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Invited Commentary

THE IMPORTANCE AND CHALLENGES ASSOCIATED WITH MULTI-SCALE HETEROGENEITY FOR GEOLOGICAL STORAGE

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ABSTRACT

Understanding multi-scale heterogeneity in porous media has become increasingly critical as the world transitions from fossil fuel production to geological storage of CO_2 and H_2 for climate change mitigation. This commentary examines why small-scale heterogeneities have taken on a heightened importance in modeling subsurface fluid migration. We identify three key factors: increased public scrutiny and stricter permitting requirements for storage projects, different risk tolerances requiring long-term monitoring, and distinct flow physics compared to traditional oil and gas extraction. Drawing from current research, we demonstrate how current models consistently underestimate CO_2 plume spread, likely due to inadequate representation of small-scale heterogeneities, which will also heavily impact H_2 storage in porous rocks. We review the current state of research on incorporating small-scale heterogeneities into field scale models, discuss relevant spatial scales for both CO_2 and H_2 storage applications, and highlight promising directions for future research in this critical area.

KEYWORDS

Multicomponent multiphase fluid, CO_2 sequestration, Hydrogen storage, Underground hydrogen storage, CCUS, Carbon capture utilization and storage

1. INTRODUCTION

1.1. Why research on multi-scale heterogeneity is more important now than ever

The movement of multiple fluids through complex porous media is ubiquitous in nature and beyond. Historically, flow in geologic media focused on oil and gas production. However, more recent research has shifted towards the geologic storage of CO_2 and H_2 as a greenhouse gas mitigation technique (7). There is now an increased importance placed on accounting for small-scale heterogeneities in large-

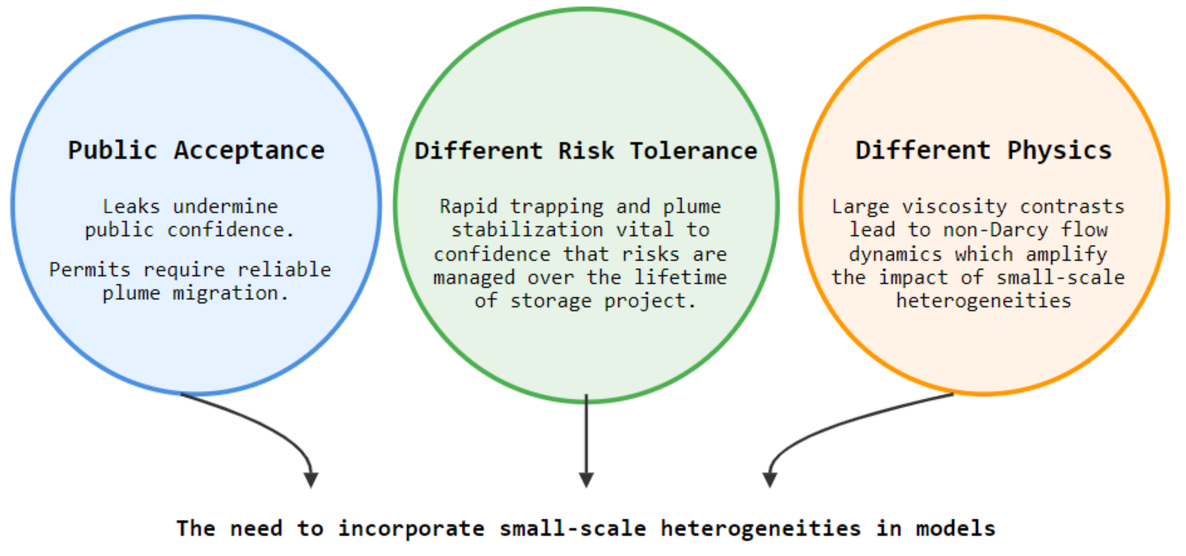

Figure 1: Overview to why small-scale heterogeneities have increased importance in geologic storage applications.

scale reservoir models; this is highlighted in **Figure 1**. The first significant difference between geological storage projects and historical oil and gas production is a social concern about retention. Accurate modeling of small-scale heterogeneities and the impact on a project's plume migration and pressure buildup is integral to developing safe storage projects. Secondly, the risk tolerance for geological storage differs from that of oil and gas production. While the latter is driven by market demand and commodity prices, the former is often incentivized by policy frameworks aimed at reducing greenhouse gas emissions. This introduces additional layers of complexity as storage projects must navigate regulatory requirements, public perception, and long-term liability concerns. Permits for CO_2 storage projects require monitoring of the plume until stabilization has occurred (31, 92). The extended timelines and costs associated with monitoring and verification further underscore the need for robust, predictive models that can inform decision-making and policy development. For H_2 storage projects, the H_2 is extracted as and when required, this means that the plume must be well contained, with little trapping. Lastly, different physics and flow dynamics are at play in storage projects. Instead of extracting a viscous non-wetting phase, such as in conventional oil extraction, geologic storage involves injecting a low-viscosity non-wetting phase. Flow rates for both phases are sufficiently low for flow to be within the capillary-dominated regime (53).

In many previous geological CO_2 storage projects, modeling predictions have differed greatly from what occurs during injection by underestimating the spread of CO_2 in the subsurface. History matching has been performed for these projects; however, matches are only achieved using model parameters outside the range of observations at wells. For example, this scenario occurred at the Sleipner project in Norway (16, 88), In Salah in Algeria (60, 67), and the Frio and IBDP projects in the United States (12, 21, 30, 33, 37, 76). Small-scale heterogeneities have been shown to control flow and could explain why accurately predicting the CO_2 plume migration in the subsurface has been so challenging (33, 80). This includes the presence of permeable fractures that are below seismic imaging resolution (12). While the aforementioned examples are for CO_2 storage, the same risk on migration and trapping exists for H_2 storage. In both storage scenarios, a small plume is desirable. However, in the case of H_2 storage, trapping is undesirable. Thus, for the geological storage of CO_2 and H_2, one of the most significant challenges to successfully predicting the subsurface migration and trapping (or lack of) of fluids is incorporating or accounting for small-scale heterogeneities in field-scale models.

