

I²CNER - efforts to achieve effective, safe CO₂ storage

The International Institute for Carbon-Neutral Energy Research (I²CNER) is studying CO₂ behavior from molecular to field scale to achieve better CO₂ storage.

By Takeshi Tsuji, CO₂ Storage Division, I²CNER, Kyushu University

CO₂ storage division at I²CNER

At the CO₂ Storage Division of I²CNER, we develop methods to characterize CO₂ injection reservoirs to allow pre-injection site selection and post-injection predictions of the fate of CO₂. We also monitor injected CO₂ to help ensure safe and permanent CO₂ sequestration.

To accomplish these goals, we are pursuing fundamental research to elucidate CO₂ behavior over a wide range of scales (Figure 1). In particular, we are studying the influence of molecular-scale (or pore-scale) characteristics on field-scale CO₂ behavior; i.e., determining the relationships between multi-scale phenomena. For example, the wettability of each mineral calculated at the molecular scale could influence the kilometer-scale CO₂ behavior in a reservoir.

Here we report our recent work on the characterization of CO₂ behavior from molecular to field scale.

Molecular to pore scale

Modeling of CO₂ mineralization

Mineralization (i.e., geochemical CO₂ trapping) is considered a safe way to store CO₂. This trapping mechanism converts CO₂ to insoluble minerals (e.g., CaCO₃) via geochemical interactions with rock and formation water.

It was believed until recently that CO₂ mineralization takes several hundreds to thousands of years. However, the Iceland-based pilot project demonstrated that CO₂ mineralization takes less than two years in basaltic rock. We have revealed the microscopic mechanism of mineralization through first-principles calculations (ab initio molecular dynamics simulations).

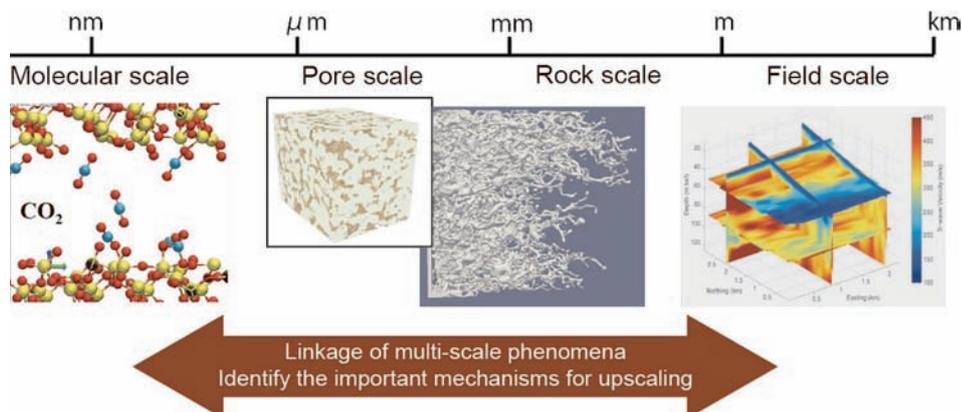


Figure 1. Injected CO₂ behavior from the molecular scale to the field scale. We aim to understand the relationships between multi-scale phenomena

To do this, we calculated the reaction process between supercritical CO₂ and host rock (e.g., igneous rock), and showed how carbonate ions (CO_3^{2-}) are generated on the surface of the host mineral (Figure 2). If suitable cations (e.g., Ca²⁺ or Mg²⁺) are present in the vicinity of CO_3^{2-} , insoluble carbonate minerals will form. These kinds of cations are abundant in igneous rocks like basalt.

We have also investigated fluid mixtures of CO₂ and hydrogen sulfide (H₂S) by a similar

approach because H₂S is a major concomitant geothermal gas of CO₂. The overall cost of CO₂ capture and storage (CCS) could be lowered substantially by injecting a mixture rather than pure CO₂.

This research provided microscopic insights into geochemical trapping of CO₂. Our molecular dynamics simulations also revealed interfacial properties, such as wettability, of the fluid mixtures.

