

CRYSTAL GROWTH IN POROUS MEDIA

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ABSTRACT

Crystalline silicate minerals and carbonates make up 90% to 95% of the Earth's lithosphere, the rigid outermost shell comprising the crust and uppermost solid mantle. Crystalline materials are continuously modified by fluid–rock interactions including crystal growth occurring along fractures and within pore spaces. Crystals form under conditions dictated by extrinsic factors, such as temperature, pressure, fluid composition, and pore confinement, as well as intrinsic factors such as crystal structure, chemical bonding, and anisotropy. While the thermodynamic stability and structure of crystals are well established, their rates of heterogeneous nucleation and growth remain poorly constrained. This is particularly true in porous media, where nucleation is frequently a distinct and rate-limiting step rather than a negligible precursor to growth, especially where non-classical pathways preclude a single, well-defined interfacial free energy.

In this commentary, we outline how crystal nucleation and growth in porous media control pore-scale structure, flow, and transport, and we evaluate how these processes can be represented in numerical models across scales. We examine the distinct roles of nucleation pathways, growth kinetics, interfacial and confinement effects, and crystallization pressure in governing transient porosity, stress localization, and self-organized crystalline networks. Furthermore, we discuss how fluid flow and mixing modulate where and when these processes occur. These principles are illustrated through examples spanning well-controlled synthetic crystal growth in materials science to geo-energy and geoscience applications, such as basaltic CO₂ mineralization, where probabilistic nucleation, reactive transport, and evolving pore architecture jointly control macroscopic behavior. Finally, we assess the potential of machine learning and surrogate modeling approaches to bridge the persistent gap between molecular-scale mechanisms and field-scale predictions. By emphasizing mechanistic understanding over system-specific details, our goal is to help porous media scientists judge when crystallization is likely to matter, and to guide the selection of modeling approaches that remain both physically grounded and computationally tractable.

KEYWORDS

Crystal nucleation; Crystal growth kinetics; Crystallization pressure; Reactive transport; Mineral precipitation; CO₂ mineralization; Pore Confinement; Machine learning; Surrogate modeling; Porous media

WHY THIS PAPER MATTERS

Crystal nucleation and growth can progressively clog pore spaces, redirect fluid pathways, and transform the mechanical and transport behavior of porous rocks across scales. Is it possible to use information we have about nanoscale processes to predict reservoir-scale changes? This InterPore Commentary article synthesizes how confinement, interfacial free energies, and crystallization pressures control where crystals appear, how fast they grow, and when they damage or seal flow networks in natural and engineered systems. It then outlines how machine learning can be used to connect molecular, pore, and field scales for predictive modeling.



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1. CRYSTALS

What is it that fascinates humans about crystals? Their vivid colors, translucence, metallic luster, and the striking symmetry of their forms seem to captivate everyone who encounters them. Who has not experienced the joy of finding perfectly cubic crystals of “fool’s gold” (pyrite), or quartz crystals that resemble diamonds for the untrained eye? Constrained only by atomic arrangement and thermodynamic stability, crystals can take on an almost infinite variety of forms (**Fig. 1**); even minerals of identical chemical composition can express strikingly different macroscopic shapes depending on the physical and chemical conditions present during growth. This morphological mutability spans from the highly symmetrical, perfectly cubic habits of pyrite, to the elongated, diamond-like faceting of quartz, the tabular, desert-rose clusters of baryte, and the massive, translucent columns of gypsum.

Yet crystals are far more than objects of beauty. For Earth scientists, understanding the chemical and physical conditions under which crystals form, or dissolve, estimating their growth rates, and predicting how they interact with their surroundings are questions of profound scientific and societal importance. How do we remove white scale deposits caused by calcium carbonate and calcium sulfate from household pipes, industrial heat exchangers, and geothermal boreholes (150, 80, 196, 98)? How do we prevent salt crystallization within porous stone and concrete, one of the leading causes of degradation in heritage buildings and monuments worldwide (64, 223)? Answering such questions requires a thorough, mechanistic understanding of crystal formation and the factors that govern it.