1.2. The challenge

While the need to account for small-scale heterogeneities at the field scale has been identified, there are still outstanding questions on how to incorporate experimental observations of the impact of small-scale heterogeneities in field-scale models, so that accurate predictions of plume migration and trapping can be made. The effect of small-scale heterogeneities depends on the type and degree of the heterogeneity. Researchers have observed a wide range of different impacts across a range of spatial scales. How to generalize these observations and upscale them for inclusion in field scale models is non-trivial.

In this work, we present an overview of the wide range of heterogeneity observed by researchers and discuss its impact on flow and trapping. We highlight the importance of modeling these small-scale heterogeneities to predict plume migration and trapping efficiency successfully. We discuss different methods for accounting for these small-scale heterogeneities without modeling them directly at the field scale. We provide commentary on the current state of research and the scales of interest for CO_2 and H_2 storage and showcase interesting avenues for future research.

2. SCALES OF HETEROGENEITY

The influence of heterogeneity on fluid flow needs to be accounted for at the field scale to accurately predict the migration and trapping of fluids in the subsurface. Historically, samples on the order of centimeters were cored, and measurements from these experiments were applied in reservoir simulations (77). These experiments are referred to as core-scale experiments. However, in more recent years, improvements in X-ray tomography has led to research on smaller scales, resolving dynamics down to the scale of individual pores (the pore-scale) (13). The imaging of fluids in situ for pore-scale and core-scale experiments is typically done using X-ray tomography. Due to X-ray attenuation, image resolution is proportional to image size (18, 87). This means that high resolution images require smaller samples. Thus, for pore-scale observations, samples are in the range of < 10 mm in both length and diameter, and flow is observed to be dominated by heterogeneity on the order of millimeters. For core-scale observations, heterogeneities on the order of centimeters appear to dominate flow and at the field scale, bedding planes on the orders of meters heavily influence flow. This wide range of scales is illustrated with examples in **Figure 2**.

While larger scale heterogeneity influences fluid flow at the field scale, small-scale heterogeneity also plays a role in plume migration and trapping at this scale. The incorporation of small-scale permeability heterogeneity in field scale models was linked to faster plume migration (33). This suggests that the lack of representation of these small-scale heterogeneities in field scale models could be the reason why, historically, CO_2 plume migration has been poorly predicted (and often underestimated). Small-scale heterogeneity also influences residual trapping (33, 36). Thus, it will influence plume stabilization times and storage security (40).

Incorporating small-scale heterogeneities at the field scale is non-trivial. A typical pore-scale experimental resolution is 4 µm (73). With this resolution, we would need $\approx 10^{16}$ grid cells per cubic meter.

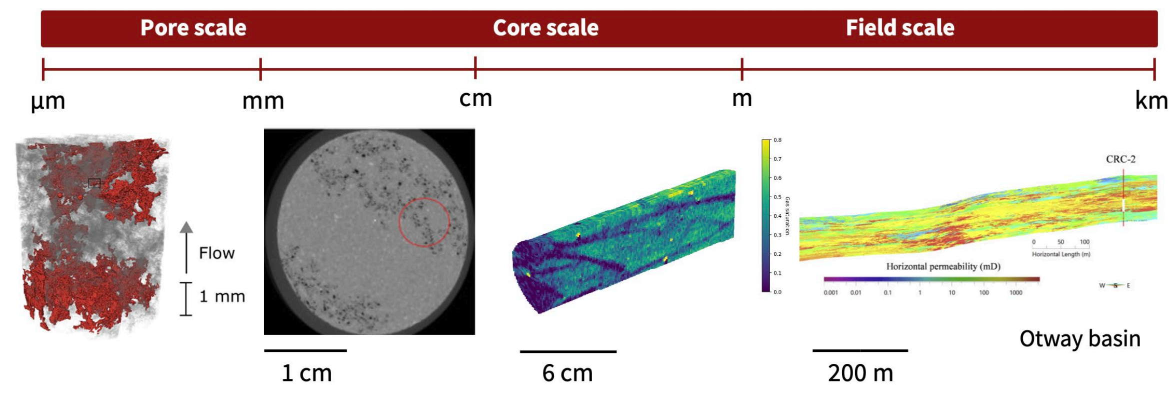

Figure 2: The manifestation of heterogeneity across different spatial scales, from the order of millimeters in pore-scale experiments, to hundreds of meters at the field scale. Pore-scale images taken from Spurin et al (72, 74), core-scale image of a core from the Otway basin, with permeability from the Otway basin cross section taken from Mishra et al (52).

In comparison, current field scale simulations have ≈10^6 grid cells to capture an area on the order of hundreds to thousands of cubic meters (65). Thus, from a computational point of view, modeling pore-scale dynamics even at the meter scale is infeasible (9). However, even if computational resources did not limit the modeling of pore-scale dynamics, we are unable to resolve the subsurface pore space at the field scale. This is because imaging of the subsurface in the field is done using seismic surveys. These surveys have a resolution of around 50 m (12). While improvements are being made to seismic imaging capabilities, the resolution is linked to sensor spacing. This means that a resolution on the order of millimeters is infeasible due to the size of sensors, and how many sensors this would require. There is research that tries to capture the impact of small-scale heterogeneities at the field scale without modeling the impacts directly. This includes flow rate dependency in relative permeability curves (10) and composite relative permeability curves (52).

