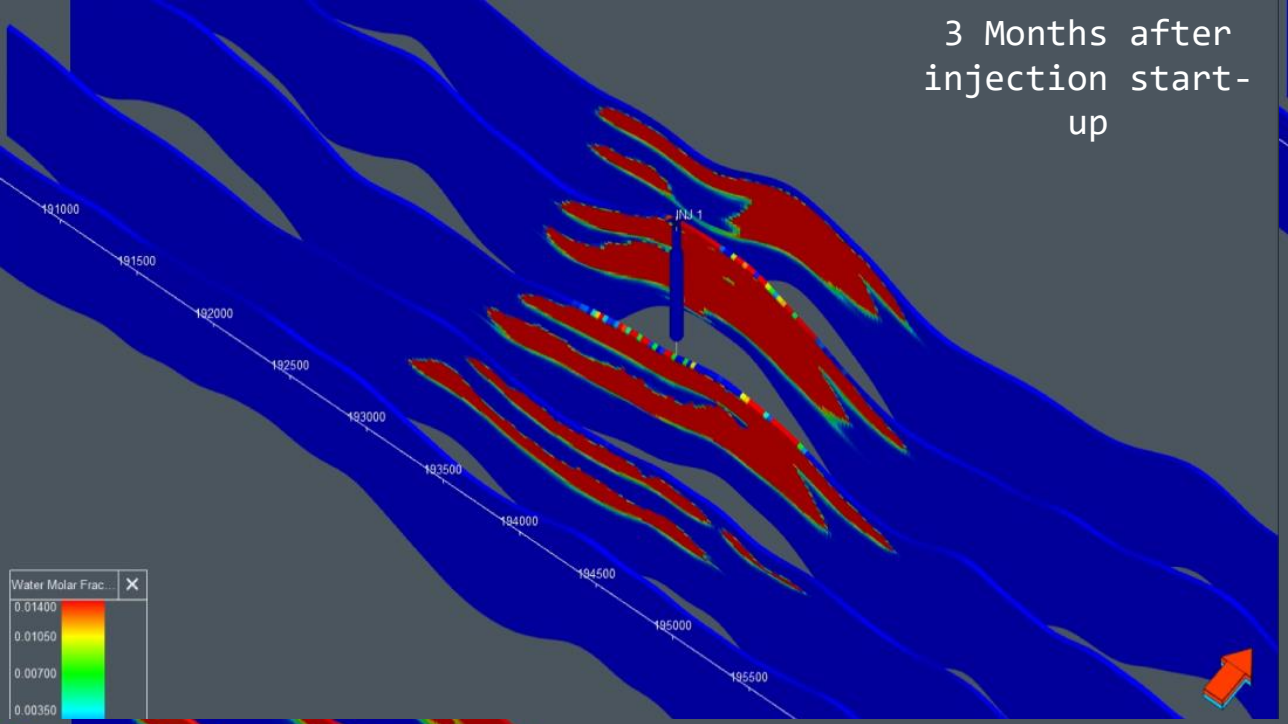


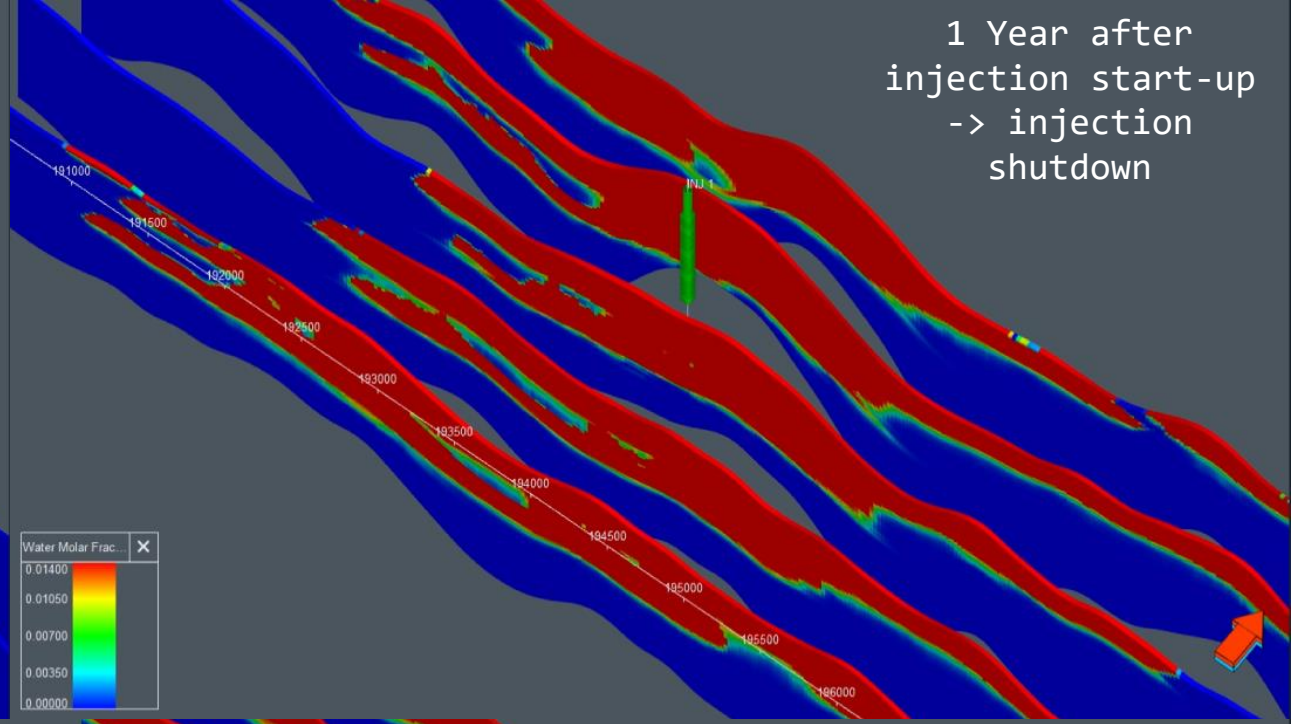


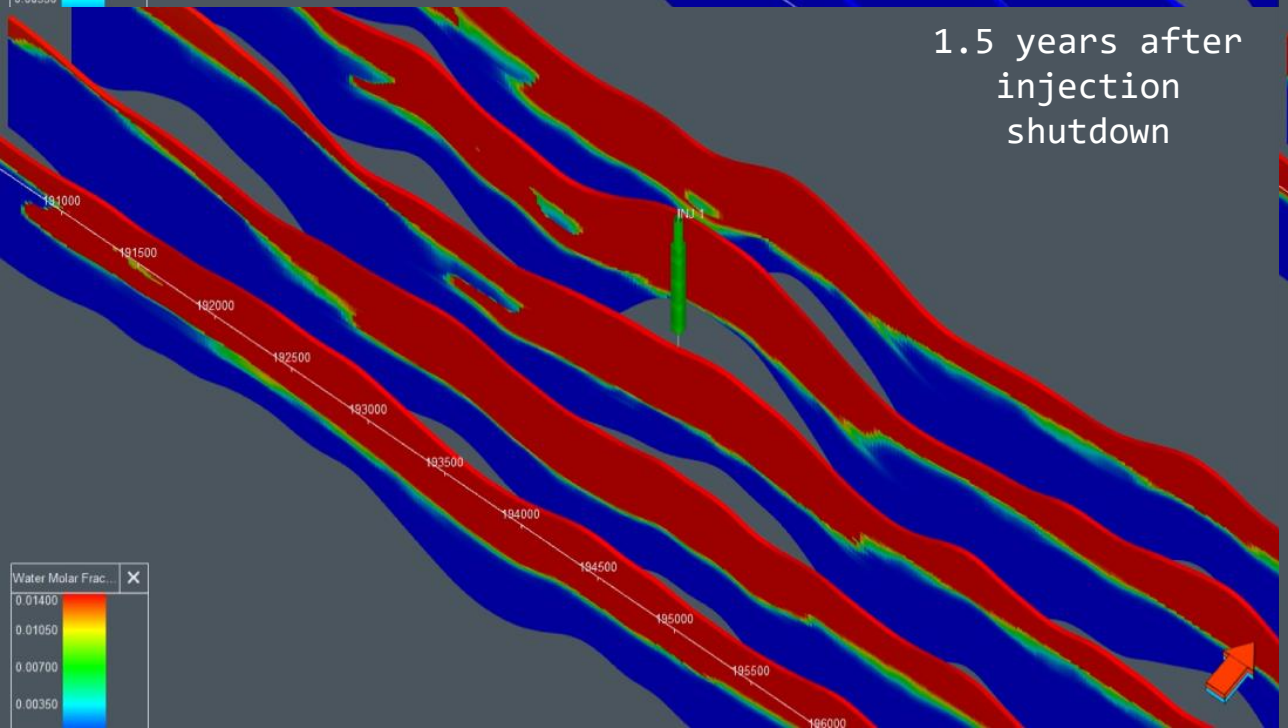
Model SCA3

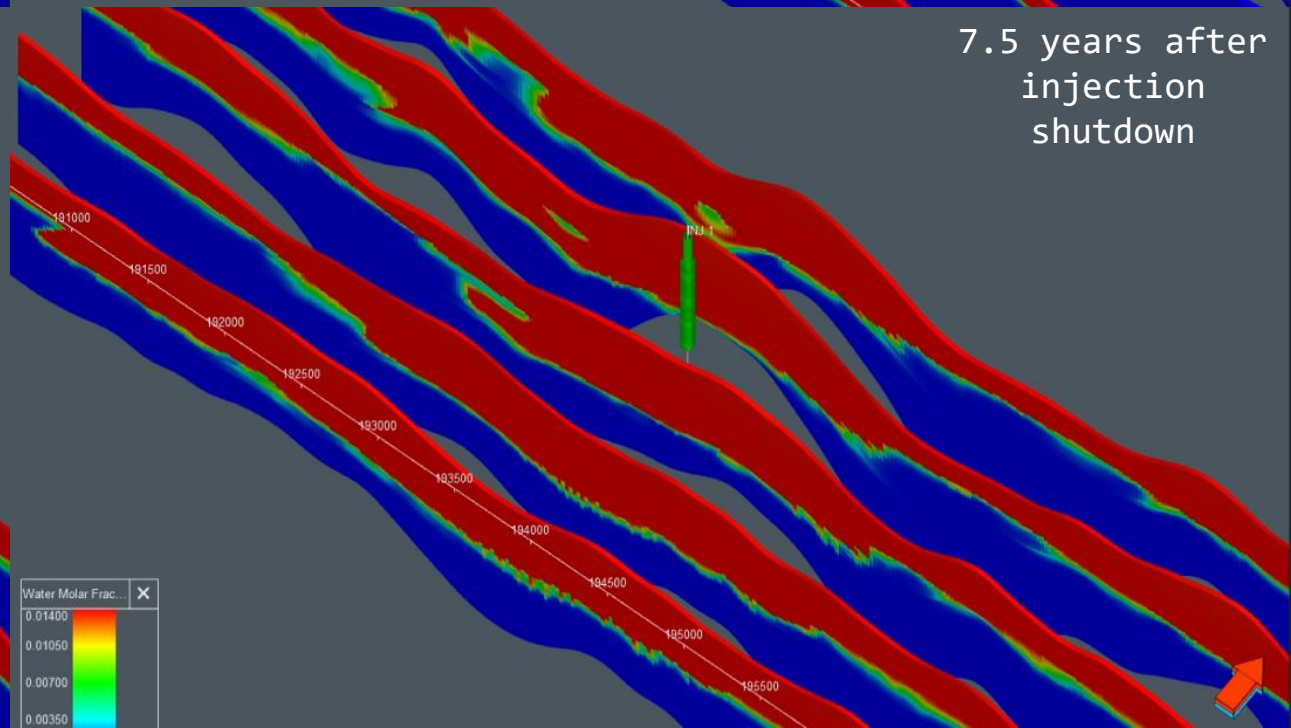

Net to Gross Ratio
1.00000
0.75000
0.50000
0.25000
0.00000
191000
191500
192000
192500
193000
193500
194000
194500
195000
195500
196000
INJ 1

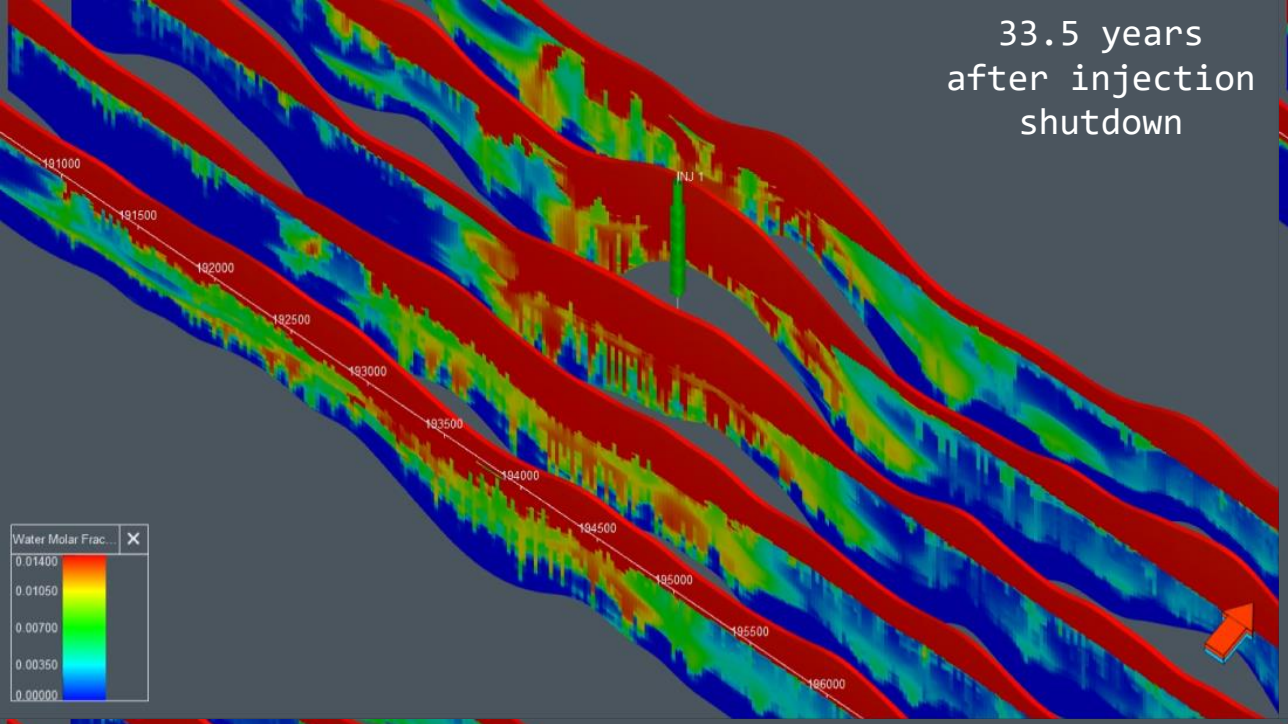

ings Files Reports Help
Run till Step:
3/01/2013
Auto Sync
General Settings
XY Aspect Ratio
Z Scaling
Axes 3D
Axes' Captions 3D
Show Compass
Show Grid
Transparent
Opacity:
Framework only
Line Thickness:
Grid Lines
Line Thickness:
Show Palette
Show Wells
Well Names
Well Status
Show All Wells
Draw Trajectories
Fractures
Stream Lines
Use Cut
Cut
Show Cross-Section
Cross-Section 1
Grid Lines
Cut Front Side
2D
3D
Histogram
INJ 1
191000
191500
192000
192500
193000
193500
194000
194500
195000
195500
196000
Water Molar Frac...
0.01400
0.01050
0.00700
0.00350
0.00000
Z scaling: 6.009
Paused