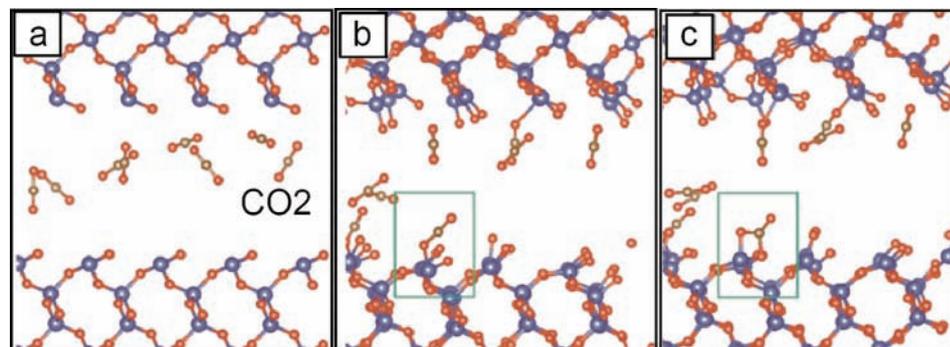


Figure 2. Example of an ab initio molecular dynamics simulation of a supercritical CO₂ reaction, showing snapshots after (a) 0 fs (initial configuration), (b) 594 fs, and (c) 750 fs. The green frames in (b) and (c) indicate formation of CO_3^{2-} ion

Accurate porous flow characterization by considering slip flow at the fluid–solid interface

Hydrological properties such as permeability play a major role in determining the storage capacity of a geological site. The typical length scale of pores available in these sites is of the order of a few micrometers. At this small scale, the slip effect starts to appear at the fluid–solid interface and affects the permeability of the rock.

We incorporated the slip effect into a lattice Boltzmann simulation by using a diffusively reflecting solid wall boundary condition. We used a simple homogeneous porous medium to validate that this boundary condition was capable of reproducing the effect of slip (Figure 3a).

An increased slip velocity inside the pore throat was obtained upon using an appropriate diffusively reflecting boundary condition (right in Figure 3a) compared with that using the conventional boundary condition (left in Figure 3a).

To evaluate the extent of the influence of slip on bulk properties like permeability, we calculated the permeability with different Knudsen numbers (Kn). Kn is defined as the ratio of the molecular mean free path to characteristic macroscopic length, and is inversely related to pore size. The rise in slip velocity results in increased permeability with decreasing pore size (Figure 3b). This effect is generally not considered in conventional numerical methods.

Pore to rock scale

Identifying suitable reservoir conditions for effective, safe CO2 storage

We have tried to identify suitable reservoir conditions (e.g., pressure) for effective, safe CO2 storage. The behavior and saturation of CO2 in a reservoir is influenced by many reservoir parameters, including the viscosity and density of the fluids, interfacial tension, pore structure, and other porous medium characteristics like wettability and surface roughness. Therefore, it is challenging to identify suitable conditions for CO2 storage.

We calculated CO2 displacements in 3D natural sandstone under various conditions using two-phase lattice Boltzmann simulations, and characterized the influence of reservoir condi-