2.1. Sub-pore scale heterogeneity

This commentary explores flow physics from the pore-scale up. Both CO_2 and H_2 typically act as the non-wetting phase in storage scenarios, meaning they minimize contact with the rock surface, while the water or brine occupies the smaller regions of the pore space (2, 23, 78). However, sub-pore processes may influence larger scale fluid dynamics. Firstly, wetting, which results from molecular forces acting within and between fluids and a solid surface, is influenced by the chemical and structural heterogeneity of the solid surface. Coverage of grains for instance, by clay, cement or other contaminants, but also roughness, may cause local variation which can change macroscopic responses (62, 94). Furthermore, if the CO_2 or H_2 occupies narrow regions of the pore space, molecular interactions may be significant (90).

In many cases, these small-scale effects may be neglected, however, researchers have observed situations where this is not the case, and these small-scale effects have altered the larger scale responses in regards to flow or structural integrity (63, 64). These effects may be more significant for H_2 storage, due to its small molecular size (38). H_2 has the ability to reach smaller pores, raising questions on differences in regards to adsorption or structural alteration of the clay. Investigations of different minerals have shown that the small molecular size would allow for hydrogen to penetrate for instance clay (91). Moreover, hydrogen can trigger microbial activity (20, 79) which further triggers questions on combined processes within a single pore.

Most studies indicate the contribution of sub-pore fluid dynamics to the overall saturation change is small (24, 89). These studies, however, were limited to model systems, not accounting for variability in rock and the time scales involved. How heterogeneities at this length scale impact larger scale responses is still subject to investigation, so our focus in this commentary remains on the pore-scale and larger dynamics. However, we acknowledge the potential significance of sub-pore processes, particularly for H_2 storage.

3. THE OBSERVED IMPACT OF SMALL-SCALE HETEROGENEITY

A wide range of heterogeneities have been observed in experiments conducted across all spatial scales. Here, we highlight the range and potential impact for different classifications of small-scale heterogeneity observed by researchers. We focus on capillary barriers, highly channelized flow, flow rate dependency in the capillary dominated regime, the influence of the orientation of heterogeneity with respect to flow direction, and how pore space heterogeneity may evolve with time. This section is by no means exhaustive, but it shows the wide range of impact small-scale heterogeneities have on larger scale flow properties such as trapping, and hopefully highlights to the reader that there is no 'silver bullet' or single adaptation that could address the influence of all types of small-scale heterogeneity at the field scale. We highlight the need for further research, and for careful consideration of if experiments are translatable to the field scale depending on experimental methodology and/or sample size.

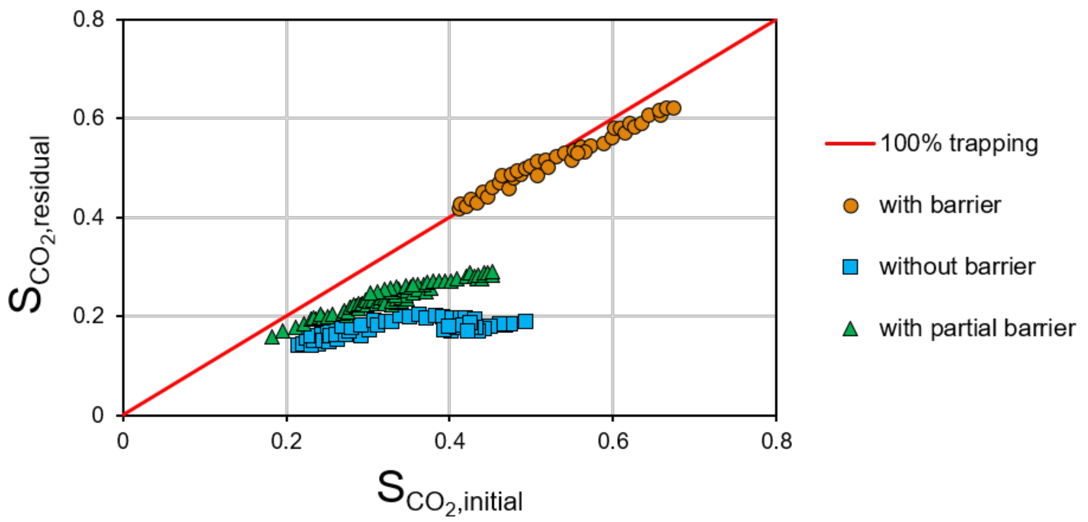

Figure 3: The impact of a capillary barrier on trapping efficiency. Points with a complete capillary barrier (with barrier) and without barrier are from Krevor et al (42), points for a partial capillary barrier are from Oh et al (54)

3.1. Capillary barriers

Capillary barriers are regions of low porosity or permeability, that inhibit the movement of the non-wetting phase (the CO_2 or H_2). At the core-scale, experiments by S. C. Krevor et al (41) explored a core with a complete capillary barrier at the end of the core. Behind this barrier, CO_2 was able to build up, improving trapping (shown in **Fig. 3**). The barrier was removed, and the experiment was repeated. Without the barrier, the trapping significantly decreased, suggesting that the presence of a capillary barrier improves trapping in the subsurface.

However, other experiments with a less extreme capillary barrier (denoted as a partial capillary barrier in **Fig. 3**) have an intermediate trapping efficiency to the results by S. C. Krevor et al (41) and Oh et al (54). In the subsurface, a complete capillary barrier is unlikely, as the CO_2 or H_2 can move laterally, in a way that is restricted in core- and pore-scale experiments. Thus, upscaling the observations with a complete capillary barrier, or no capillary barrier at all, will likely misrepresent the trapping in the subsurface.

Overall, the presence of a capillary barrier heavily influences the trapping efficiency. **Figure 3** highlights a wide range of trapping efficiencies, which introduces uncertainty in predicted field scale values. Small-scale heterogeneities improve the trapping efficiency and so could be desirable for geologic CO_2 storage (and undesirable for H_2 storage). However, the impact of these capillary barriers in small samples might not be representative of what will happen at the larger scale where there are more options for the CO_2 and H_2 to move in space.