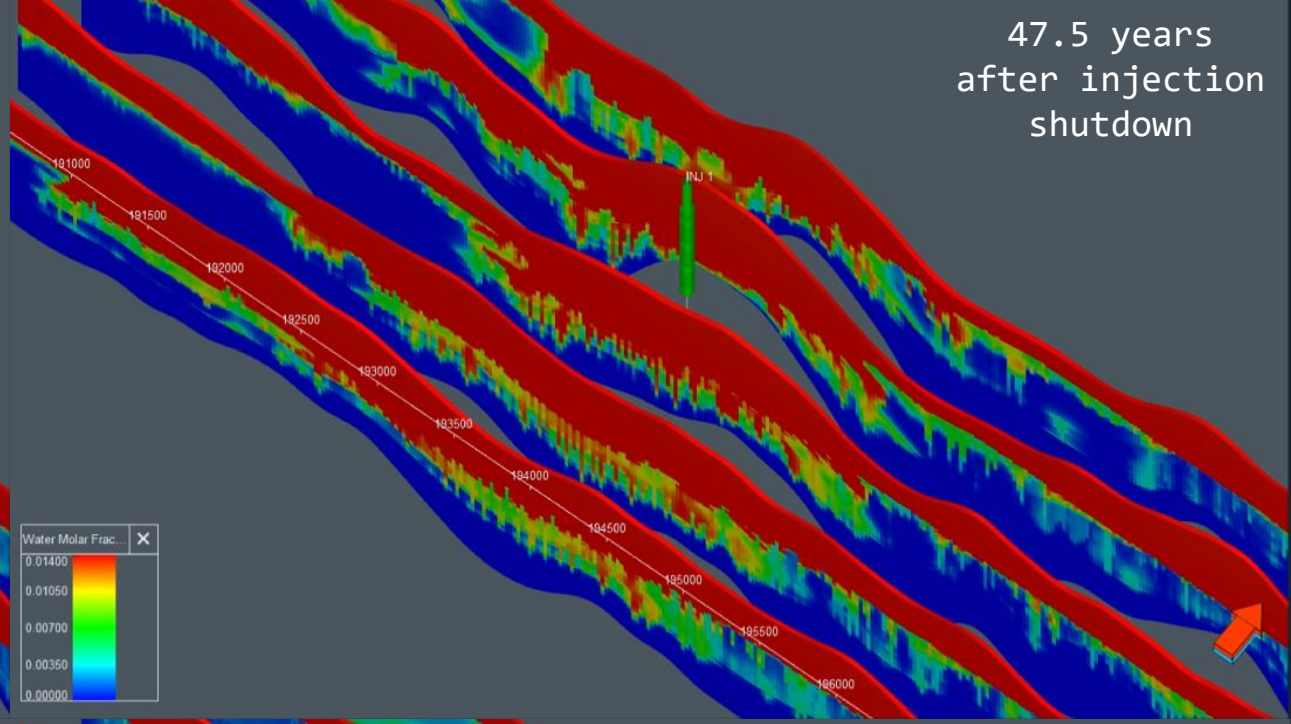

3 Months after injection start-up
INJ 1
191000
191500
192000
192500
193000
193500
194000
194500
195000
195500
Water Molar Frac...
0.01400
0.01050
0.00700
0.00350

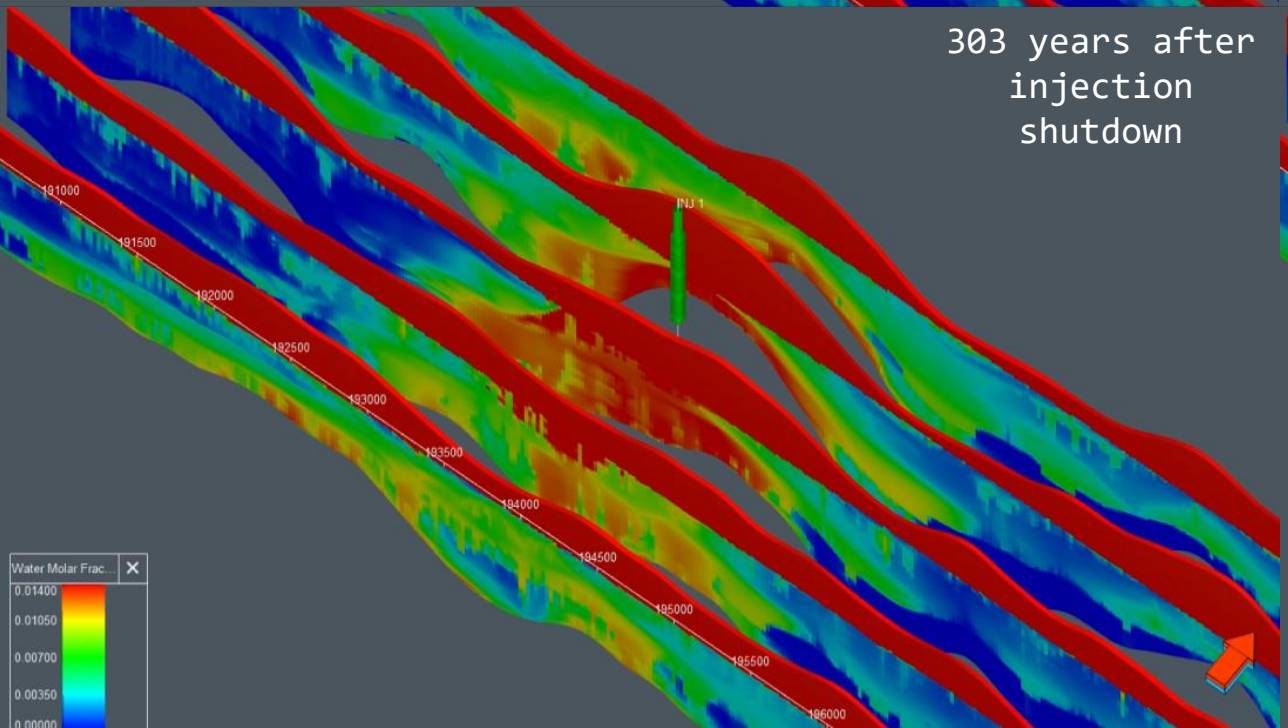

1 Year after injection start-up -> injection shutdown
INJ 1
191000
191500
192000
192500
193000
193500
194000
194500
195000
195500
196000
Water Molar Frac...
0.01400
0.01050
0.00700
0.00350
0.00000

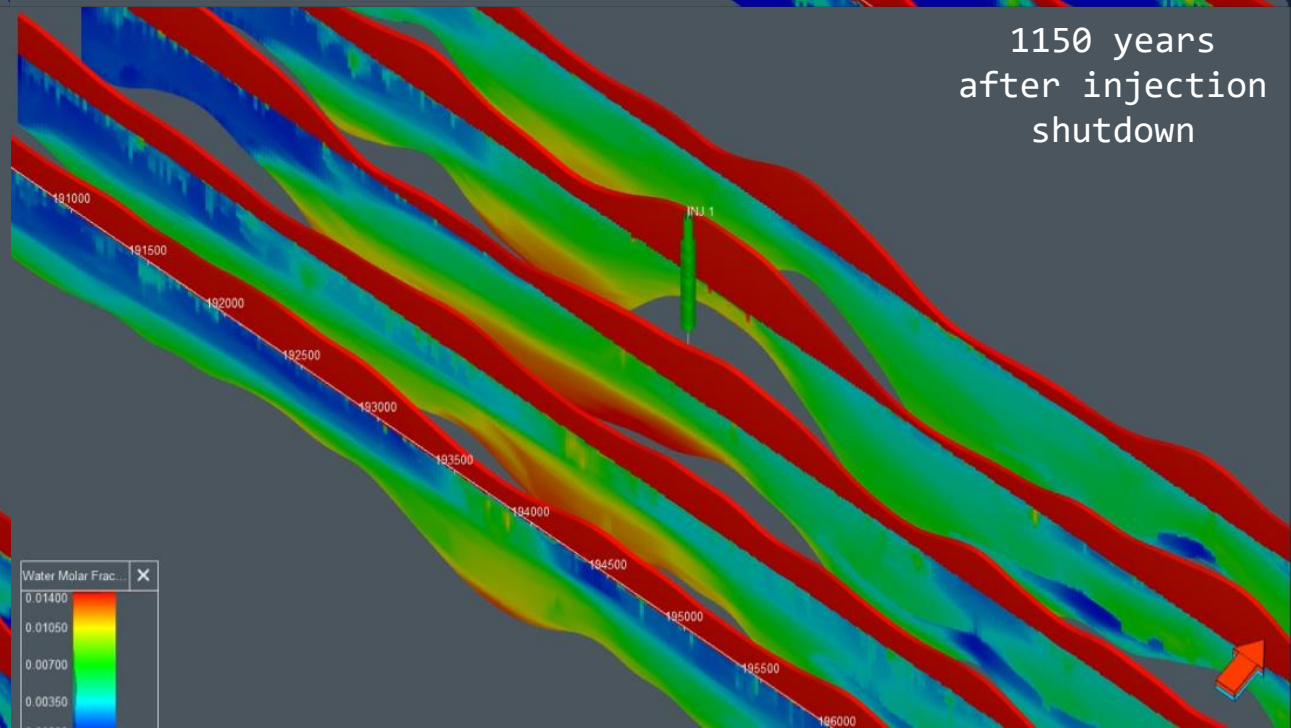

1.5 years after injection shutdown
INJ 1
191000
191500
192000
192500
193000
193500
194000
194500
195000
195500
196000
Water Molar Frac...
0.01400
0.01050
0.00700
0.00350


7.5 years after injection shutdown
INJ 1
191000
191500
192000
192500
193000
193500
194000
194500
195000
195500
Water Molar Frac...
0.01400
0.01050
0.00700
0.00350

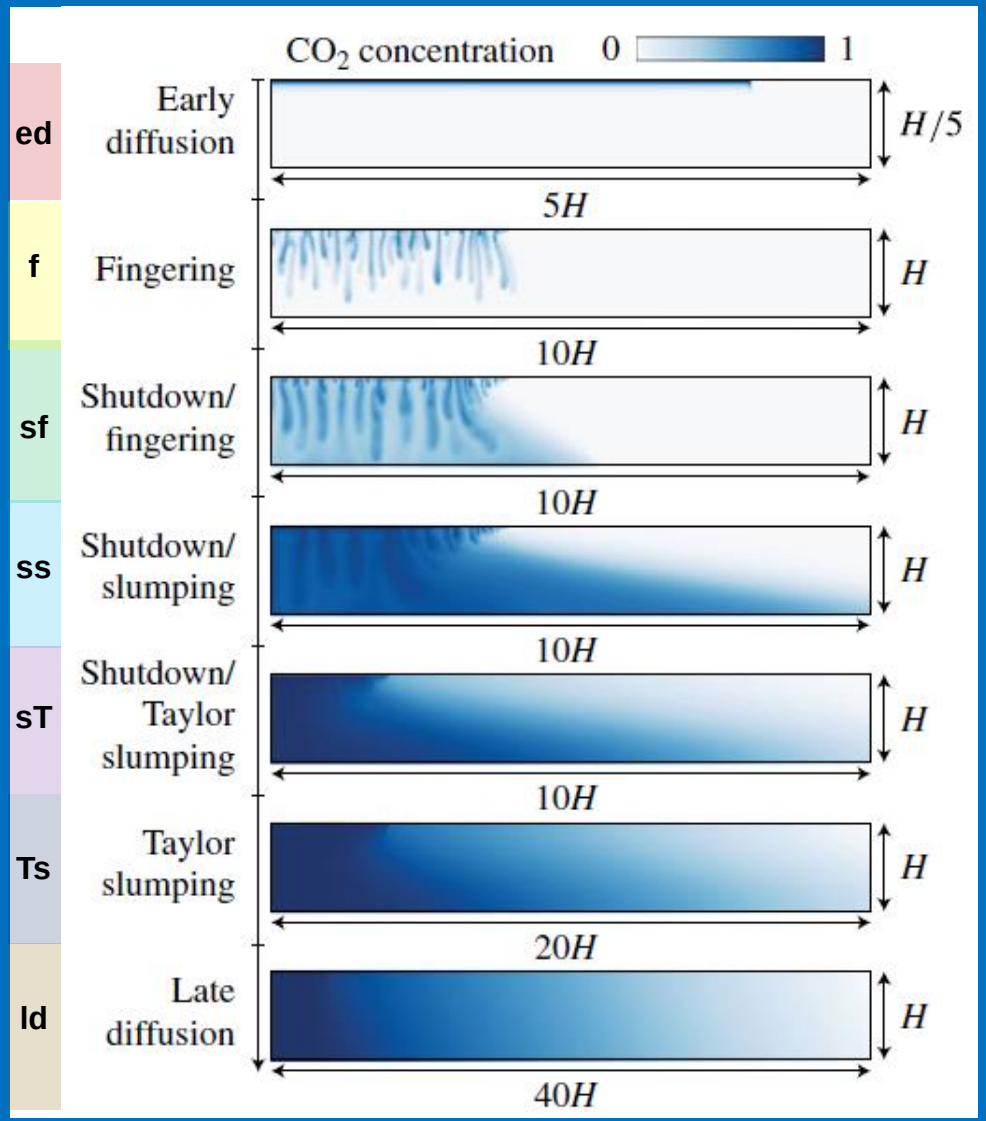

33.5 years
after injection
shutdown
INJ 1
191000
191500
192000
192500
193000
193500
194000
194500
195000
195500
196000
Water Molar Frac...
0.01400
0.01050
0.00700
0.00350
0.00000