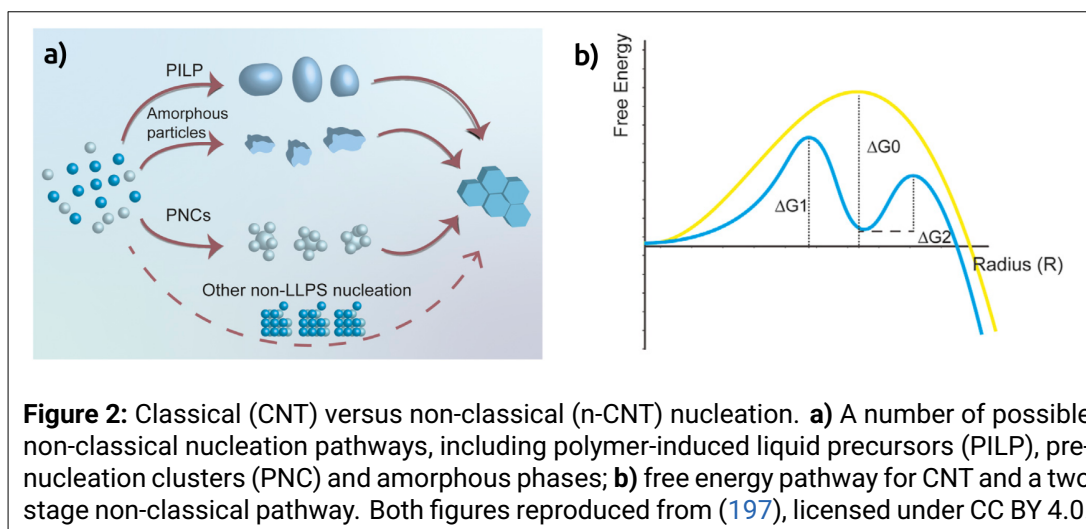
With this knowledge, scientists can also make crystallization work *for* us. Carbonate minerals can co-precipitate with lead, cadmium, and zinc, effectively locking these pollutants into stable, low-solubility phases and limiting their mobility in soils and groundwater (228, 170). Mineral formation can likewise capture CO₂ in solid form over geological timescales (275, 162, 181), making carbon mineralization one of the most secure mechanisms for long-term carbon storage and climate mitigation (10, 109, 110). Crystals also carry memory. Their isotopic compositions, trace element distributions, and structural defects record the temperature, pressure, fluid chemistry, and atmospheric conditions present at the time of their formation. Carbonate and ice-core archives, for example, have been central to reconstructing past climates and tracing environmental change over millions of years (55, 53). In this sense, a single crystal can serve as a window into a world long gone.

These diverse roles converge on a single fundamental question: what controls **how** and **when** crystals form? The answer lies in a set of interacting physical and chemical factors, from bulk fluid supersaturation and temperature to the physical properties of the liquid-solid interface, pore



confinement, and the presence of foreign ions or organic molecules. In highly controlled laboratory and industrial settings, where these factors can be isolated and precisely tuned, scientists have developed robust theoretical frameworks that allow the production of synthetic crystals and functional materials with well-defined crystal chemistry and remarkable precision in size and defect distribution. The semiconductor industry offers a compelling illustration: using molecular beam epitaxy (MBE) or metal-organic vapor-phase epitaxy (MOVPE), III-V semiconductor nanowires such as GaAs can be grown at predefined positions with lateral placement accuracy of just a few nanometers, yielding arrays of nearly defect-free monocrystalline structures (149, 144).

However, applying the same deterministic frameworks to natural porous media remains far from trivial. Predicting how newly formed crystals distribute across pore space, and thus how fluid flow shapes crystallization, is a particularly difficult challenge: even gentle advection alters local supersaturation gradients and ion supply rates, shifting where and when crystals nucleate (190, 247). A further obstacle is the description of pore walls, which exhibit a mosaic of surface chemistries,



charges, and defect densities that exert a strong, yet poorly characterized, influence on local solution chemistry and nucleation kinetics (43, 243). Natural systems introduce additional complexity because groundwater almost always contains trace ions and organic molecules whose concentrations are rarely fully known, yet even at nanomolar levels these species can dramatically inhibit or catalyze crystal growth (44, 201).