3.2. Highly Channelized flow

Highly channelized flow arises when the non-wetting phase (the CO_2 or H_2) travels in a restricted region of the rock sample. The non-wetting phase saturation is high in these locations, but the overall non-wetting phase saturation is low. These highly channelized flows lead to rapid migration due to small pore volume utilization. Furthermore, with few possible pathways through the sample, and low connectivity, intermittent flow pathways could be expected (70). This leads to a time dependent relative permeability and dynamics not currently incorporated in field scale models.

Highly channelized flow has been observed to significantly impact trapping efficiency. In H_2 experiments conducted by Boon and Hajibeygi (10), the H_2 saturation at the end of drainage was high, but during

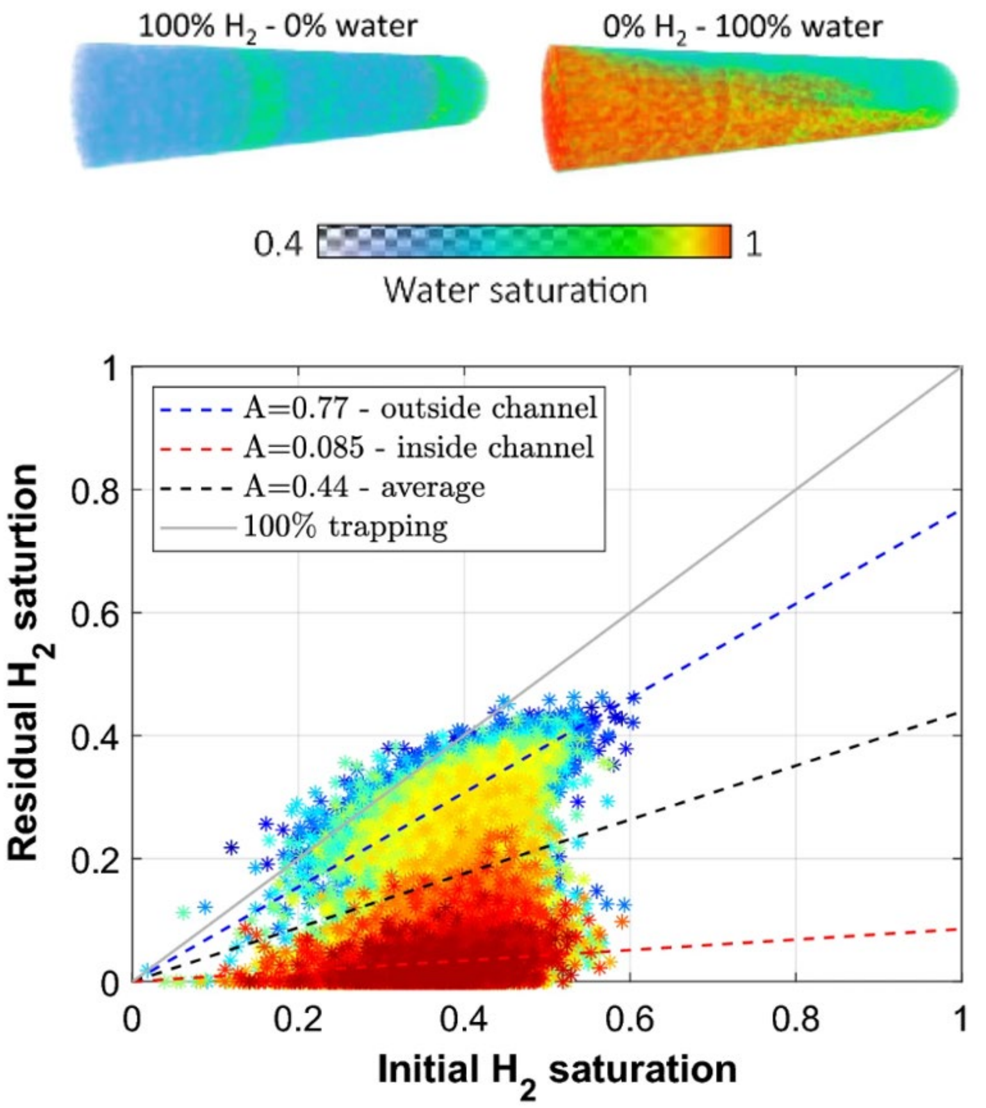

Figure 4: The impact highly channelized flow on trapping efficiency in H_2 experiments conducted by Boon and Hajibeygi (10). The water saturation across the core at the end of drainage and imbibition are shown at the top. For the trapping curve, color corresponds to vertical location in the core. Blue is the top of the core and red is the bottom of the core. The dashed lines denote the best-fit linear trapping relationships. The grey line denotes 100% trapping.

imbibition, the water formed fingers that evolved into channels. Outside the channel, the trapping of the H_2 was high, while trapping in the location of the fingers was close to zero (as shown in **Fig. 4**). This led to trapping efficiencies between 0 and 100% depending on location in the rock sample. More complex patterns of heterogeneity (i.e. beyond layers) have also been observed, with some highlighted in **Figure 5**. Some of these patterns arise from features such as compaction bands or cross-bedding (**Fig. 5b**) (61). In other work, the porosity was homogeneous, but the saturation distribution was highly heterogeneous (the Bentheimer sandstone in **Fig. 5c**) (66). This makes it difficult to predict fluid distributions prior to the experiment and inhibits our ability to make predictions based off porosity.

Analytical models have been created to incorporate the impact of highly channelized flow (11, 85). While these models are able to successfully capture the impact of high permeability layers (such as those in **Fig. 5a**), other experiments cannot be replicated even with history matching (47, 86). This is likely due to heterogeneity below the resolution of the images.