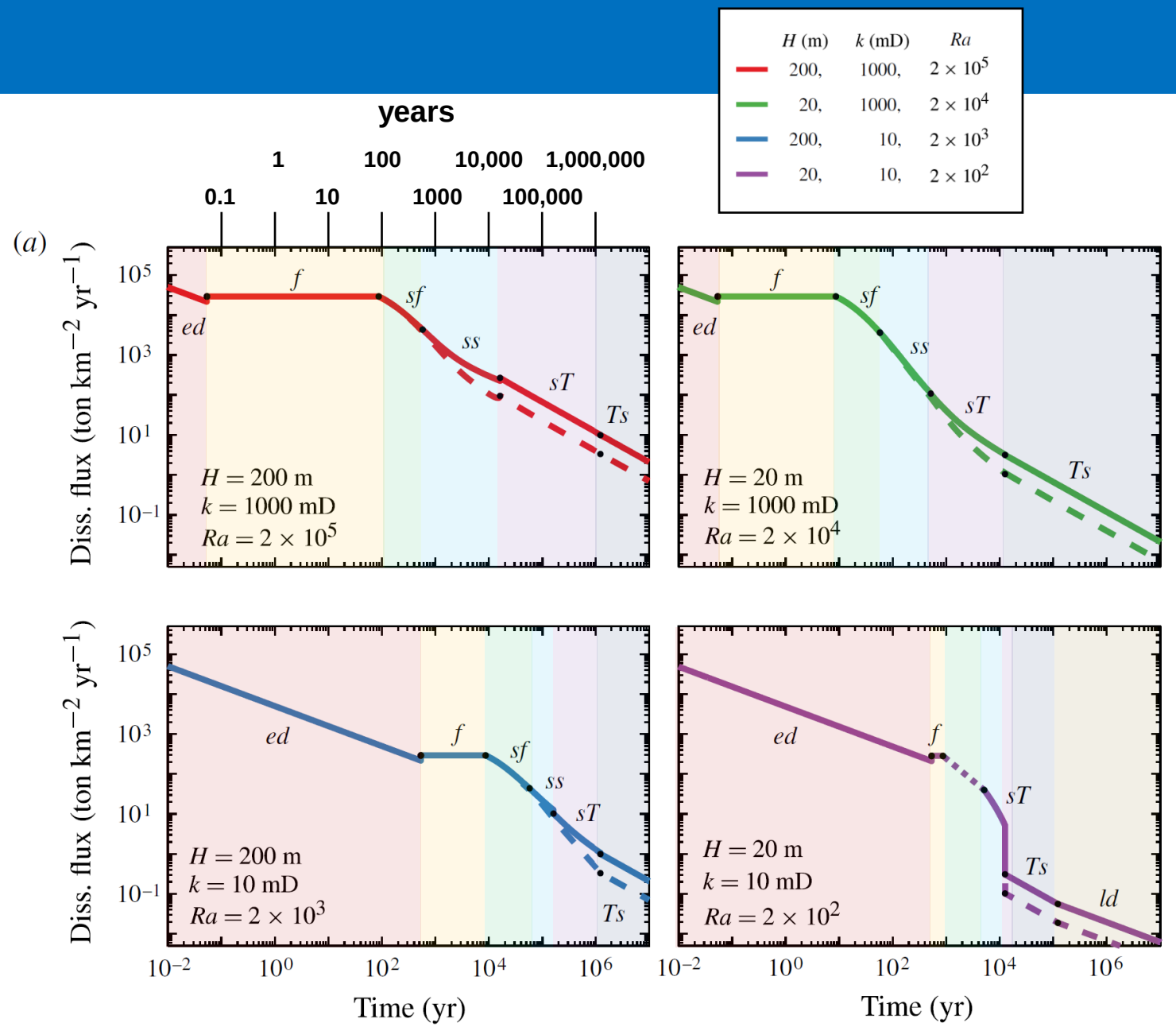

47.5 years
after injection
shutdown
INJ 1
191000
191500
192000
192500
193000
193500
194000
194500
195000
195500
196000
Water Molar Frac...
0.01400
0.01050
0.00700
0.00350
0.00000


303 years after
injection
shutdown
INJ 1
191000
191500
192000
192500
193000
193500
194000
194500
195000
195500
196000
Water Molar Frac...
0.01400
0.01050
0.00700
0.00350
0.00000


1150 years
after injection
shutdown
INJ 1
191000
191500
192000
192500
193000
193500
194000
194500
195000
195500
196000
Water Molar Frac...
0.01400
0.01050
0.00700
0.00350
0.00000

Flux Regimes





Szulczewski et al. 2013

Rayleigh Number (Ra) & Dissolution Flux Regimes

- **Key variable for convection onset**
- **Geology**: Reservoir heterogeneity causes local Ra variability

$$V = \frac{\Delta\rho \cdot g \cdot k}{\mu \cdot \phi} \qquad Ra = \frac{V \cdot H}{D} = \frac{\Delta\rho \cdot g \cdot k \cdot H}{\mu \cdot \phi \cdot D}$$

Where:

- $\Delta\rho$ = density contrast (CO_2-rich vs fresh brine)
- k = permeability
- H = interface thickness
- μ, D, ϕ = viscosity, diffusivity, porosity

Regime	Dominant Process	Ra Range
Early Diffusion	Molecular diffusion only	Ra < 100
Transition	Onset of unstable fingers	100 < Ra < 2000
Fingering	Fully developed convection	Ra > 2000
Shutdown/Taylor Slumping	Saturation-controlled	–

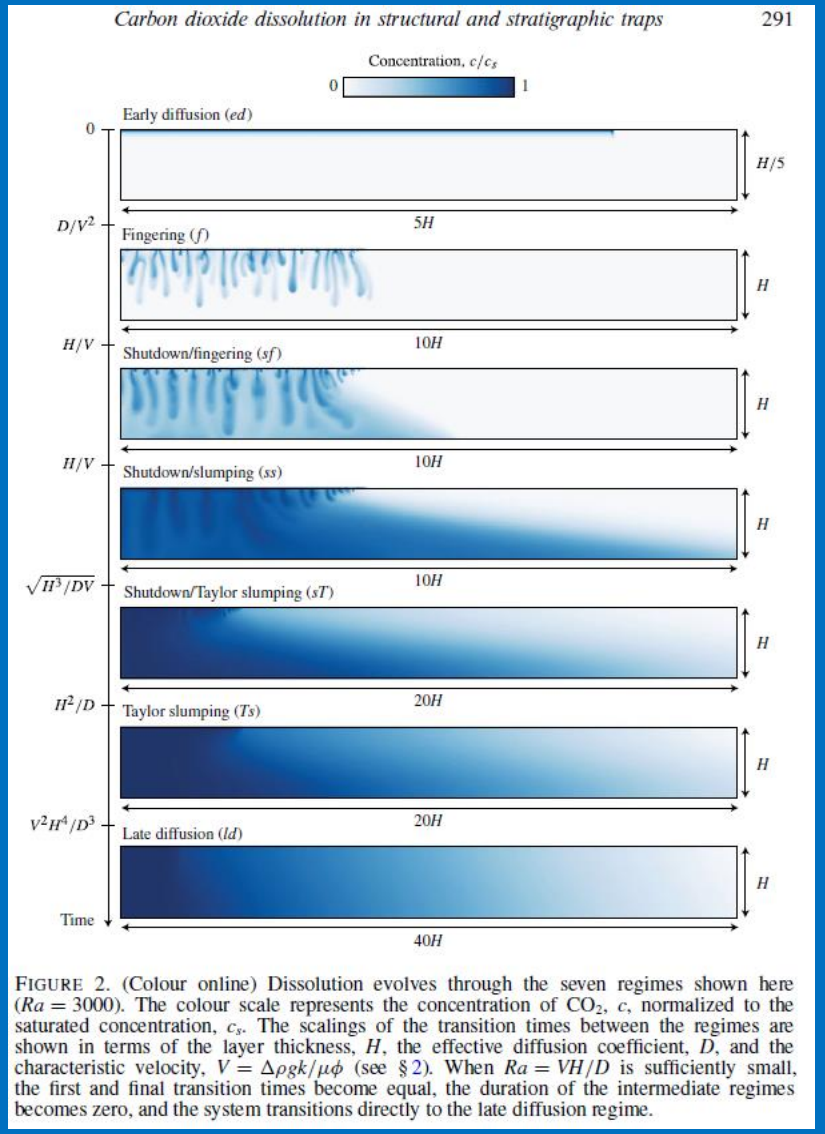


FIGURE 2. (Colour online) Dissolution evolves through the seven regimes shown here ($Ra = 3000$). The colour scale represents the concentration of CO_2, c, normalized to the saturated concentration, c_s. The scalings of the transition times between the regimes are shown in terms of the layer thickness, H, the effective diffusion coefficient, D, and the characteristic velocity, $V = \Delta\rho gk/\mu\phi$ (see §2). When $Ra = VH/D$ is sufficiently small, the first and final transition times become equal, the duration of the intermediate regimes becomes zero, and the system transitions directly to the late diffusion regime.

Szulczewski et al. 2013

H : layer thickness

D : effective diffusion coefficient

V = characteristic pore velocity Δρgk/μφ

Ra = VH/D

c : CO2 concentration

c_v : saturation concentration

k : permeability

μ : dynamic viscosity

φ : porosity

p : pressure

g : gravitational acceleration

ρ : density

Δρ : difference between freshwater and CO2-saturated water

take the following as constants:

D, k, μ, φ

Flux Regime Durations & Rates

Regime	Typical Duration	Flux Formula (kg/m²/s)	Description / Trigger
Early Diffusion (ed)	$0 - t_f \approx D/V^2$	$f(t) = c_s\sqrt{\frac{D}{\pi t}}$	Diffusion from a fixed CO_2-brine interface; no convection yet
Fingering (f)	t_f to $t_{sf} \approx 15H/V$	$f = 0.017 \cdot c_s \cdot V$	Onset of convection (Ra > 2000); steady fingering flux
Shutdown / Slumping (sf)	t_{sf} to $t_{sT} \sim (H^3/VD)^{1/2}$	$f(t) \approx c_s V\left(\frac{H}{Vt}\right)^{1/2}$	Interface becomes saturated; mixing slows
Taylor Slumping (sT)	t_{sT} to $t_{ld} \sim H^2/D$	$f(t) \sim \frac{c_s H}{W}\left(\frac{H^4V^2}{Dt^3}\right)^{1/4}$	Edge-driven convective mixing
Late Diffusion (ld)	$> H^2/D$	$f(t) \sim t^{-1/2}$	Final decline; no fresh brine available to convect

How to Calculate Regime Transition Times

Onset of Fingering (end of early diffusion):

$$t_f = \frac{D}{V^2}$$

Start of Shutdown / Slumping:

$$t_{sf} = \frac{15 \cdot H}{V}$$

Taylor Slumping Onset:

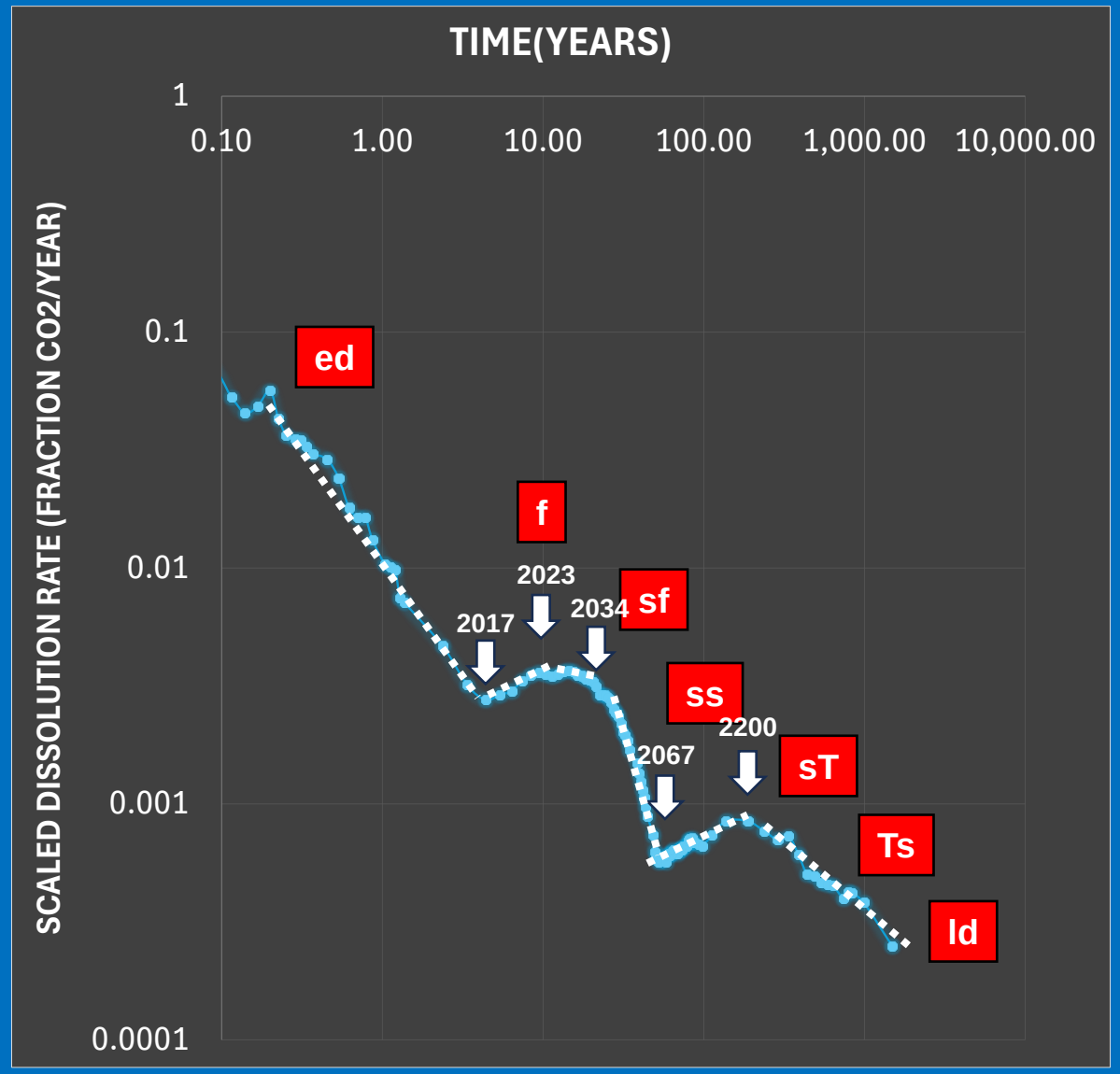
$$t_{sT} = \left(\frac{H^3}{V \cdot D}\right)^{1/2}$$

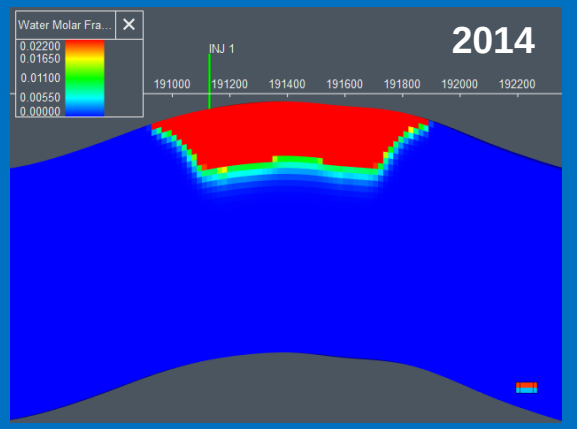
Late Diffusion Onset:

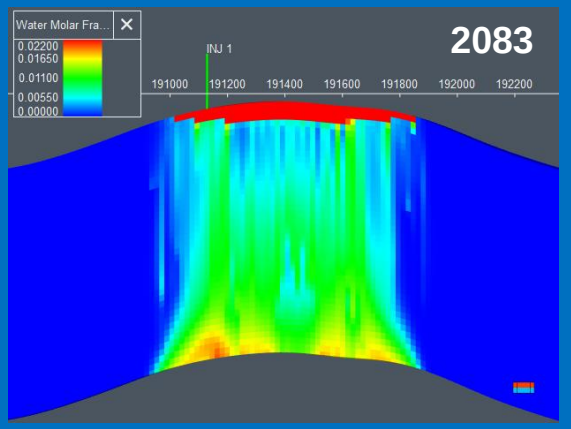
$$t_{ld} = \frac{H^2}{D}$$

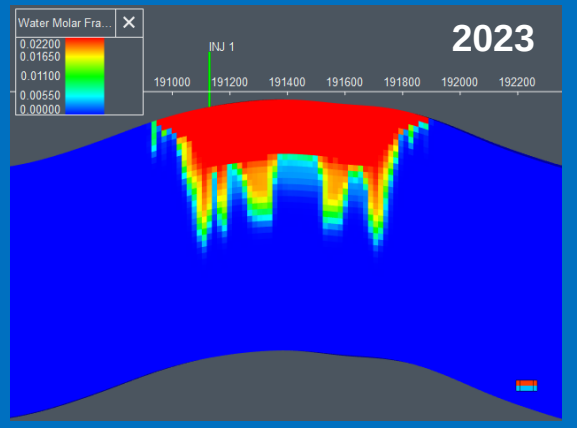
Szulczewski et al. 2013

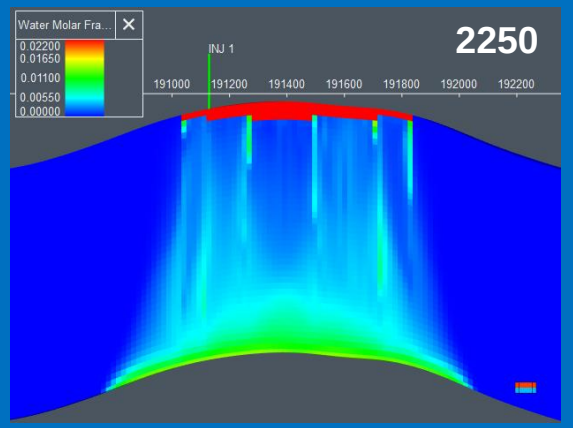
Test Model

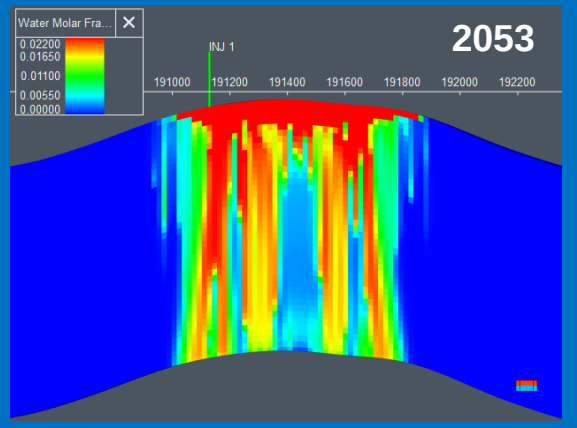

TIME(YEARS)
1
0.10
1.00
10.00
100.00
1,000.00
10,000.00
SCALED DISSOLUTION RATE (FRACTION CO2/YEAR)
0.1
0.01
0.001
0.0001
ed
f
2023
2017
2034
sf
ss
2200
2067
sT
Ts
ld

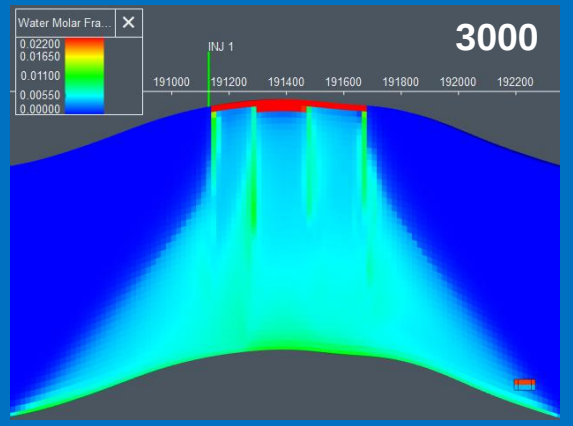

Water Molar Fra...
0.02200
0.01650
0.01100
0.00550
0.00000
INJ 1
191000
191200
191400
191600
191800
192000
192200
2014


Water Molar Fra...
0.02200
0.01650
0.01100
0.00550
0.00000
INJ 1
191000
191200
191400
191600
191800
192000
192200
2083

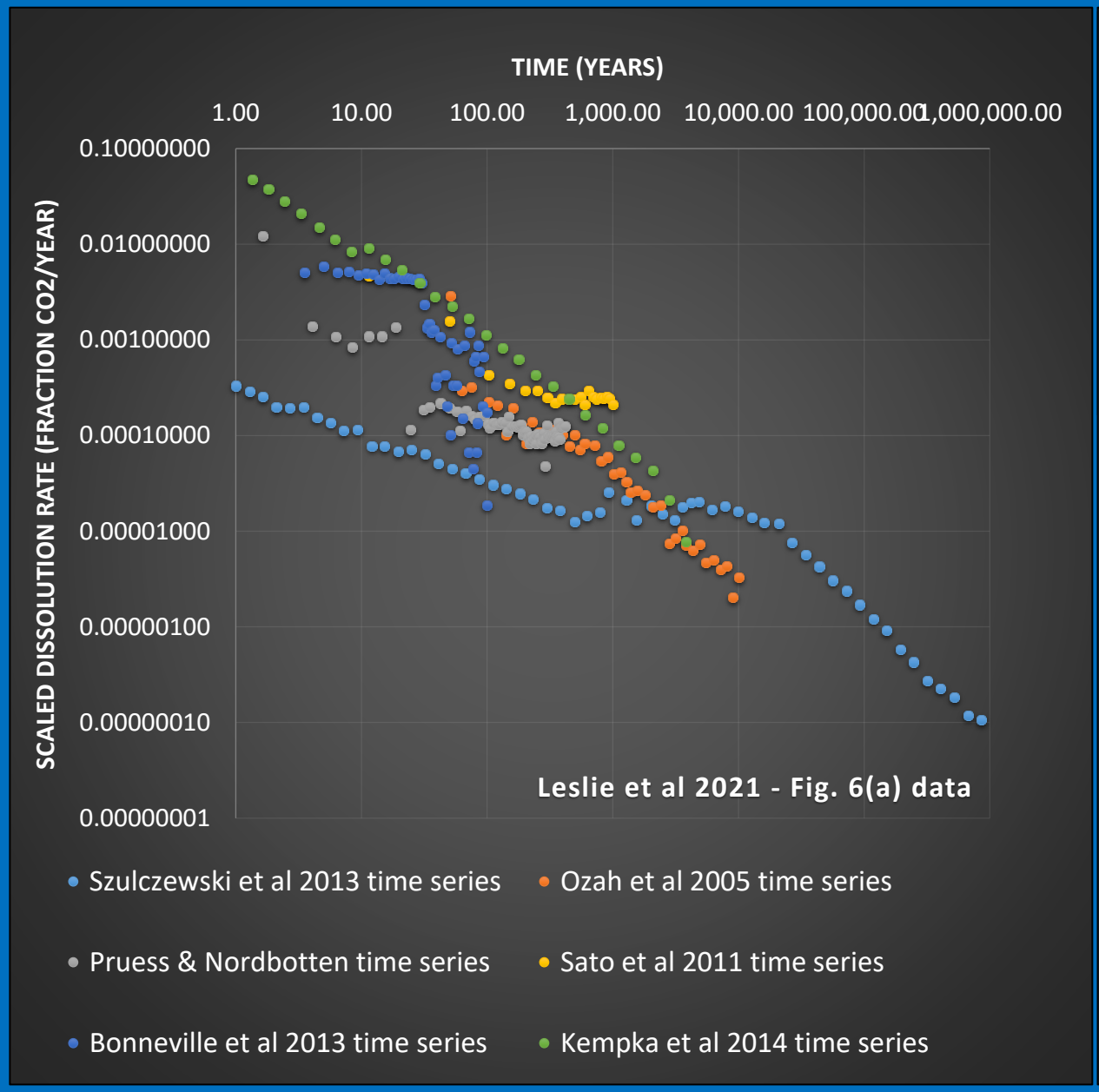

Water Molar Fra...
0.02200
0.01650
0.01100
0.00550
0.00000
INJ 1
191000
191200
191400
191600
191800
192000
192200
2023

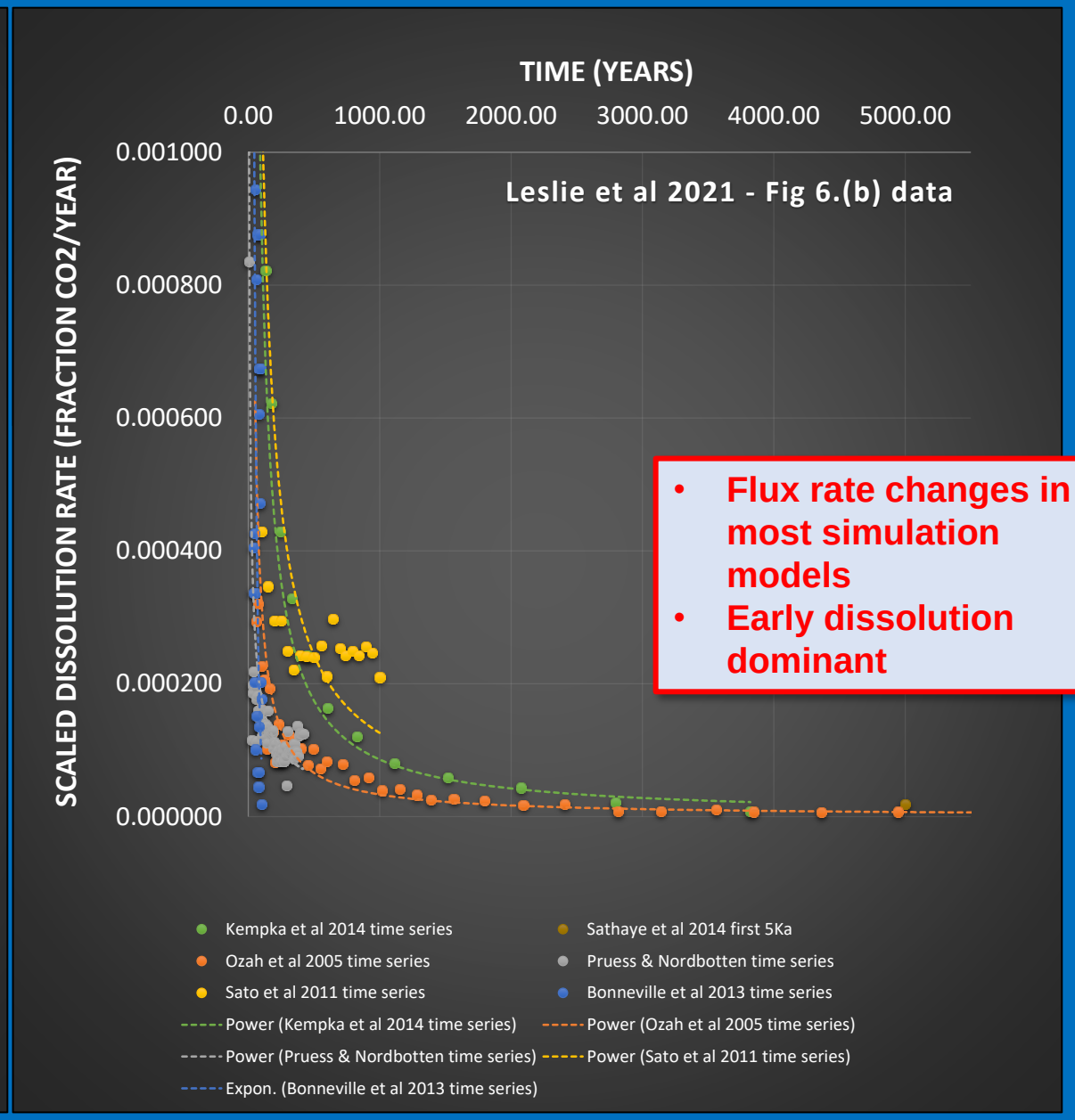

Water Molar Fra...
0.02200
0.01650
0.01100
0.00550
0.00000
INJ 1
191000
191200
191400
191600
191800
192000
192200
2250


Water Molar Fra...
0.02200
0.01650
0.01100
0.00550
0.00000
INJ 1
191000
191200
191400
191600
191800
192000
192200
2053

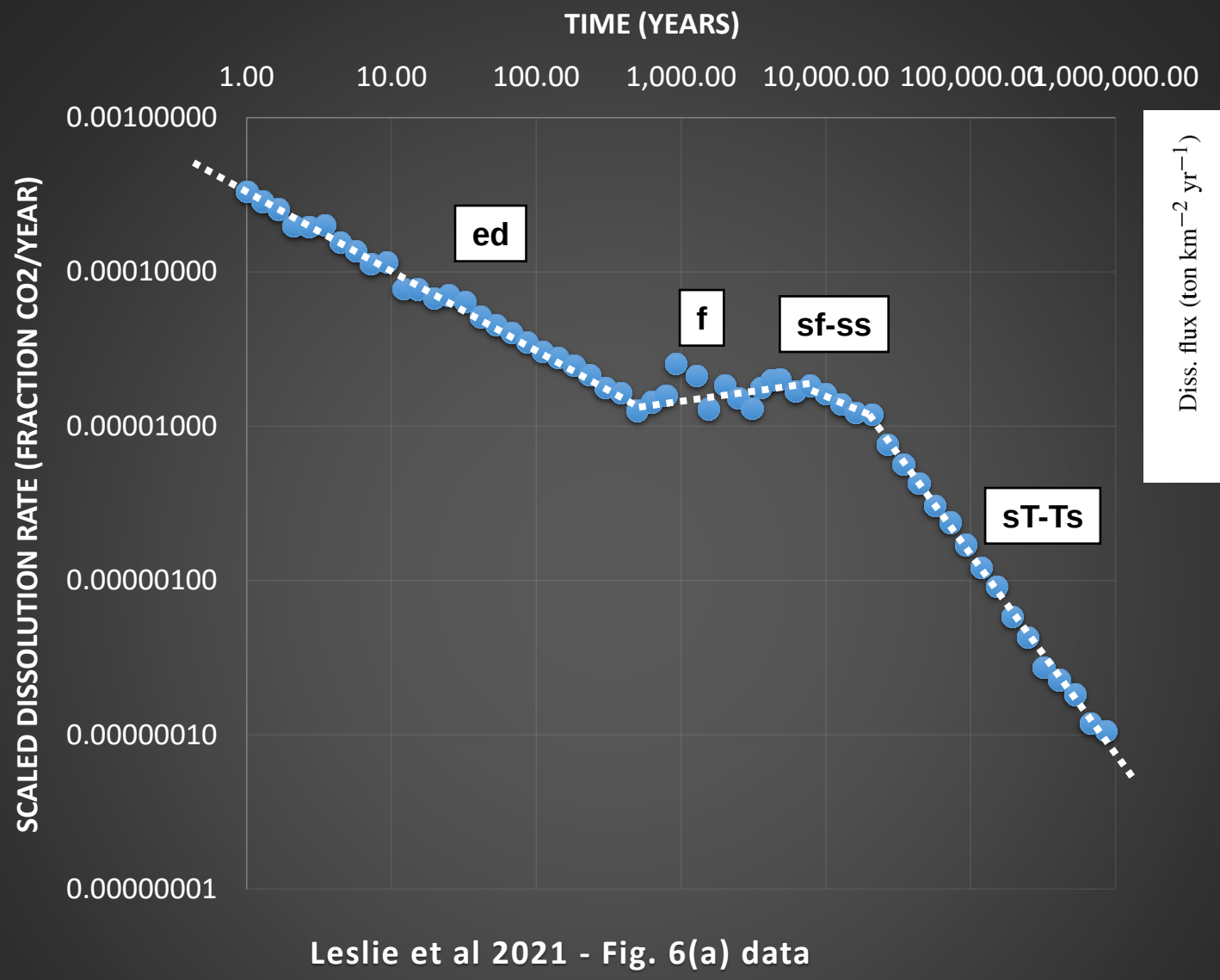

Water Molar Fra...
0.02200
0.01650
0.01100
0.00550
0.00000
INJ 1
191000
191200
191400
191600
191800
192000
192200
3000