Nevertheless, a great deal can be learned from geological observations: the gradual filling of pore space during diagenesis, the mineralization of fractures under hydrothermal fluid flow, and microbially induced mineral precipitation all comprise natural experiments in which the outcome is observable even when the initial conditions are not. Crystal nucleation and growth have been incorporated into reactive-transport models, but important questions persist: how can nucleation and growth be represented efficiently without sacrificing the underlying physics, and how can such models be genuinely predictive rather than merely descriptive? Perhaps the greatest challenge is upscaling, translating mechanisms that operate at the nanoscale or microscale into continuum-scale formulations that remain both physically sound and computationally tractable (33).

In this commentary, we present a perspective on crystal formation in porous media to guide decisions about whether and how to incorporate crystallization into numerical models. We organize this discussion around the physical processes that govern crystallization at each scale: nucleation pathways and their stochastic nature (Section 2), crystal growth and recrystallization kinetics and the role of confinement and crystallization pressure in deforming the host medium (Section 3), the intrinsic and evolving properties of the solid-fluid interface (Section 4), and the influence of fluid flow and mixing on where and when crystals form (Section 5). We then turn to how these mechanisms are, and are not, currently represented in numerical models (Section 6), and assess the emerging potential of machine learning and surrogate approaches to bridge molecular-scale mechanisms and field-scale predictions (Section 7). Throughout these sections, we address two guiding questions: when is it necessary to treat nucleation and growth explicitly, rather than rely on simplifying approximations, and how can nanoscale and microscale mechanisms be represented at the continuum scale without sacrificing predictive power?

2. NUCLEATION - THE BIRTH OF A CRYSTAL

No crystal can be grown without shaping a stable nucleus first. The necessity of nucleus formation for crystal growth is a fundamental constraint. However, in many cases, computational models of mineralization phenomena neglect the nucleation stage when predicting crystal growth rates in porous media. For example, it remains common to assign a hypothetical initial surface area to secondary phases that begin with zero mass, effectively bypassing the nucleation step entirely for

numerical modeling of carbonate mineral trapping during geological CO₂ storage (273, 60, 35, 173). This choice is pragmatic: existing modeling frameworks largely lack fast, low-cost nucleation schemes, and omitting nucleation reduces computational cost, allowing simulations of larger, more complex systems over longer timescales. Incorporating nucleation processes into these models remains challenging. However, their omission risks introducing systematic bias into predictions of crystal growth rates in porous media. As an illustrative example, we can take a flask containing a supersaturated solution of sodium acetate. At room temperature, sodium acetate is more thermodynamically stable in solid form than in solution, however the liquid can remain transparent for a long time because nucleation is kinetically inhibited. Once a tiny seed crystal is introduced, solid “hot ice” rapidly propagates throughout the volume, and the liquid transforms within seconds into a white, opaque crystalline mass. Likewise, a model that assumes an initial crystal surface area everywhere effectively presumes that the seed crystal is already present throughout the porous medium, and will predict immediate, pervasive growth even in regions where nucleation would never be triggered over any realistic timescale.

Therefore, the nucleation step introduces a temporal delay: crystals appear later and are less abundant at shorter timescales than models without nucleation would predict (181, 88, 85). This has direct consequences for the interpretation of laboratory experiments: when measurements stop before the induction time (the interval required for detectable nuclei to form), models that neglect nucleation will incorrectly infer that no crystals will ever appear. Such misreadings of “no crystals yet” as “no crystals ever” are common, and they highlight the need for a more careful treatment of nucleation mechanisms in both theory and experiment.