Overall, highly channelized flow leads to low non-wetting phase saturations in experiments. This introduces large uncertainty in relative permeability values for higher non-wetting phase saturations,

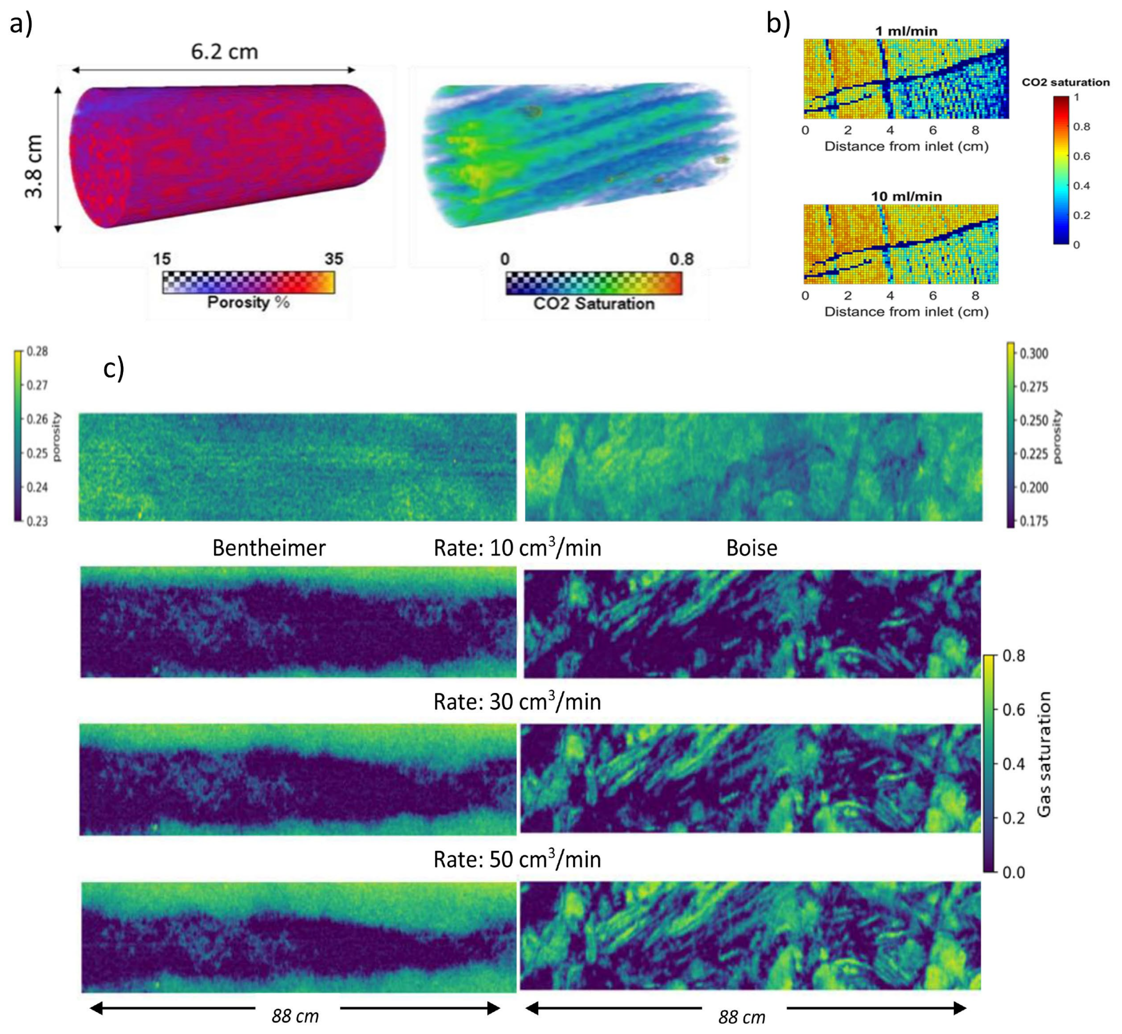

Figure 5: The impact of highly channelized flow on fluid distribution **a)** high permeability layers causing channeling of CO_2 (11), **b)** compaction bands causing channeling of CO_2 (61), and **c)** channeling of the non-wetting phase for a relatively homogeneous Bentheimer sandstone compared to a heterogeneous Boise sandstone (66).

which might be present in the plume at the field scale due to upwards migration of the non-wetting phase. Highly channelized flow also leads to reduced water relative permeabilities. This impact could be represented at the field scale.

3.3. Flow rate dependency in capillary dominated regime

Another observation is the influence of flow rate on residual trapping. While a difference is expected between the capillary dominated regime and the viscous dominated regime (7, 11), researchers have seen large changes in the relative permeability and trapping even in: **1)** the capillary dominated regime, and **2)** with very small changes in flow rate.

In experiments by Manoorkar et al (47), the capillary number was varied between 10^{-5} and 10^{-6} (so purely in the capillary dominated regime, with the flow rate increased by a factor of 10), but the trapping efficiency was significantly less for the higher flow rate experiment. Furthermore, the Land trapping model only fitted the trapping data for the lower flow rate experiments. This was attributed to the impact of millimeter and centimeter scale heterogeneity in the samples. This dependency on flow rate in the capillary regime was also observed in variable flow rate experiments (74). Here, the same flow rates were used, but the injection sequence was either high flow to low flow, or vice versa. The order of injection rate influenced the amount of trapping observed at the end of the experiment.

Analytical frameworks have been derived to capture this. They highlight that incredibly low capillary numbers are necessary for flow dynamics to stabilize (44, 45, 55). However, field scale simulations typically only have a viscous dominated relative permeability curve to simulate flow near the injection well, and a capillary dominated relative permeability curve to simulation flow away from the injection well. These simulations are not influenced by the injection sequence, just total flow rates and duration of injection. Thus, the flow rate dependency in the capillary dominated regime is not currently captured at the field scale.