CO2 Flux Quantification

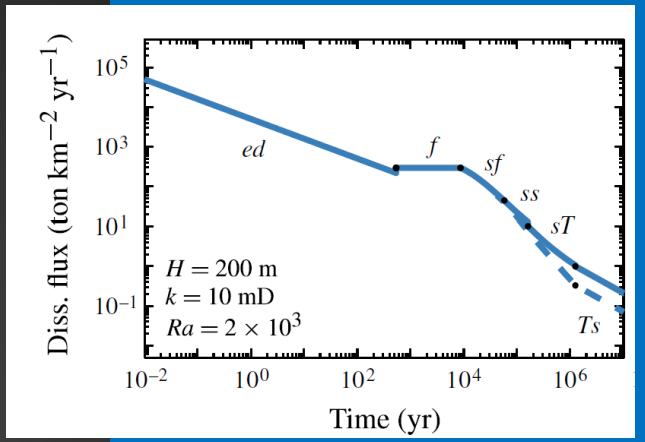




- **Flux rate changes in most simulation models**
- **Early dissolution dominant**



Leslie et al 2021 - Fig. 6(a) data



- Szulczewski et al 2013 time series

Summary of Key Variables Affecting CO_2 Dissolution Flux

Variable	Influence on Dissolution Flux	Direct or Indirect Effect?	Notes
CO_2 Solubility (c_s)	Increases flux linearly: $f \propto c_s$ ↑ P (↑c_s); ↑T & ↑Salinity (↓c_s)	✅ Direct	Determines max CO_2 that can dissolve into brine
Density Contrast (Δρ)	Increases buoyancy velocity V, hence flux: $f \propto \Delta\rho$	✅ Direct	Drives convective fingering; depends on c_s
Permeability (k)	Increases velocity $V \propto k$, hence flux	✅ Direct	Higher k = faster convection
Viscosity (μ)	Higher viscosity decreases V, hence reduces flux	✅ Direct (inverse)	Viscosity increases with salinity and temperature
Porosity (ϕ)	Higher porosity reduces V, hence reduces flux	✅ Direct (inverse)	Appears in denominator of velocity term
Diffusivity (D)	Higher D delays fingering onset, reduces early-time Ra	⚠ Indirect	Affects regime transitions, not flux directly. ↑ T and ↑ P (↑D); Sal↓ μ ↓ (↑D)
Salinity (g/L)	Reduces c_s (↓ solubility) but increases $\Delta\rho$	⚠ Both (nonlinear)	Flux first increases, then declines with salinity
Temperature / Pressure	Affects c_s, μ, and $\Delta\rho$	⚠ Indirect	Elevated T typically ↓ solubility; ↑ P increases it

Note: Interface Area and Reservoir Heterogeneity also key

Down-Dip Injection

Critical Role of Dissolution:

Dissolution is a key trapping mechanism for CO2 in geological storage. It immobilizes the CO2 by converting it into a denser, dissolved phase within the brine, significantly reducing the risk of upward migration and leakage.

Impact of Background Flow:

Background flow initially enhances dissolution by bringing fresh brine into contact with CO2.

Strong flows can slow dissolution by transporting dissolved CO2 away, reducing interaction at the CO2-brine interface.

Plume Dynamics:

The CO2 plume decelerates as dissolution and residual trapping reduce its mobility.

Over time, convective mixing dominates, leading to further plume fragmentation and dissolution.

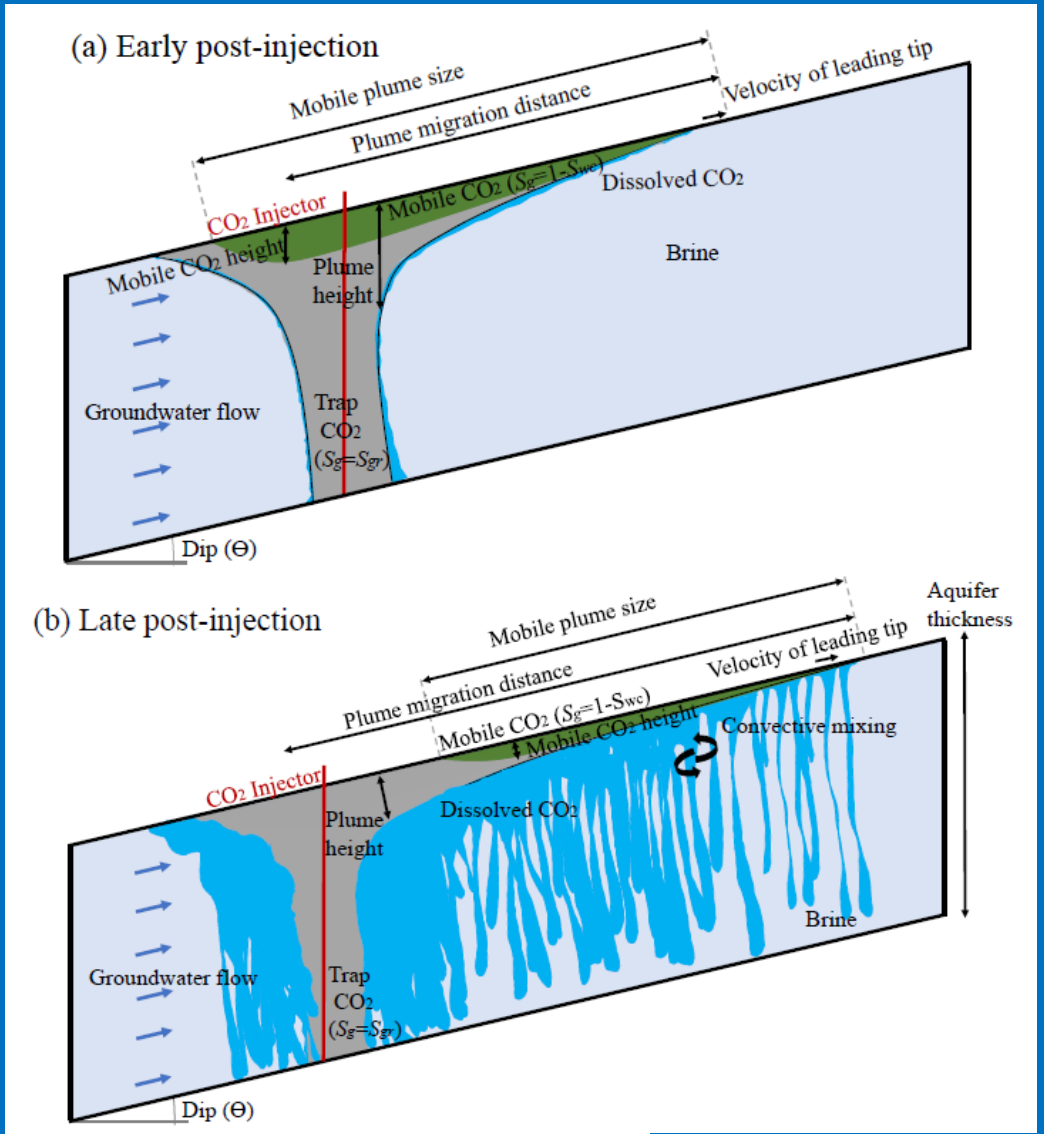


Fig. 1. the migration of a plume of CO_2 in a conceptual dipping aquifer system with updip groundwater flux during the early and late post-injection periods. Region 1 comprises mobile CO_2 and a connate water saturation S_{wc} (green); Region 2 contains the residual CO_2 S_{gr} and mobile water (grey); Region 3 indicates the dissolved CO_2 in water (blue).(a) Early post-injection and (b) Late post-injection.

Promotes up-dip migration and contact with more brine

Awag et al. 2024

UNIVERSITY OF ABERDEEN

Stacked Reservoirs

Benefits of Injecting CO2 into Stacked Multiple Reservoirs vs. a Single Reservoir

Pressure Management:

- Stacked reservoirs distribute pressure across multiple layers, reducing the risk of overpressure in a single formation. This prevents fracturing and maintains seal integrity.

Enhanced Storage Capacity:

- Utilizing multiple reservoirs increases the overall storage volume, as each layer contributes independently to the total capacity.

Improved Efficiency:

- Stacked systems allow for concurrent injection in separate layers, optimizing the injection process and mitigating the risk of injection interference.

Reduced Risk of Leakage:

- The presence of interbedded seals between stacked reservoirs adds additional barriers to CO2 migration, enhancing long-term containment security.

Scalability:

- Stacked systems are more adaptable to varying injection rates and capacities, offering flexibility for scaling up storage operations.
- This approach leverages the geological heterogeneity of reservoirs to optimize storage while minimizing risks and operational challenges

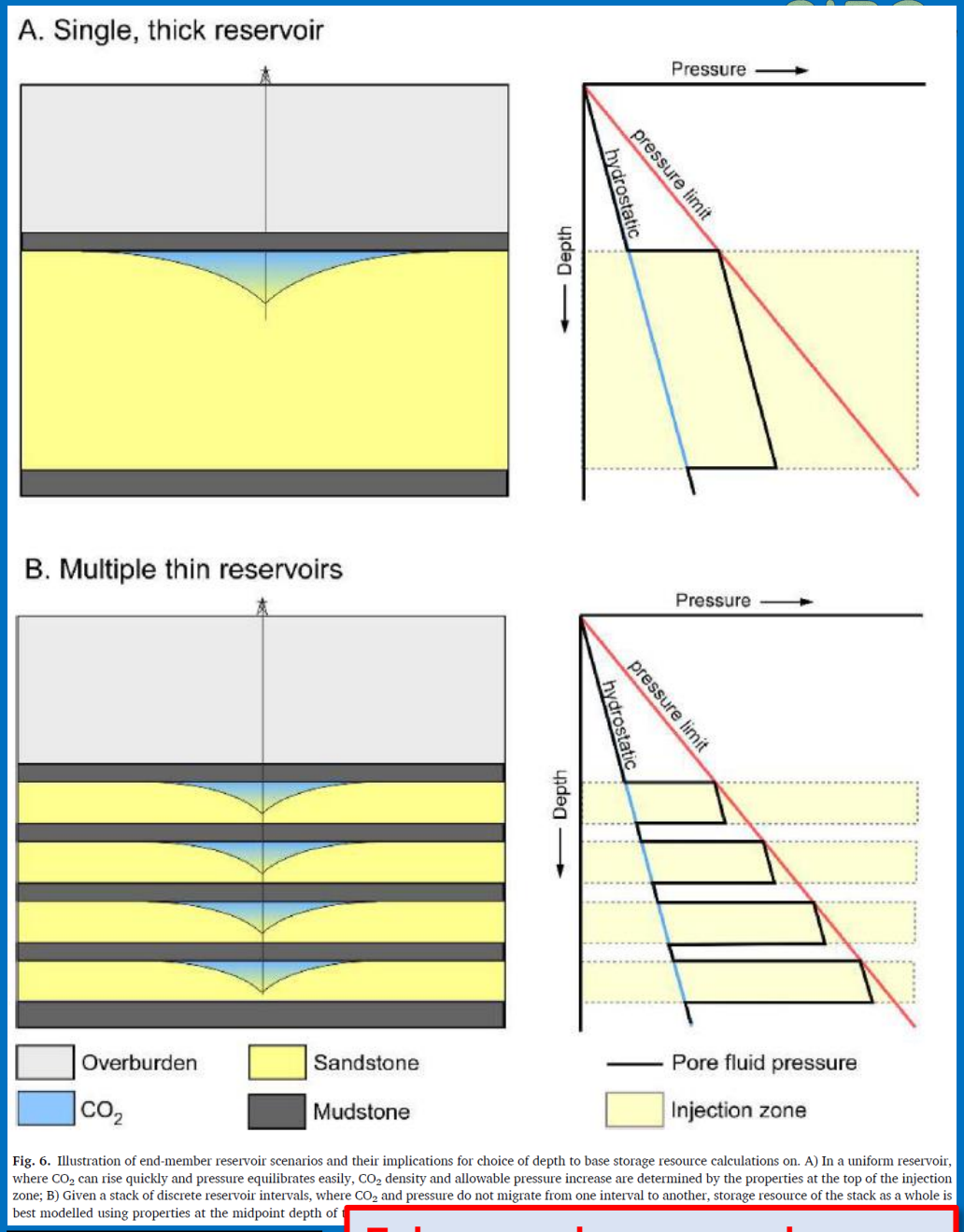


Fig. 6. Illustration of end-member reservoir scenarios and their implications for choice of depth to base storage resource calculations on. A) In a uniform reservoir, where CO_2 can rise quickly and pressure equilibrates easily, CO_2 density and allowable pressure increase are determined by the properties at the top of the injection zone; B) Given a stack of discrete reservoir intervals, where CO_2 and pressure do not migrate from one interval to another, storage resource of the stack as a whole is best modelled using properties at the midpoint depth of t

Bump et al. 2024

Enhances plume spread across different permeability layers

Summary

CO_2 injection and storage can now be reliably modelled using 2-phase 3D reservoir simulation frameworks.