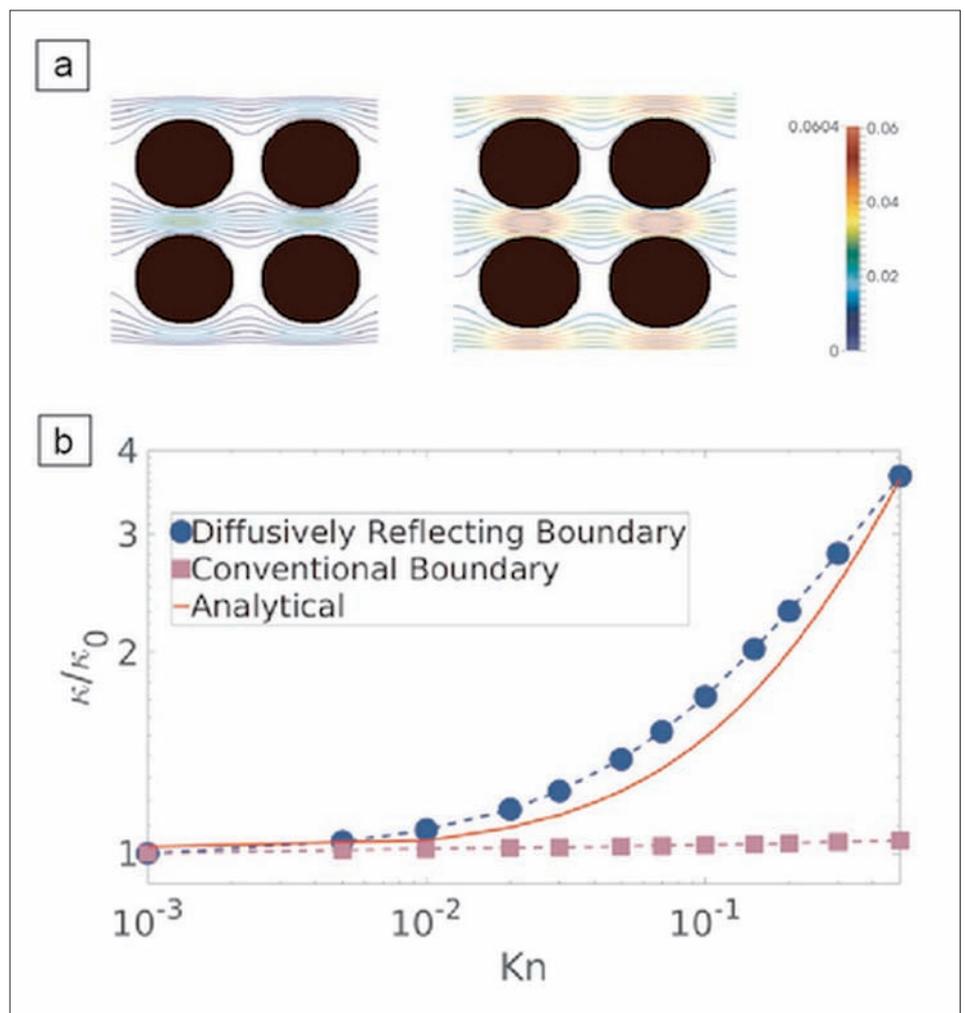


Figure 3. (a) Steady-state streamlines and fluid velocity using (left) a conventional boundary condition and (right) our boundary condition considering slip. (b) Permeability correction factor (κ/κ_0) with respect to Knudsen number (Kn). The permeability predicted from our analysis agrees with analytical one

tions on CO2 and water flow (Figure 4a) [1]. The results of simulations conducted under more than 50 combinations of conditions were used to classify the resulting two-phase flow behaviors into typical fluid displacement patterns in plots of capillary number (Ca) against the viscosity ratio of CO2 to water (M). In addition, the saturation of the non-wetting phase (CO2) was calculated and mapped on the Ca–M diagrams.

In CCS, we should consider the domain of $M < 1$ (the areas indicated by red rectangles in the bottom panels of Figure 4). Our results demonstrated that CO2 saturation is controlled by Ca and M, and the optimum CO2 saturation scales with Ca and M (bottom of Figure 4a).

Similar analysis of a different type of rock (2D homogeneous model in Figure 4b) revealed that its CO2 saturation and behavior were quite different from those of 3D natural rock.

These important differences between two-phase flow in 3D natural rock and the 2D homogeneous model could be caused by the heterogeneity of pore geometry and differences in pore connectivity.

Our approach provides useful information to determine suitable reservoir conditions for effective CO2 storage (e.g., high CO2 saturation) by quantifying CO2 behavior in a target reservoir rock under various conditions (i.e., saturation mapping on the Ca–M diagram).

Quantifying CO2 saturation in reservoirs from monitoring data

Time-lapse seismic surveys are suitable to monitor CO2 distributions within reservoirs, but it is difficult to quantify CO2 saturation from time-lapse seismic data. To estimate CO2 saturation from seismic velocity, the relationship between CO2 saturation and seis-

mic velocity must be determined (Figure 5a). However, this relationship is difficult to quantify because the response of seismic velocity to CO₂ saturation is affected by multiple factors, and is also influenced by the CO₂ distribution in the pore spaces of rock (see Figure 4). Therefore, quantitative monitoring requires both hydrological and geophysical approaches.