3.4. Orientation of heterogeneity with respect to flow direction

The orientation of heterogeneity has also been observed to influence flow and trapping. In this section we cover two topics: **1)** the orientation of heterogeneity relative to flow direction is an important consideration when conducting or upscaling experiments, and **2)** that the influence of heterogeneity varies in the direction of flow relative to upwards migration (assumed to be perpendicular to the flow direction).

Firstly, the orientation of heterogeneity influences trapping efficiency in core-scale experiments (58). Numerical models exist that allow researchers to reorientate the heterogeneity and assess the impact of this on larger scale flow properties such as trapping and relative permeability (32). Despite the recognized importance of the orientation of heterogeneity, the orientation of cores is often not documented once a core is drilled, leading to uncertainty when upscaling predictions. If there are dipping beds, the core should be drilled in the direction of the beds, rather than horizontally. The presence of thin mudstone, siltstone, shale or other low permeability layers will significantly influence the vertical relative permeability while having little impact on the horizontal relative permeability.

At the field scale, the treatment of anisotropic relative permeabilities remains inconsistent. Some studies do not incorporate anisotropic relative permeabilities (25). Others incorporate anisotropic relative permeability by reducing the vertical component by a given factor (3). Some studies explicitly account for directional variations in relative permeability with distinct relative permeability curves (1). This lack of methodological consensus introduces additional uncertainty in upscaling reservoir characterization and predictive modeling, highlighting the need for more robust and systematic approaches to representing anisotropic flow behaviors in heterogeneous geological systems.

3.5. Dynamic changes in pore space heterogeneity

Pore space heterogeneity can evolve with time due to phase changes such as dissolution and precipitation. The morphology of a dissolution front exhibits significant variability, ranging from uniform to the formation of distinct wormholes and channels. This variability is governed by the interplay between mixing rates, dissolution kinetics, and the inherent heterogeneity of the pore space (69). This creates a feedback loop where small-scale heterogeneities influence dissolution patterns, which in turn modify the pore-scale architecture. When wormholes or channels develop, they can dramatically alter flow patterns, leading to preferential flow paths (57). These dissolution-induced modifications to pore structure have significant implications for both CO_2 and H_2 subsurface storage applications (35). While mineral precipitation primarily affects CO_2 storage scenarios (17), both CO_2 and H_2 storage in saline aquifers face challenges related to salt precipitation (27). These precipitation processes, like dissolution, are influenced by existing heterogeneities while simultaneously modifying the pore structure (46, 57).

This dynamic evolution of pore space heterogeneity through phase changes introduces additional complexity to modeling efforts. The temporal variation of heterogeneity, coupled with its role in driving further changes, creates a complex feedback system that must be carefully considered in pore-scale modeling approaches.

4. DIFFERENCES IN DYNAMICS ACROSS SCALES

Experiments conducted at the pore-scale, with experimental parameters such as capillary number and viscosity ratio matched to core-scale experiments, have highlighted some differences in dynamics across scales. It is important to quantify these differences in order to predict how they might manifest at the field scale.

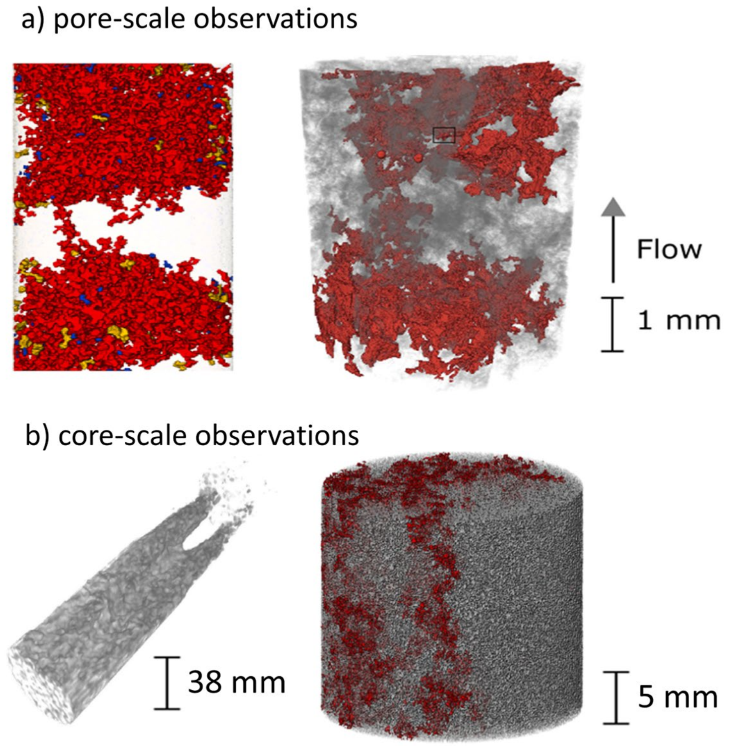

Figure 6: a) pore-scale observations highlighting a single pore controlling flow across the sample, for H_2 on the left (36), and N_2 on the right (72), and **b)** core-scale observations highlights multiple channels for the flow to move, for H_2 of the left (10), and N_2 on the right (83) The experiment in the bottom right image matches the experimental conditions of the top right image. Few core-scale H_2 experiments have been conducted, with no known replication of the top left experiment.

Pore-scale experiments have shown a fluid flow phenomena termed intermittent pathway flow that heavily influences energy dissipation and trapping (59). The amount of fluid fluctuating was observed to increase with increasing capillary number (71, 93). However, while experiments conducted in larger samples observed this trend at very low capillary numbers. There was a decrease in the amount of intermittent pathway flow observed at higher capillary numbers, that was attributed to the increased importance of viscous forces (even with very low capillary numbers $\ll 1$, at around 10^{-7}) (83). A single critical flow pathway has been observed in pore-scale observations (see **Fig. 6**). However, more pathways are possible in larger cores, which controls the amount of dynamics, but also the impact of the dynamics on the relative permeability.