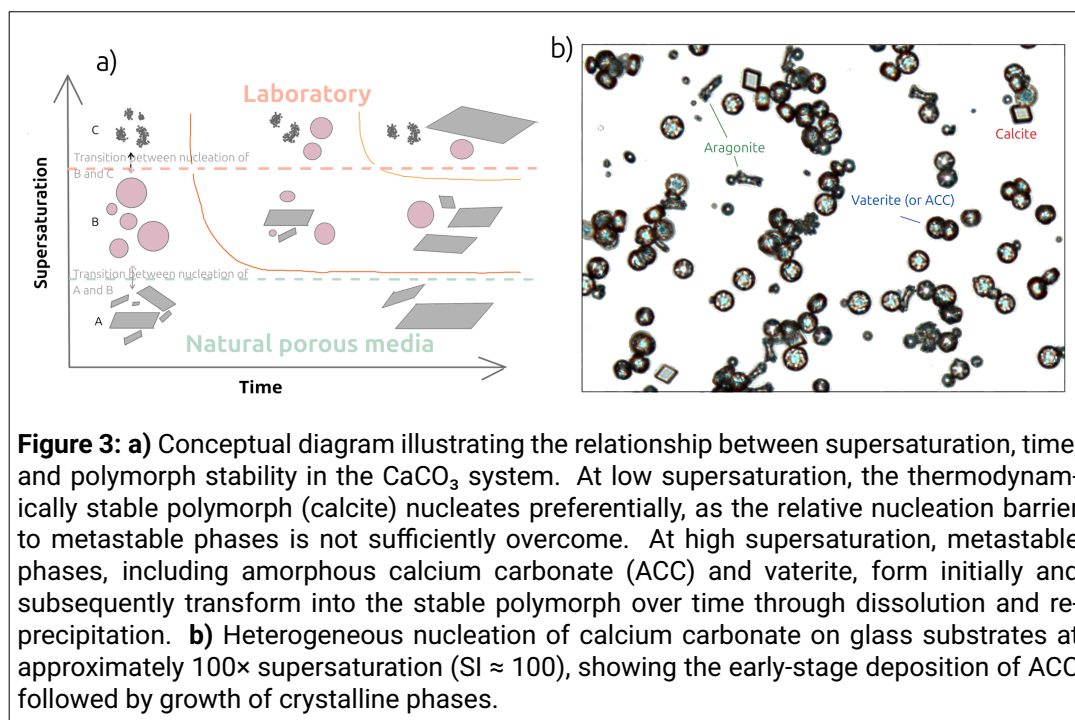
The following section explores three central aspects of crystal nucleation, particularly relevant in the context of porous media:

1. **Classical versus non-classical nucleation pathways** — the fundamental mechanisms by which stable nuclei form.
2. **Probabilistic versus deterministic models for heterogeneous nucleation** — how we describe and predict where and when nucleation occurs.
3. **Laboratory challenges in studying heterogeneous nucleation** — the practical difficulties of observing and quantifying nucleation experimentally.

2.1. Classical versus non-classical pathways for the formation of stable nuclei

The understanding of nucleation has advanced tremendously over the recent years (31). Classical nucleation theory (CNT) conceptualizes phase transitions as a single-step process, in which constituent building blocks (e.g., atoms or molecules) attach directly to an ordered crystal nucleus that has the same structure as the stable crystallite. In this framework, the nucleus continues to grow by structural unit attachment until supersaturation is depleted. In contrast, non-classical models (n-CNT) propose multi-step pathways for phase transitions, where crystallization is preceded by solution phase separation manifested in formation of metastable liquid-like droplets, amorphous intermediates, or thermodynamically stable pre-nucleation clusters (Fig. 2). In recent years, experimental studies have increasingly demonstrated that non-classical pathways govern the nucleation of a number of industrially important compounds, in particular CaCO₃ (200, 237, 71) and BaSO₄ (210, 266, 12).

Non-classical pathways lower the energy barrier required to form a nucleus. However, the hydrated amorphous phases that form through these pathways have lower thermodynamic stability than the crystalline end product, and therefore require higher supersaturation to reach critical nucleus size (200). This may create a supersaturation-dependent competition between the classical and non-classical pathways. When a solution is supersaturated with respect to the stable crystalline