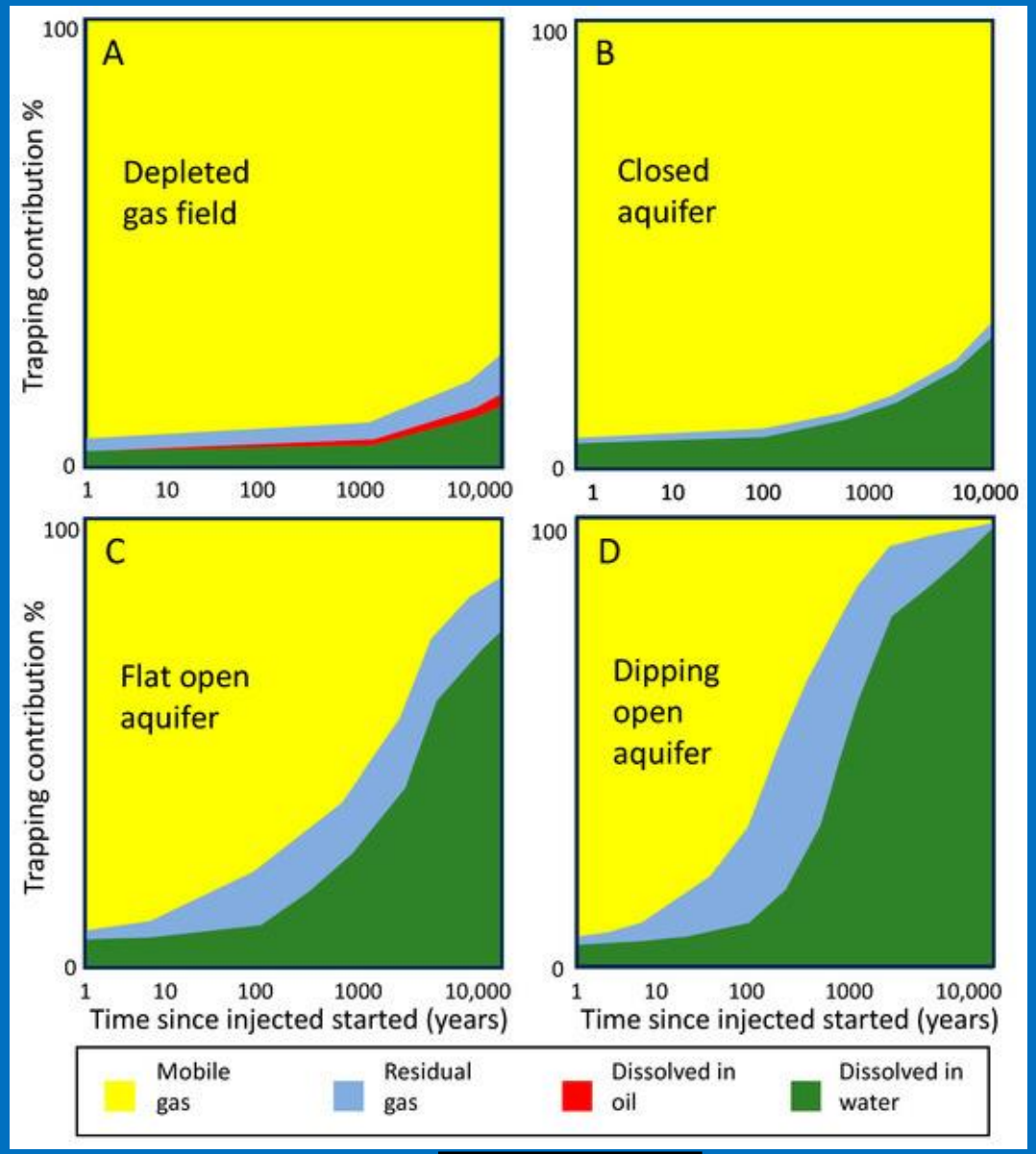
These models capture key **flux regimes** such as:

- **Plume initiation and growth**
- **Early diffusion and Rayleigh–Taylor fingering**
- **Convective shutdown**, **slumping**, and **late-time diffusion**

Each has characteristic timescales and flux behaviours that depend on reservoir properties and geometry.

Dissolution trapping is slow but powerful, and remains underutilized in many CCS projects.

CO_2 dissolution provides irreversible immobilization and reduces free-phase mass over time, enhancing long-term storage security.



Worden 2024

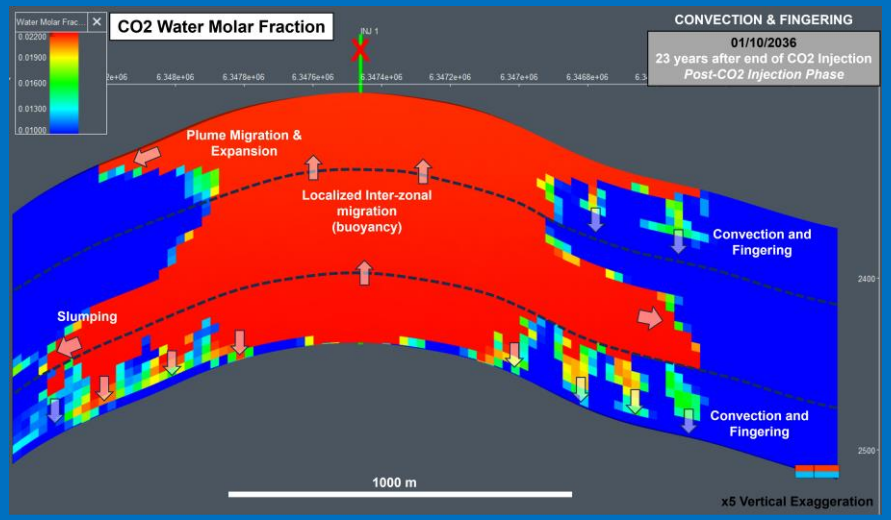
Conclusions

Rayleigh number (Ra) is a critical predictive tool for:

- *Diagnosing onset and strength of convection*
- *Pre-screening reservoir suitability*
- *Guiding injection and monitoring strategies*

Reservoir heterogeneity and architectural layering have a **first-order control** on:

- Convective onset and shutdown
- Slumping behaviour
- Dissolution surface area and interface longevity



Simulation and monitoring should ideally match the physical regimes expected:

- **Fine-gridded models** and **long durations** for high-Ra systems
- **Brine chemistry calibration**, **EOS accuracy**, and **saturation tracking** are essential

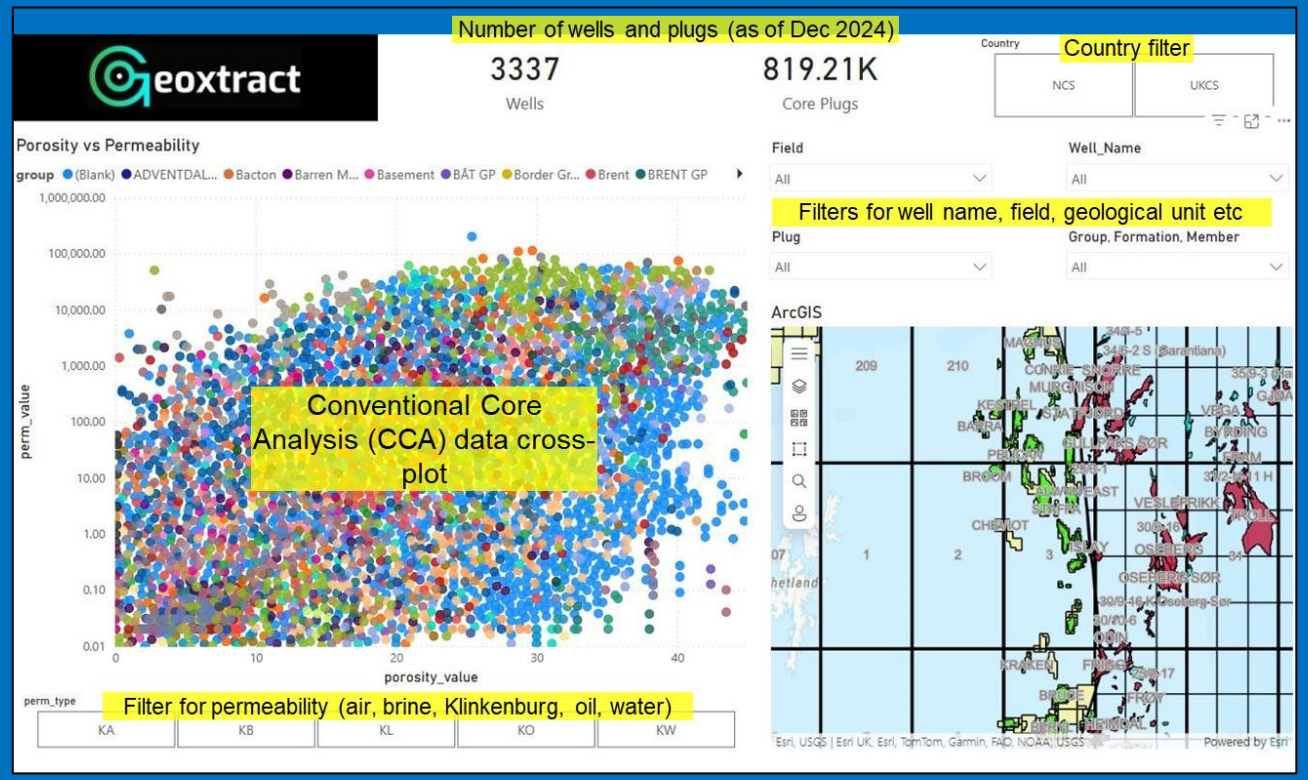
Alternative engineered injection strategies:

- **Downdip well placement**, **multi-zone targeting** can enhance interface growth and drive more dissolution.
- Engineer for **higher Ra to boost early dissolution**
- Prefer **downdip injection** to maximize interface
- Use Ra + D + cs maps to pre-screen reservoir quality

→ Shift from **containment-only thinking** and design to **dissolution-enhanced CCS**.

UNIVERSITY OF ABERDEEN

SIRG



https://www.geoxtract.com/

GeoXtract – North Sea Core Database

yousef.abuyousef@abdn.ac.uk
matthew.brettle@abdn.ac.uk

- **By Q2 2025 ALL North Sea CCA data (+5000 wells) loaded**
- Stratigraphy applied per plug for cored wells
- Dean Stark analysis (Saturation, Fluid summation)
- Core photographs (Concatenated original operator's and BGS)
- RFT formation pressure data
- Well log viewer
- Planned future data packages: SCAL, fluid properties, petrographic data ++

Scan QR code for a video or a free demo of the database

UoA GCS Research Project Proposal

1495 UNIVERSITY OF ABERDEEN

PROPOSAL FOR RESEARCH FUNDING

Short and long-term containment of CO_2 associated with Geological Carbon Storage in Saline Aquifers and Depleted Fields:

Delivery of data, workflows, cellular models and dynamic simulation results in the northern North Sea post-rift succession

Dr. Matt Brettle, Dr. Rene Jonk, Dr. Danica Jablonska,

Dr. Sean Kelly

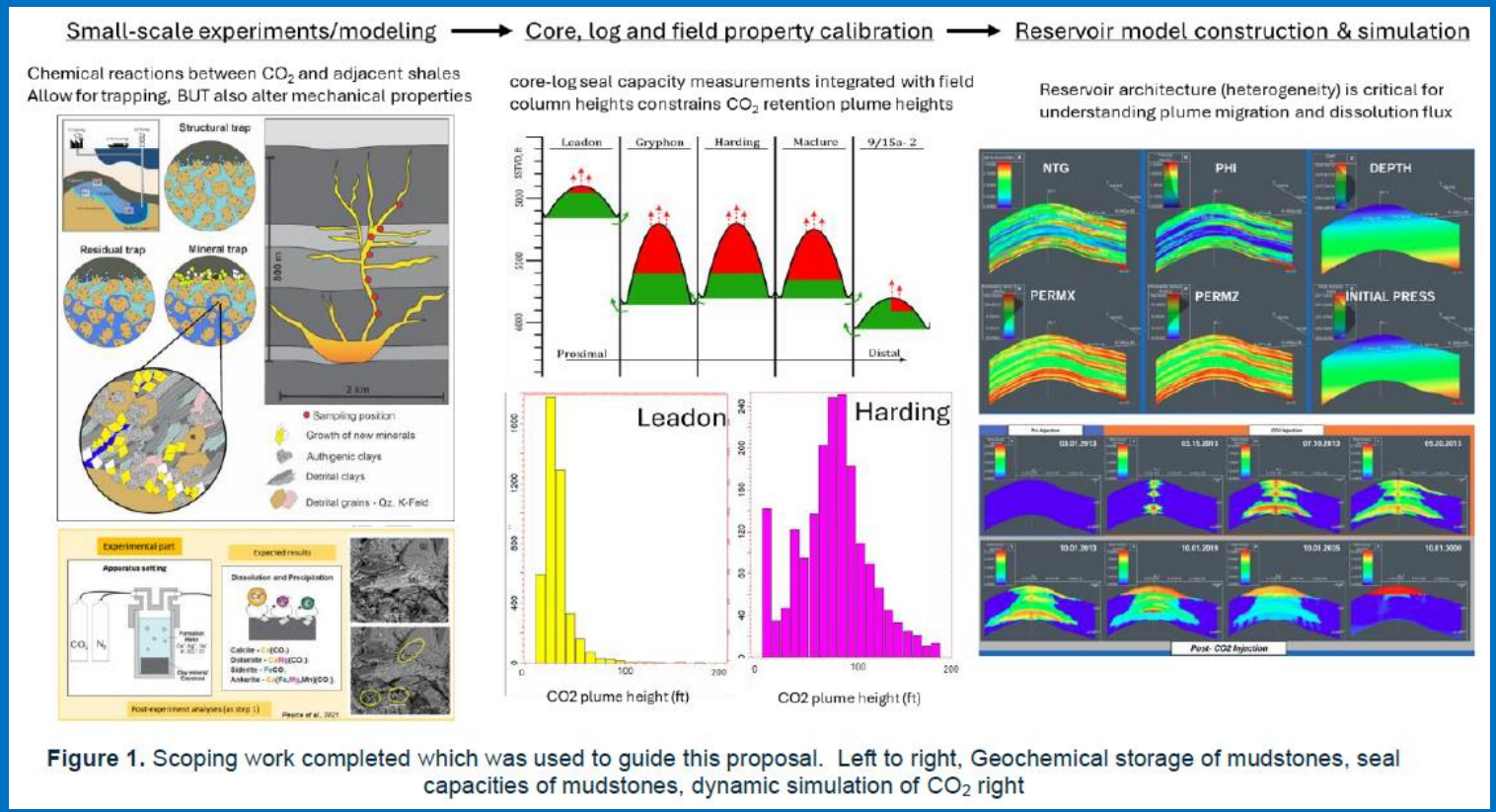


Figure 1. Scoping work completed which was used to guide this proposal. Left to right, Geochemical storage of mudstones, seal capacities of mudstones, dynamic simulation of CO_2 right