We evaluated the influence of CO₂ behavior within rock pores on the relationships between seismic velocity and CO₂ saturation (Figure 5a) [2]. We conducted two computational studies with different injection pressures using (1) a two-phase lattice Boltzmann method to simulate CO₂ injection (i.e., hydrologic simulation) and (2) wave propagation simulation with a finite difference approach to evaluate seismic velocity (i.e., elastic simulation).

We identified a difference in the relationships between seismic velocity and CO₂ saturation in a few cases; i.e., lower seismic velocity was observed when Ca was high than when Ca was low at the same saturation (Figure 5a).

The difference in velocity response to CO₂ saturation was controlled by CO₂ distribution features. Ca (or the pressure gradient) depends on the distance from the injection well (Figure 5b). Low Ca values are expected far from the injection well and high ones near the well.

This study demonstrated that Ca at each reservoir location should be considered to accurately estimate CO₂ saturation from seismic monitoring data.

Rock to field scale

Reservoir characterization in high resolution (application to the Tomakomai CCS project)

Geological heterogeneity influences CO₂ behavior in reservoirs. In particular, if there are localized fractures in CO₂ storage sites, they may behave as CO₂ leakage paths. To detect localized heterogeneity in high resolution (i.e., downscaling), we developed an advanced seismic processing method using surface waves [3].

Our method allowed us to characterize local heterogeneity by integrating S-wave velocity and attenuation. We applied the method to 3D seismic data acquired at the Tomakomai CO₂ storage site, Japan, and successfully extracted a high-resolution S-wave velocity

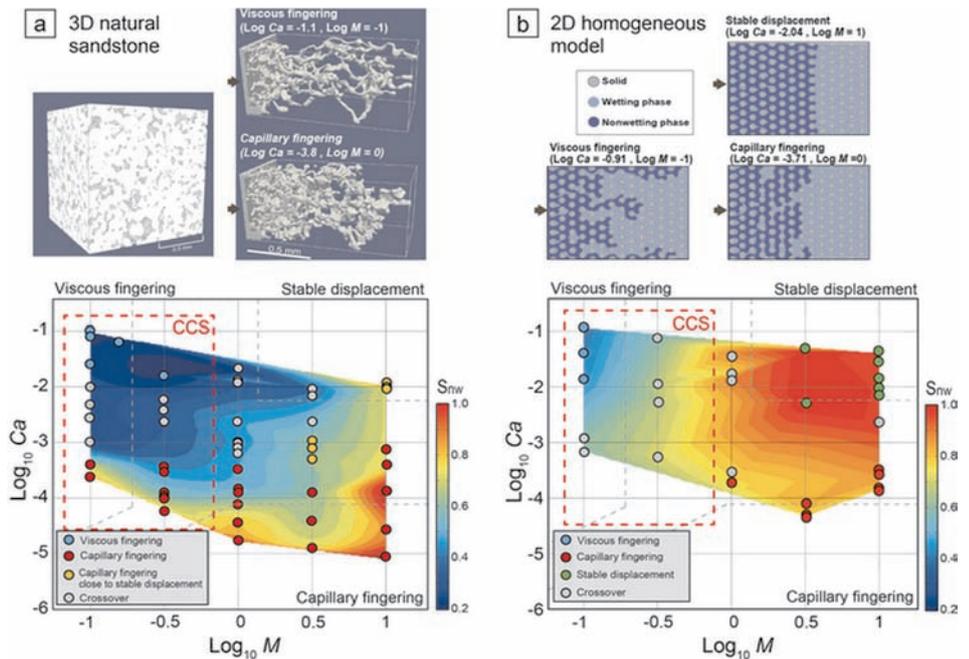


Figure 4. (a) 3D pore geometry of natural sandstone (top left), and CO₂ behavior in 3D natural sandstone under viscous fingering and capillary fingering regimes (top right). The bottom panel shows the displacement pattern and CO₂ saturation plotted on a diagram of capillary number Ca against viscosity ratio M [1]. The dots indicate the calculation conditions. The color map on the phase diagram shows the CO₂ saturation. (b) CO₂ behavior in the 2D homogeneous pore model under different conditions (top). The displacement pattern and CO₂ saturation for the 2D homogeneous pore model are plotted on a diagram of Ca against M (bottom)

structure and attenuation coefficient (Figure 6b and c, respectively).