In other work, two samples from the typical range of core-scale experiments were explored (74). The role of a variable injection rate was explored in both samples, and the observed impact was different for the different sized samples. This was attributed to the presence of a connected flow pathway across the core for the smaller sample. This creates something that might not be present in the subsurface (a pathway for the instantaneous transmission of pressure across the core). Other work explored the pressure signal of intermittent pathways versus connected pathway flow in small samples, where fluid interfaces could be resolved. When the experiments were repeated in larger samples (with the flow rate changed to match capillary numbers), the signal for connected pathway flow was not observed (75). This highlights that a connected pathway is unlikely at larger spatial scales, and experiments with a connected flow pathway across the core might not present representative dynamics. The relaxation of fluids post trapping is also influenced by sample size (22). Thus, many other important phenomena is likely dependent on the scale at which the observation was made.

Observations at the pore-scale help us understand the underlying physics. While these observations are persistent for different non-wetting phases (see **Fig. 6**), how they manifest at the larger scale might not be trivial. This is because of the possibility of more pathways encouraging connectivity and the increased importance of viscous forces even in the capillary dominated regime. Furthermore, in the subsurface, the plume is large, this creates high capillary pressure even with low velocities. This is something that might not be able to be recreated in core-or pore-scale experiments. Furthermore, in these experiments water is injected to get the trapping efficiency. This is not representative of how water will move in the subsurface. In the subsurface, more pathways are possible, meaning that the plume may bypass the region explored experimentally. Overall, there has been research that suggests that the observations made in small samples might not be representative of what happens at the larger scale. Experiments have been done in even longer cores, so that gravity effects start to play out (66). These experiments are incredibly challenging, as they require large volumes of pressurized fluid.

5. WHAT SCALE MATTERS THE MOST?

Here we examine what scale matters the most for capturing small-scale heterogeneities at the field scale. We explore what is a representative volume in experiments. Then we explore what is the minimum scale required in models to accurately capture the movement of the non-wetting phase in experiments (regardless of if the experiments are representative of larger scale fluid movement).

5.1. What sample size is representative of dynamics at the field scale?

Theoretically, a Representative Elementary Volume (REV) exists where you are imaging a representative volume, such that the observations made in that volume are representative of the continuum scale (34). By identifying an REV, a sense of what scale experiments are needed can be established, if the goal is to apply observations to the field scale movement of fluids in the subsurface. An REV is usually described as a cubic length side and is done so in this commentary.

For porosity and capillary pressure characteristic curves, the REV for both homogeneous and heterogeneous samples has been reported to be less than 2 mm by many researchers (29, 34, 68, 83). The REV for these quantities is within the range of pore-scale experimental sample sizes. In contrast, the REV for flow properties varies significantly between studies, and also between different quantities of interest. For saturation, Jackson et al (34) reported that the REV was 5.4 mm, while an REV was not observed even with a cubic length side of 20 mm in Wang et al (83). For the Euler characteristic (a measure of connectivity, see (82) for more details) the REV was not found for the non-wetting phase even at 40 mm (39). In Armstrong et al (5), the cluster length was defined as the lower boundary for the definition of the macroscopic scale, and thus indicative of an REV. This was calculated to be 54 mm for a homogeneous sandstone at low flow rates. This means that a REV for the parameters of interest have been reported to be somewhere between 5 mm and over 50 mm. Which is an incredibly wide range.

This leads to two questions: **1)** why is there such a large range? **2)** with advances in imaging capabilities and computational processing, do we aim for exploring pore-scale dynamics in larger samples? For the first question, work exploring the REV for dissolution found that the focusing effect was greater with increasing pore space heterogeneity, indicating that the REV for dissolution was far greater than the dissolution front itself (50). This non-local behavior has been seen elsewhere for non-wetting phase propagation. Armstrong et al (4) found that the zone of influence associated with a Haines jump was found to exist over a distance of multiple pores, and thus, is much larger than the correlation length of the homogeneous micro-model pattern the experiments were conducted in. This highlights the need to carefully consider what we want to capture in the REV, and to understand that REV will depend on heterogeneity. For the second question, pore scale imaging is being done in larger samples, however, if the REV is greater than 60 mm, this suggests that even some core-scale samples are smaller than an REV. These samples were deemed to be continuum-scale, and thus representative of dynamics at the larger field. This may not have been the case for heterogeneous systems, leading to uncertainty in all upscaled parameters taken from these core-scale observations.

5.2. How do we incorporate these findings into models?

In the previous sections, we have highlighted how small-scale heterogeneities heavily influence larger scale flow properties. Therefore, we want to incorporate these findings into our field scale models both through permeability and porosity data, but also through relative permeability and capillary pressure relationships.

Typical reservoir modeling assumes relative permeability is purely a function of saturation (7, 19). This is valid for connected pathway flow. In work by Picchi and Battiato (56), some dynamics, beyond connected pathway flow, can be captured with relative permeability functions and the viscosity ratio of the two fluids present. For other flow regimes, the film thickness at the pore-scale or the average pore-scale curvature was needed (which is closely related to the Euler characteristic). The evolution of the Euler characteristic can account for hysteresis observed during multiphase flow (34, 48). However, the Euler characteristic is incredibly sensitive to resolution (26). This makes it difficult to measure at even the core-scale. Thus, making predictions of their values at the field scale impractical.