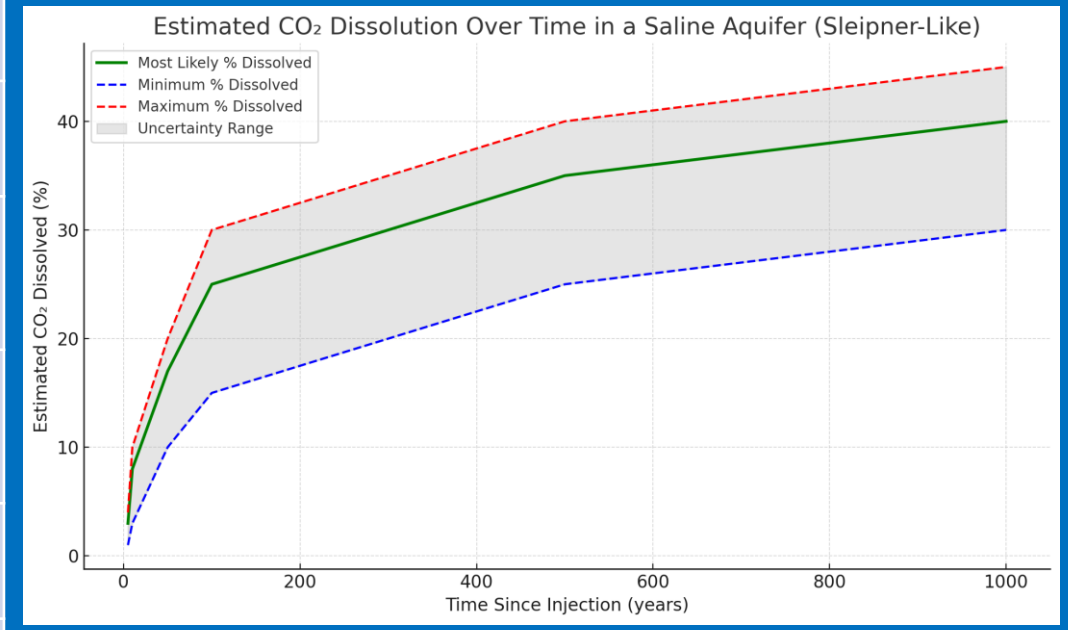
sean.kelly@abdn.ac.uk
matthew.brettle@abdn.ac.uk

END

% of CO_2 Dissolved Over Time

Estimated *Maximum* % of CO_2 Dissolved Over Time
(Assumes a moderately high Ra number system like Sleipner, with ongoing interface growth)

Time Since Injection	Likely Max % Dissolved	Notes & Reference Points
5 years	~2–4%	Early diffusion phase; small interface area. Dissolution is starting.
10 years	~7–10%	Convection begins. Onset of fingering increases flux.
50 years	~15–20%	Most of the rapid fingering and slumping phases occur within this period.
100 years	~25–30%	Some plume fragmentation and Taylor slumping. Flux slowing but still active.
500 years	~35–40%	System transitions to late diffusion. Most available CO_2 is dissolved.
1000 years	~40–45% (plateau)	Asymptotic behavior; remaining free-phase CO_2 is minimal or structurally trapped.



Sleipner type saline aquifer - assume **injection stops after a defined period** (e.g., ~20-30 years)

With vs. Without Dissolution in Saline Aquifer Site Evaluation

Aspect of Site Evaluation	With Dissolution Considered	Without Dissolution Considered
Estimated Storage Capacity	Higher effective capacity due to solubility trapping (up to 30% in monitoring period)	Capacity underestimated; design conservatism or early abandonment
Plume Size and Migration	Smaller plume footprint over time as mass dissolves	Larger plume overestimated; potential for overlap or interference
Risk of Seal Breach	Lower risk due to reduced buoyancy and plume thinning	Higher leakage risk perceived due to plume size and pressure
Pressure Management Forecast	More gradual pressure buildup; longer safe injection window	Pressure buildup may appear too fast; risk of unnecessary constraints
Monitoring Design	Monitoring optimized for saturation and flux trends	Monitoring misaligned with plume evolution; false positives or blind spots
Post-Injection Behavior	Flux transitions through well-defined regimes (e.g., shutdown, tailing)	Overestimation of mobile-phase CO_2 duration
Operational Lifespan	Extended operational lifespan; delayed saturation	Shortened modeled lifespan; overly conservative closure plans
Long-Term Security	Improved security through irreversible CO_2 immobilization	Long-term stability undervalued; containment appears more risky

Rayleigh Number

What is the Rayleigh Number (Ra)?

In the context of **geological carbon storage (GCS/CCS)**, the Rayleigh number describes the **relative strength of buoyancy-driven flow (convection)** compared to **diffusion** in a porous medium saturated with brine.

- It quantifies the **instability** of the system and helps determine when **convective fingering** (which greatly accelerates CO_2 dissolution) will occur.

In its standard form for porous media:

$$\mathrm{Ra} = \frac{g \cdot \Delta\rho \cdot k \cdot H}{\mu \cdot \phi \cdot D}$$

- Some formulations include porosity ϕ in the denominator, depending on whether **pore velocity** or **Darcy velocity** is used

Symbol	Definition	Units
g	Gravitational acceleration	m/s²
$\Delta\rho$	Density difference between saturated and unsaturated brine	kg/m³
k	Permeability of the porous medium	m²
ϕ	Porosity	-
H	Vertical height of the CO_2-brine interface (aquifer thickness)	m
μ	Dynamic viscosity of brine	Pa·s
D	Effective molecular diffusivity of CO_2 in brine	m²/s

Rayleigh Number

Why is Ra So Important in CCS?

1. Predicts Onset of Convection

- If Ra is **low** (e.g., <100), the system is **diffusion-dominated**.
- If Ra exceeds a critical threshold (Ra ≈ **2000** for CO_2-brine systems), **convective fingering** occurs.
- **Convection accelerates CO_2 dissolution by orders of magnitude**.

2. Controls Regime Transitions

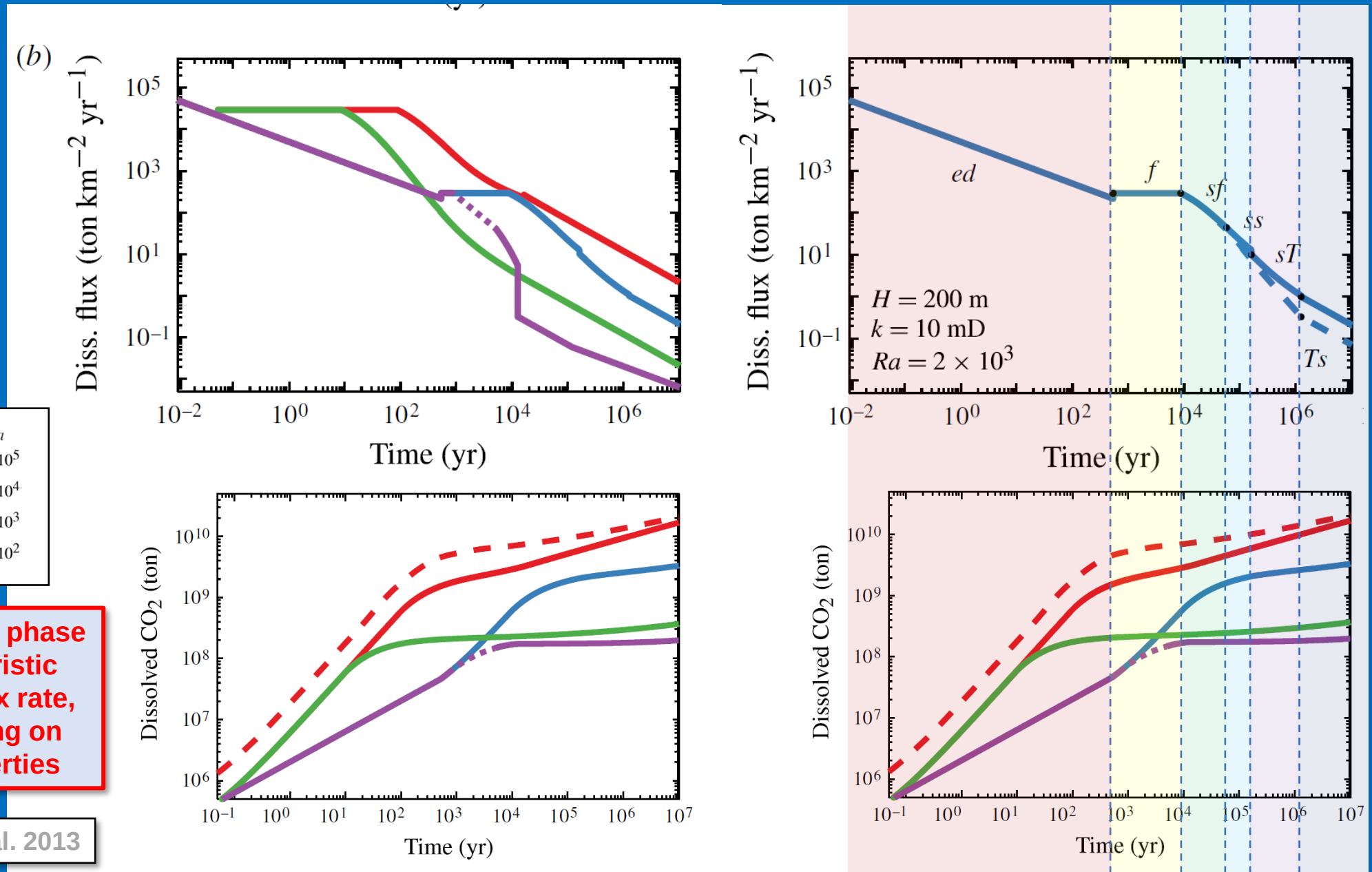
- Rayleigh number determines **which regime** of Szulczewski's flux model the system will occupy:

Regime	Dominant Process	Ra Range
Early Diffusion	Molecular diffusion only	Ra < 100
Transition	Onset of unstable fingers	100 < Ra < 2000
Fingering	Fully developed convection	Ra > 2000
Shutdown/Taylor Slumping	Saturation-controlled	–

Use Ra in Practice

- **Site Screening**: Helps assess if a formation is suitable for long-term solubility trapping.
- **Reservoir Modeling**: Guides whether high-resolution modeling of fingers is needed.
- **Injection Strategy**: Encourages designing plumes with high H, k, or temperature-adjusted μ to increase Ra.
- **Monitoring Planning**: High-Ra systems may require monitoring for finger spread; low-Ra systems evolve too slowly.

CO2 Flux Regimes & Timescales



H (m)	k (mD)	Ra
200,	1000,	2×10^5
20,	1000,	2×10^4
200,	10,	2×10^3
20,	10,	2×10^2

Each regime or phase has a characteristic timescale & flux rate, partly depending on reservoir properties

Szulczewski et al. 2013

UNIVERSITY OF ABERDEEN

Salinity, Solubility & CO2 Flux

Why the Flux First Rises, Then Falls with Salinity

The fingering flux is given by:

$$f = 0.017 \cdot c_s \cdot \frac{\Delta\rho \cdot g \cdot k}{\mu \cdot \phi}$$

So **flux increases linearly with both**:

- CO_2 solubility c_s (which decreases with salinity),
- Density difference $\Delta\rho$ (which increases with salinity).

Competing Effects:

- At **low salinity**, c_s is high, but $\Delta\rho$ is small → low buoyancy, weak convection.
- At **moderate salinity**, c_s is still reasonably high and $\Delta\rho$ has increased → optimal convection.
- At **high salinity**, $\Delta\rho$ keeps rising, but c_s drops sharply → **not enough CO_2 to dissolve**, reducing total flux.

Peak Dissolution Rate

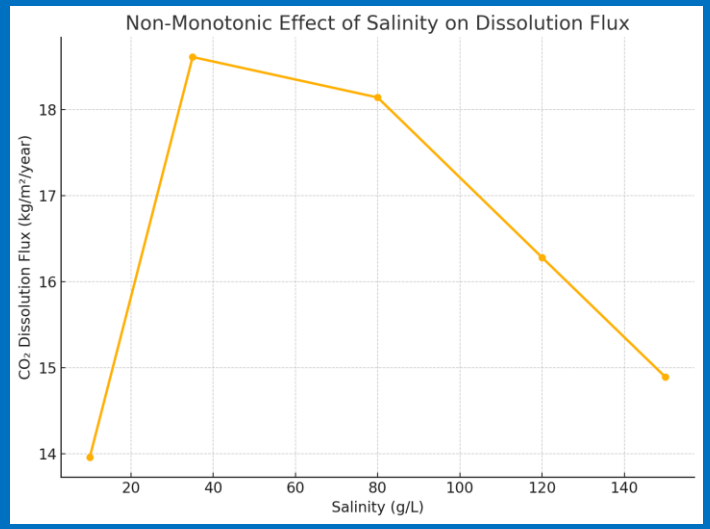
- The **maximum flux** occurs at **moderate salinities** (e.g., 35–80 g/L), where $c_s \cdot \Delta\rho$ is maximized.

Summary

- The **non-monotonic response of dissolution flux to salinity** is a **well-established behavior**, supported by experimental work and analytical theory (e.g., Hidalgo et al. 2013, Agartan et al. 2015).
- This is why reservoirs with **intermediate salinity (~seawater levels)** often show **higher dissolution efficiency** than freshwater or hypersaline systems.

CO_2 solubility (c_s) is directly and linearly linked to dissolution flux, especially in the **fingering regime**, and is one of the most influential variables in predicting and interpreting dissolution behavior.

Parameter	Symbol	Value	Units	Notes
Gravitational acceleration	g	9.81	m/s²	–
Dynamic viscosity	μ	0.000688	Pa·s	Brine viscosity at ~1000 m depth
Porosity	ϕ	0.37	–	Sleipner/Utsira
Aquifer thickness	H	200	m	Typical for Utsira
Effective diffusion	D	2×10^{-9}	m²/s	Moderate estimate
Interface area	A	4.5e6	m²	Based on top plume layer at Sleipner
Duration	–	30 years	–	Fingering regime duration



Salinity (g/L)	CO_2 Solubility c_s (kg/m³)	Δρ (kg/m³)	Notes
10	75	6	Near-freshwater, low Δρ
35	60	10	Seawater-like
80	45	13	Moderate salinity reservoir
120	35	15	High salinity (e.g., In Salah)
150	30	16	Very high salinity

Salinity, Solubility & CO2 Flux

1. Direct Relationship Between Solubility and Flux

In the **Szulczewski et al. (2013)** fingering regime, the dissolution flux is given by:

$$f = 0.017 \cdot c_s \cdot V \quad \text{where} \quad V = \frac{\Delta\rho \cdot g \cdot k}{\mu \cdot \phi}$$

So:

- $f \propto c_s$ when all other parameters are held constant.
- If you **double solubility**, you **double the dissolution flux**.
- It also means that **total CO_2 mass dissolved** over a time period t is directly proportional to c_s:

$$M = f \cdot A \cdot t \propto c_s$$

2. Solubility Role in Onset of Convection (Indirect Link)

While c_s is not explicitly in the Rayleigh number:

$$Ra = \frac{\Delta\rho \cdot g \cdot k \cdot H}{\mu \cdot \phi \cdot D}$$

it is **functionally tied to** $\Delta\rho$, because:

- The **density contrast** $\Delta\rho$ is caused by the **dissolution of CO_2 into brine**.
- This means **higher** c_s allows **higher potential** $\Delta\rho$, which can:
  - Increase Rayleigh number
  - Reduce fingering onset time
  - Strengthen convection once it begins

So: **Higher c_s → More CO_2 dissolves → Greater density contrast → Earlier and stronger fingering**.