From these results, we identified a geological boundary developed for northwest–southeast direction. This was the first demonstration of using surface waves to identify a 3D S-wave velocity distribution in a CO₂ storage site.

Because the S-wave velocity reflects the strength of a formation, the estimated S-wave velocity distribution can be used to evaluate lithology strength for geomechanical simulation (prevention of a CO₂ injection-induced earthquake).

The estimated heterogeneity also provides vital information for CO₂ geological storage,

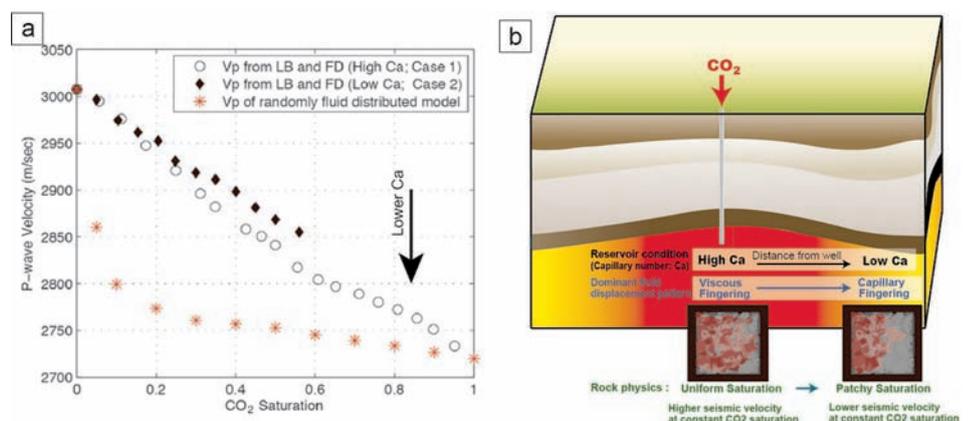


Figure 5. (a) Relationship between seismic velocity and CO₂ saturation at different capillary numbers Ca [2]. These relationships were calculated by lattice Boltzmann method fluid flow simulations and dynamic wave propagation simulations. Circles indicate the results for higher Ca and diamonds those for lower Ca. Red asterisks show results for randomly distributed models. (b) Injected CO₂ behavior under different reservoir conditions (Ca)

such as evaluation of CO₂ leakage paths and permeability heterogeneity used in reservoir simulation.

Continuous, accurate monitoring system for injected CO₂

In CCS, monitoring of injected CO₂ is crucial to (a) predict the risk of CO₂ leakage from storage reservoirs, (b) increase the efficiency of CO₂ injection and lower its cost, and (c) lower the risk of injection-induced seismicity.

Time-lapse seismic surveys have been used to monitor the distribution and migration of injected CO₂. However, the monitoring interval in time-lapse surveys is usually long because of the high cost of monitoring; it is generally too expensive to continuously monitor the injected CO₂. However, continuous monitoring of dynamic CO₂ behavior is crucial to detect incidents associated with CO₂ injection (e.g., leakage).

We developed a seismic monitoring system using a continuous, controlled seismic source (Figure 7a) [4]. Our system monitored the shallow subsurface through temporal variation of surface-wave velocity.

Compared with conventional monitoring, our system is cost-effective with high temporal resolution and accuracy. Field experiments showed that hourly variation of surface-wave velocity could be monitored with better than 1% accuracy (Figure 7b).