While it is difficult to resolve pore-scale fluid connectivity at the core-scale. There has been some success in calibrating numerical models against observed millimeter scale saturation heterogeneity, with these models able to accurately predict average pressure drop and equivalent relative permeability at the pore-scale for homogeneous sandstone samples (32, 86). However, these models already fail at making predictions for limestone rock cores with sub-resolution porosity and so might also insufficiently represent high degrees of heterogeneity in reservoir rocks (47, 86). Models have been created that incorporate this sub-resolution (or micro-porosity) (14). Here, the incorporation of micro-porosity was shown to influence the invasion of the non-wetting phase. However, determining the petrophysical parameters, and developing more advanced models, is limited by difficulties in measuring and quantifying flow in these regions where the porosity is below image resolution.

This leads to the question of: do we need to be able to resolve small features directly in models, or is there an upscaled representation of the underlying dynamics that can be applied at the field scale? The latter is preferable from a computational demand point of view. Another challenge is how to best incorporate the uncertainty in the geology into dynamic simulations. Currently, many CO_2 storage projects use a discrete geomodel to perform dynamic simulations and may perform a sensitivity study on certain reservoir parameters. However, this approach does not fully capture the uncertainty space with regards to the geology and reservoir parameters. These uncertainties can lead to significant differences in the predicted plume footprint and pressure buildups. In many cases, hundreds of simulations are required to fully characterize the subsurface (15). To mitigate the high computational cost of running the simulations needed to capture the uncertainty space, one solution is to use machine learning models. Machine learning techniques can accelerate the reservoir simulation process, enabling the necessary simulations to quantify the subsurface uncertainty and gain a probabilistic understanding of plume migration and pressure buildup throughout a project's lifecycle.

These models can be trained on a wide range of heterogeneities, and thus, fewer experiments are required to be run in order to populate a reservoir model (as these experiments are time-consuming, highly technical, and expensive) (49). However, if there are dynamics below the resolution of the images, machine learning models will have trouble incorporating them from segmented images (81). Deep learning models that can predict multiphase flow properties such as relative permeability and trapping are still lacking (84). However, there is ongoing research using machine learning to predict flow dynamics at the pore-scale, which could address these issues (28).

6. KEY OUTSTANDING QUESTIONS TO ADDRESS UPSCALING

There are a number of key outstanding questions that the authors of this commentary believe need to be addressed in future work.

1. **Does a global measure exist, that is independent of resolution, that can be used to characterize the propagation and trapping of CO_2 and H_2 in the subsurface?** Pressure is a promising metric, as it has been linked to fluid connectivity (75). However, there are some key questions to address since most experimental setups only measure the pressure drop across the core. **1)** Is spatially resolved pressure needed to link pressure fluctuations to the pore space heterogeneity and flow dynamics? **2)** Is pressure needed for just the non-wetting phase, or both fluid phases? **3)** How easy is it to resolve pore-scale pressure fluctuations at the field scale, where pressure will also be influenced by other factors such as tides (43)?

2. **Do we need to adapt experiments to be more representative of field scale plume migration?** We highlighted in this commentary that incorrectly scaling up capillary barriers and

highly channelized flow could significantly impact predictions. Most experiments measure trapping by injecting CO_2 or H_2 and then injecting water or brine. The water injection is not representative of how water migrates in the subsurface, which leads to uncertainty in the trapping estimates. Furthermore, with large plumes in the field, high capillary pressures arise under low flow rates. These are represented in experiments by injecting at high flow rates to get high capillary pressure. However, with the flow rate dependency observed, this might not be a good representation of what is occurring in the subsurface.

3. **Do we move away from a single prediction to a suite of predictions?** Machine learning allows us to perform many simulations with different subsurface realizations. This will enable researchers to quantify uncertainty in estimates of flow properties and heterogeneity. A probabilistic approach can help to characterize project risk better and lead to more informed decision-making by project stakeholders.

4. **Do we include small-scale heterogeneity using the conventional modeling framework?** Experiments dominated by small-scale heterogeneity have reduced water relative permeabilities and lower gas saturations than expected. Incorporating this to some extent will allow us to accommodate the impact of small-scale heterogeneities. But is something outside the conventional framework of relative permeability and trapping efficiency needed to successfully predict the migration and trapping of CO_2 and H_2 in the subsurface?

7. CONCLUSIONS

In this commentary, we highlighted the impact of small-scale heterogeneities on plume migration and trapping. We want to encourage future research on this topic that spans many orders of spatial and temporal scales to capture the full range of important dynamics. Efforts are also needed in upscaling and for accounting for differences across scales so that accurate predictions of plume migration can be made.

One avenue of interest would involve conducting many pore-scale experiments and then using data-driven algorithms and pressure data to determine the spectral signature of different event types, sizes, and frequencies. This could be used, in turn, in core-scale experiments to determine what dynamics persist and if new dynamics arise outside the signature of events recorded at the pore-scale. This approach would help elucidate the scalability of pore-scale experiments. Pressure data can also be measured at the field scale at different locations. If the underlying pore-scale dynamics can be deduced from this pressure data, it becomes possible to determine the most critical factors for modeling at the field scale. This represents a non-trivial task, as fluctuations in the pressure data caused by pore-scale dynamics would need to be separated from other factors influencing the signal, such as tides, vehicles, and other environmental influences.

While modeling small-scale heterogeneities is no easy feat, small-scale heterogeneities are not necessarily a negative feature of storage reservoirs. In fact, small-scale heterogeneities could be exploited to maximize trapping in CO_2 storage projects, making highly heterogeneous sites favorable. This is an area of ongoing research at the Otway International Test Center, where a deliberately heterogeneous site was chosen to explore the impact of heterogeneity on trapping (6). The injection of CO_2 at this site ended in January 2025, with analysis currently underway.

STATEMENTS AND DECLARATIONS

Author Contributions

All authors contributed to the preparation of this article, including the drafting, revising, and final approval.

Conflicts of Interest

The authors have no conflicts of interest to declare.

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