Salinity, Solubility & CO2 Flux

3. Dependency on Salinity, Pressure, and Temperature

CO_2 solubility c_s is not constant; it's a **function of**:

- **Salinity**: ↑ salinity ⇒↓ c_s
- **Pressure**: ↑ P ⇒↑ c_s (until close to critical point)

Temperature: Complex — but often ↑ T ⇒↓ c_s at typical reservoir depths

Example from Sensitivity Analysis

If:

- $c_s = 70\,\text{kg/m}^3$: high flux (e.g., 22 kg/m²/yr)
- $c_s = 60\,\text{kg/m}^3$: moderate flux (18.6 kg/m²/yr)
- $c_s = 45\,\text{kg/m}^3$: low flux (~13.8 kg/m²/yr)

Total mass dissolved over 30 years also scales directly.

Key Insight on Salinity:

Salinity affects **both**:

- **CO_2 solubility c_s → lowers** it
- **Density contrast $\Delta\rho$ → raises** it

Because $f = 0.017 \cdot c_s \cdot V$, and $V \propto \Delta\rho$, flux has a **non-monotonic relationship with salinity**:

- **Increases at first** (due to rising $\Delta\rho$)
- **Decreases at high salinity** (because c_s drops sharply)

Variable	Influence on Flux	Direct or Indirect?
Solubility c_s	Proportional to flux and total mass dissolved	Direct
Δρ	Proportional to flux and Ra	Direct
k, μ, φ	Control buoyancy velocity V	Direct via V
D	Affects regime onset and Ra	Indirect

Flux Regime Duration Example Calculation (Sleipner-Like Composite Plume Case)

Example Calculation (Sleipner-Like Case)

Assume:

- $H = 200\,\text{m}$
- $D = 2 \times 10^{-9}\,\text{m}^2/\text{s}$
- $k = 1.5 \times 10^{-12}\,\text{m}^2$
- $\mu = 0.000688\,\text{Pa·s}$
- $\phi = 0.37$
- $\Delta\rho = 10\,\text{kg/m}^3$

Symbol	Definition	Units
c_s	CO_2 solubility in brine	kg/m³
V	Characteristic buoyancy velocity	m/s
H	Thickness of aquifer	m
D	Effective diffusion coefficient (including tortuosity)	m²/s
Ra	Rayleigh number: ratio of buoyancy to diffusion	–
A	Interface area (CO_2–brine contact)	m²
$f(t)$	Dissolution flux at time t	kg/m²/s
t	Time since injection started	s or years

Step 1: Compute Velocity

Compute Velocity

$$V = \frac{10 \cdot 9.81 \cdot 1.5 \times 10^{-12}}{0.000688 \cdot 0.37} \approx 5.78 \times 10^{-7}\,\text{m/s}$$

Step 2: Regime Times

- $t_f = \frac{2\times10^{-9}}{(5.78\times10^{-7})^2} \approx 6.0 \times 10^3\,\text{s} \approx 0.07\,\text{days}$

In real reservoirs, convection likely begins a bit later due to vertical constraints; field data suggests ~2–5 years for fingering onset.

- $t_{sf} = \frac{15\cdot200}{5.78\times10^{-7}} \approx 5.2 \times 10^9\,\text{s} \approx 165\,\text{years}$
- $t_{sT} = \left(\frac{(200)^3}{5.78\times10^{-7}\cdot2\times10^{-9}}\right)^{1/2} \approx 1.66 \times 10^8\,\text{s} \approx 5.3\,\text{years}$
- $t_{ld} = \frac{(200)^2}{2\times10^{-9}} = 2 \times 10^{10}\,\text{s} \approx 635\,\text{years}$

Flux Rate and Total Example Calculation (Sleipner-Like Composite Plume Case)

Step 1: Characteristic Buoyant Velocity V

From Szulczewski et al.:

$$V = \frac{\Delta\rho \cdot g \cdot k}{\mu \cdot \phi}$$

Substitute values:

$$V = \frac{10 \cdot 9.81 \cdot 1.5 \times 10^{-12}}{0.000688 \cdot 0.37}$$

$$= \frac{1.4715 \times 10^{-10}}{2.5456 \times 10^{-4}} = 5.78 \times 10^{-7} \text{ m/s}$$

Step 2: Fingering Flux Rate per Area

Fingering regime flux (Szulczewski):

$$f = 0.017 \cdot c_s \cdot V = 0.017 \cdot 60 \cdot 5.78 \times 10^{-7} = 5.89 \times 10^{-7} \text{ kg/m²/s}$$

Convert to **kg/m²/year**:

$$f_{\text{year}} = f \cdot \text{seconds per year} = 5.89 \times 10^{-7} \cdot 31{,}557{,}600 = \boxed{18.61 \text{ kg/m²/year}}$$

Step 3: Total Mass Dissolved over 30 Years

We are targeting:

$$M_{\text{total}} = 2.94 \text{ Mt} = 2.94 \times 10^{6} \text{ tonnes} = 2.94 \times 10^{9} \text{ kg}$$

Let:

A_{eff} = unknown effective interface area

f = 5.89×10^{-7} kg/m²/s (from above)

t = total duration in seconds = 30 × 365.25 × 86400 = 946,728,000 s

We solve:

$$M = f \cdot A_{\text{eff}} \cdot t \Rightarrow A_{\text{eff}} = \frac{M}{f \cdot t} = \frac{2.94 \times 10^{9}}{5.89 \times 10^{-7} \cdot 9.467 \times 10^{8}} = \boxed{5{,}267 \text{ m²}}$$

Convert to km²:

- $A_{\text{eff}} = 0.00527$ km²

Quantity	Value
Characteristic velocity V	5.78×10^{-7} m/s
Fingering flux f	18.6 kg/m²/year
Effective area A_{eff}	5,267 m² (0.0053 km²)
Duration	30 years
Total dissolved CO_2	2.94 Mt

Salinity & Viscosity

1. Salinity (How salty the water is)

- **What it is**: How much dissolved salt is in the brine.
- **Impact on dissolution**:
  - ⬇ **Reduces CO_2 solubility** → salty brine can hold **less CO_2**.
  - ⬆ **Increases brine density** → makes CO_2-saturated brine **even denser**, which helps **trigger convection**.
  - ⬆ **Increases viscosity slightly** → makes the brine more resistant to flow.
- **Analogy**: Salt water is "thicker" and "heavier" than fresh water — it can slow things down but also set up stronger sinking when CO_2 dissolves.

2. Viscosity (How thick or resistant the brine is)

- **What it is**: A measure of how easily the fluid flows.
- **Impact on diffusion and convection**:
  - ⬆ Higher viscosity = slower movement (including convection).
  - Appears in the **denominator of the Rayleigh number**, so **higher viscosity reduces the likelihood of convection**.
- **Rule of thumb**: The more viscous the brine, the **less mobile** the CO_2-rich fingers will be.

Solubility & Diffusivity

3. Solubility (cs) – How much CO_2 can dissolve in the brine

- **What it is**: The maximum amount of CO_2 that can dissolve in the brine at given pressure, temperature, and salinity.
- **Dependence on other factors**:
  - ⬆ **Increases with pressure**.
  - ⬇ **Decreases with temperature**.
  - ⬇ **Decreases with salinity**.
- **Why it matters**: Higher solubility means more CO_2 enters solution per unit time — **directly boosts flux**.
- **Key point**: Solubility is the “fuel” for dissolution. Less solubility = smaller flux ceiling.

4. Diffusivity (D) – How fast CO_2 molecules spread in brine

- **What it is**: The molecular diffusion coefficient — how fast dissolved CO_2 spreads through brine **before convection begins**.
- **Impact**:
  - Sets the rate of **early diffusion** (slow phase before fingering).
  - Affects the **onset time of convection**: higher *D* slightly **delays** the density instability.
  - Lower *D* = faster convection onset (sharper density contrast builds up sooner).
- **Key point**: Diffusivity controls the **early behavior** of CO_2 dissolution, before the system “kicks into gear.”

Salinity, Viscosity, Solubility & Diffusivity

- **How They Work Together in Real Aquifers**

Parameter	What Happens When It's High	Net Effect on Dissolution
Salinity	⬇ solubility, ⬆ density, ⬆ viscosity	Mixed: reduces solubility but can strengthen convection
Viscosity	Slows flow and fingering	Generally slows dissolution
Solubility	More CO_2 can dissolve	Increases dissolution flux directly
Diffusivity	Smoother gradients, slower fingering onset	Speeds early diffusion, delays convection onset

In Summary – Natural Aquifer Scenarios

In natural aquifers:

- **Moderate salinity** (e.g. 30–60 g/L) often gives the **best balance**: decent solubility, strong density contrast.
- **High salinity** (e.g. 100–150 g/L) may **limit CO_2 solubility too much**, reducing the overall effectiveness of dissolution trapping.
- **Lower viscosity** brines (warmer, less saline) promote better convection and faster mixing.
- Solubility and diffusivity are **temperature- and pressure-dependent**, so deeper aquifers may perform better despite higher temperature, due to **high pressure** boosting c_s.

Key challenges in simulating CO_2 dissolution in CCS/GCS projects - I

1. Capturing Density-Driven Convective Mixing

- **Description**: Convective dissolution—driven by the density contrast between CO_2-rich and ambient brine—is a key mechanism that accelerates CO_2 solubility trapping.
- **Challenges**:
  - Requires **high spatial and temporal resolution** to resolve fine-scale "gravity fingers."
  - **Numerical dispersion** in coarse grids can artificially mimic or obscure fingering.
  - Difficult to simulate **both fingering instability and large-scale plume migration** simultaneously.
  - Existing commercial simulators often smooth out these instabilities unless adapted with specialized modules or fine meshes.

2. Integrating Dissolution with Multiphase Flow and Transport

- **Description**: CO_2 dissolution is governed by a combination of advection, diffusion, and convection, each occurring at different scales.
- **Challenges**:
  - **Coupling molecular diffusion, advective flow, and convective mixing** remains a complex task, especially when feedbacks are nonlinear.
  - Misrepresentation of this interplay can result in incorrect predictions of plume evolution and dissolution efficiency.
  - Modeling of **residual trapping and hysteresis** also interacts with dissolution processes.

3. Accurate Representation of Fluid Properties

- **Description**: CO_2 solubility, density, and viscosity depend strongly on **pressure (P)**, **temperature (T)**, and **salinity**.
- **Challenges**:
  - Slight variations (e.g., <1% in density) can control whether convective mixing is triggered.
  - **Non-isothermal conditions** influence solubility and buoyancy but are often neglected for simplicity.
  - Lack of site-specific P–T–x data (especially for **formation-specific brines**) hampers accurate model calibration.

4. Modeling Reservoir Heterogeneity

- **Description**: Subsurface heterogeneity governs the structure of the CO_2 plume and the brine-CO_2 contact area.
- **Challenges**:
  - Requires **multi-scale representation** of features like thin baffles, layered heterogeneity, or anisotropy.
  - Impacts **convective onset**, fingering structure, and lateral spreading of dissolved CO_2.
  - Traditional grid-based models struggle to represent fine-scale heterogeneity without excessive computational cost.

Key challenges in simulating CO_2 dissolution in CCS/GCS projects - II

5. Uncertainty in Petrophysical Properties

- **Description**: CO_2-brine-rock interaction is governed by permeability, porosity, capillary pressure, and relative permeability.
- **Challenges**:
  - These properties are **difficult and expensive to measure** at relevant scales.
  - **Large uncertainties** in relative permeability and capillary pressure can affect predictions of residual trapping and plume mobility.
  - The spatial variability in these parameters introduces **input uncertainty** that propagates through simulations.

6. Coupling Geochemical Reactions with Fluid Flow

- **Description**: Dissolved CO_2 can react with minerals, affecting long-term trapping and reservoir properties.
- **Challenges**:
  - Geochemical reactions can **alter porosity/permeability**, affecting fluid movement and subsequent dissolution.
  - **Kinetics of mineral trapping** (e.g., calcite, dawsonite) are slow and uncertain, but must be captured for long-term predictions.
  - Fully coupled **reactive transport models** are computationally intensive and require detailed kinetic and thermodynamic data.

7. Multi-Scale Integration (Time and Length Scales)

- **Description**: Dissolution occurs at the mm–m scale over timeframes from minutes to >10^4 years.
- **Challenges**:
  - Requires **upscaling** of pore-scale processes to reservoir scale without losing key features (e.g., convective onset).
  - Many simulation tools cannot resolve fine-scale behavior (e.g., diffusion layers) within large domains.
  - Modelers often resort to **heuristic or semi-analytical approximations** (e.g., enhanced effective diffusivity) that may not generalize.

8. Numerical Artifacts and Grid Sensitivity

- **Description**: Simulation results are sensitive to **grid resolution, discretization schemes**, and numerical solvers.
- **Challenges**:
  - Coarse grids may **underpredict dissolution rates** due to missed fingering or **overpredict** due to artificial dispersion.
  - Simulation **stability** is sensitive to time-step size and phase transition handling (e.g., supercritical to aqueous).
  - Discretization can impose directional bias in fingering or underestimate saturation gradients.

Key challenges in simulating CO_2 dissolution in CCS/GCS projects - III

9. Lack of Long-Term Field Calibration

- **Description**: Most CCS projects are <30 years old, while dissolution evolves over centuries.
- **Challenges**:
  - Limited data for **validating long-term model predictions** (e.g., over 1000+ years).
  - Geophysical monitoring (e.g., seismic, gravity) typically cannot resolve dissolved CO_2 distributions directly.
  - Direct **sampling of in-situ formation water** to measure CO_2 content is rare and difficult.

10. Computational Expense

- **Description**: Full-physics 3D models with high resolution and coupled reactive transport are **computationally intensive**.
- **Challenges**:
  - Fine-grid simulations that resolve convection can require **millions of grid cells** and **weeks to months of compute time**.
  - **Monte Carlo or UQ analyses** (for risk assessment) become intractable unless surrogate models or upscaled simplifications are used.

Recommendations for Overcoming Challenges

- **Adaptive meshing** or local grid refinement (LGR) to resolve fingering where it matters most.
- **Hybrid models** combining fine-scale dissolution modules with coarse reservoir flow models (e.g., vertical equilibrium (VE) approximation).
- **Upscaling of fingering dynamics** into enhanced dissolution terms (e.g., Sherwood number-based corrections).
- Development of **field-calibrated effective models** using controlled injection pilot tests.
- **Improved brine sampling methods** (e.g., wireline formation testers with downhole chemistry tools) for field validation.

Conclusion

- Simulating CO_2 dissolution in CCS/GCS is a multi-faceted challenge that blends fundamental fluid physics with the practical limitations of field-scale reservoir modeling.

- Addressing these issues requires a **balance between physical fidelity and computational feasibility**, and hinges on better site characterization, improved monitoring, and integrated modeling frameworks that resolve fine-scale physics within large-scale domains.