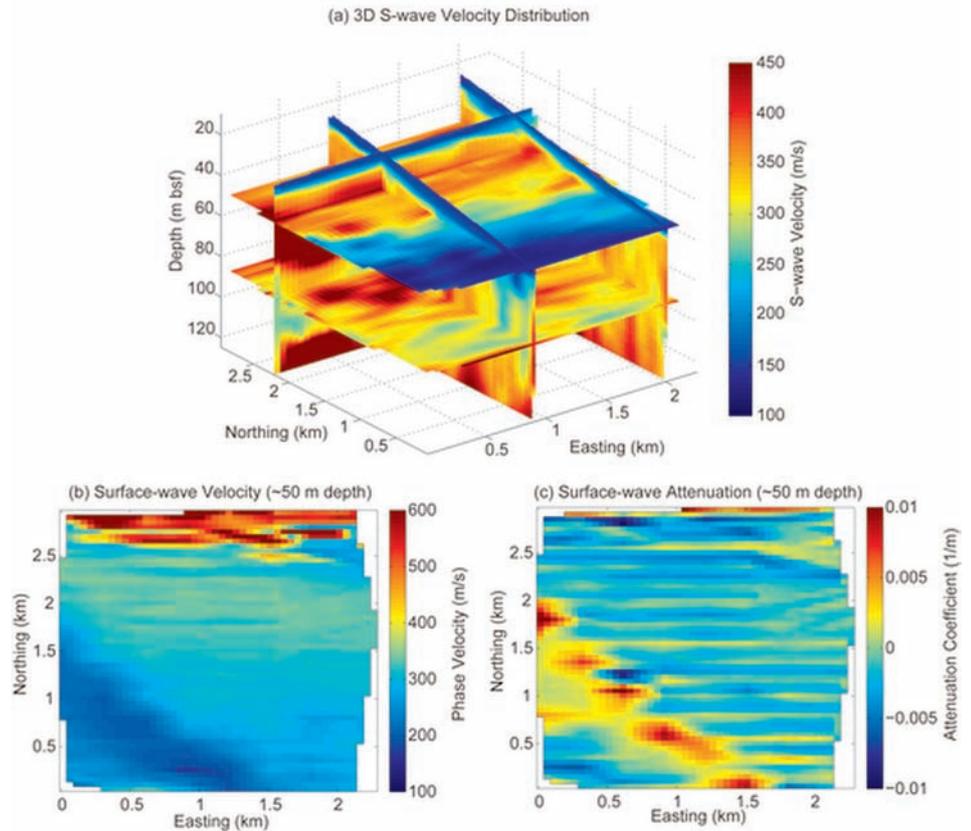


Figure 6. (a) The estimated 3D S-wave velocity model for the Tomakomai CO₂ storage site. Horizontal slices (map views) of the estimated (b) surface-wave velocity and (c) attenuation ~50 m below the seafloor [3]

This temporal stability provides the possibility to detect changes in seismic velocities associated with CO₂ leakage through fault zones. Recently, we used this monitoring system in the Aquistore CCS project in Canada, and

clearly identified seasonal variation associated with the degree of freezing in shallow sediments.

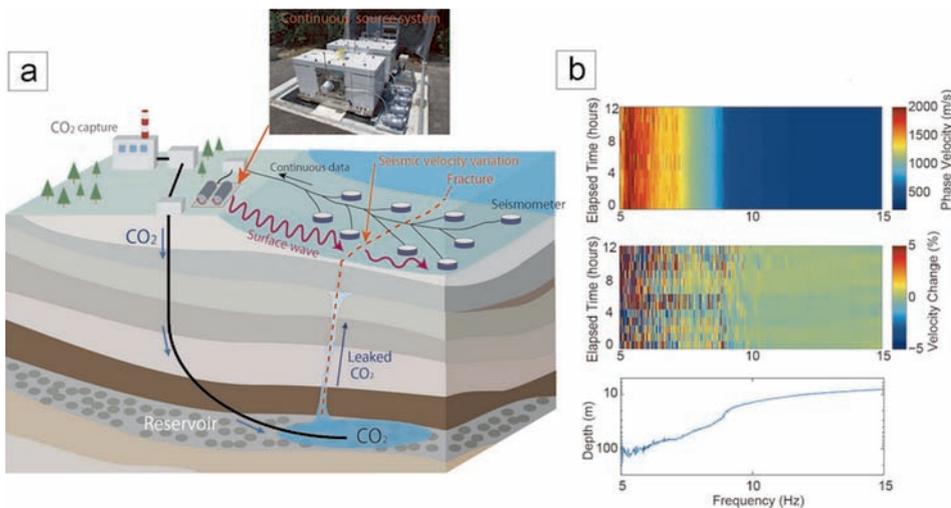


Figure 7. (a) Continuous seismic monitoring of injected CO₂ and detection of leaked CO₂. The photograph shows the monitoring device, which generates a continuous, accurate source signal. (b) Hourly variation of (upper) surface-wave velocity, (middle) velocity change for averaged velocities, and (lower) sensitive depth in field experiments [4]

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More information
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