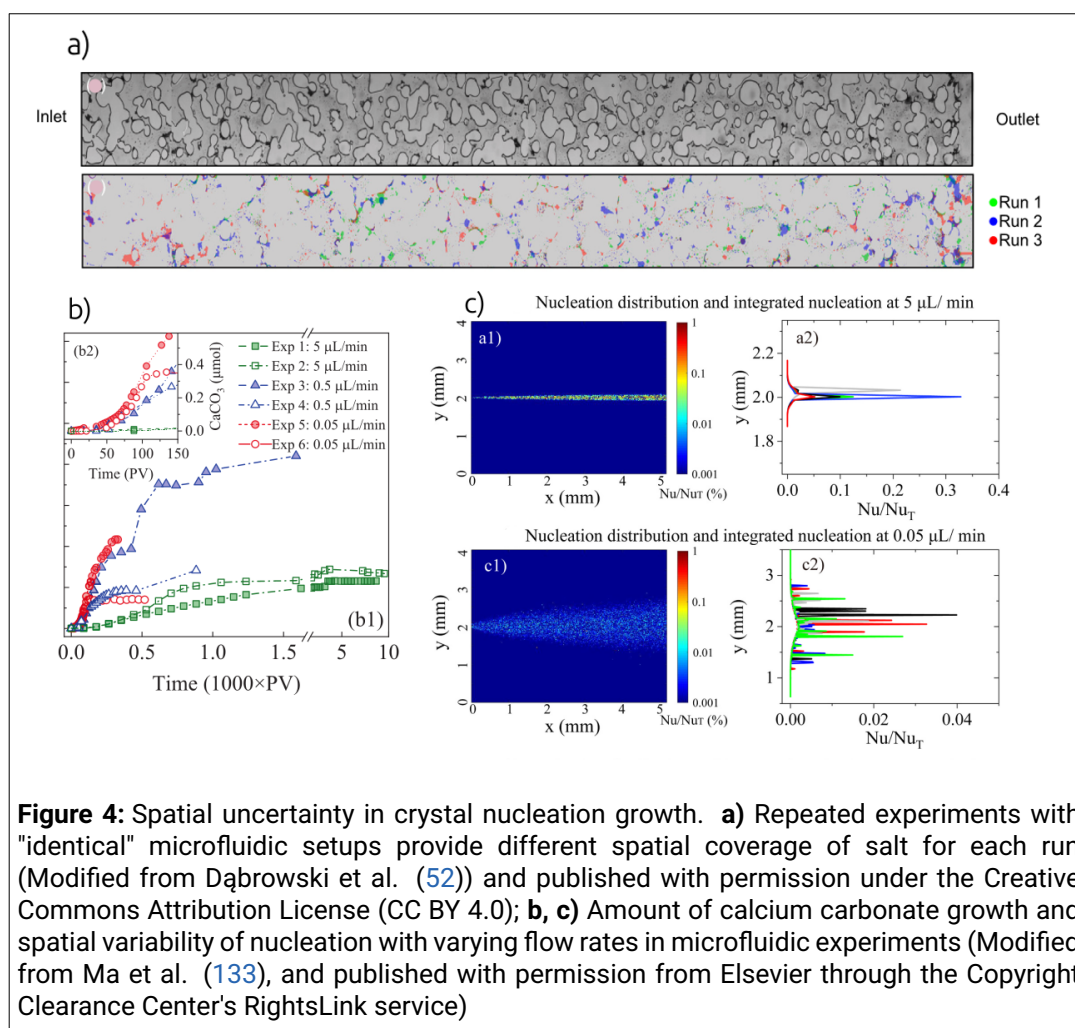
phase, but not yet supersaturated enough to stabilize hydrated amorphous phases or metastable polymorphs, only the classical pathway is thermodynamically accessible, so the stable crystalline phase nucleates directly, without a metastable intermediate (124). However, it may also be that all (or most) nuclei form through the non-classical pathway, and that polymorph selection mainly occurs after a stable nuclei has formed.

The distinction between CNT and n-CNT is not merely conceptual — understanding the nucleation pathway has direct practical consequences for predicting nucleation and the resulting mineral growth rates. Unlike CNT, where the energy barrier is well constrained by a single interfacial free energy, n-CNT lacks this constraint: the energy barrier scales with the interfacial free energy between the nucleus and water, and this energy varies substantially across crystalline and amorphous phases, with hydrated phases showing much lower interfacial free energy than crystalline polymorphs (126). If nucleation proceeds through a sequence of increasingly dehydrated, increasingly stable phases, no single interfacial free energy value can be used to estimate nucleation rates, thereby undermining a core simplifying assumption of classical models.

This ambiguity is reflected experimentally: for example, laboratory studies routinely observe multiple CaCO_3 polymorphs forming concurrently (133) (Fig. 3). This pattern is consistent with two distinct explanations: true co-nucleation of multiple phases at transitional supersaturations, or sequential regrowth and recrystallization of initially unstable phases into more stable ones (see Section 3). Distinguishing between these scenarios requires detailed monitoring of individual nuclei and crystals, which remains technically challenging in most experimental setups.

2.2. Probabilistic versus deterministic nucleation models – when do we need the probabilistic models?

To better account for the nucleation step in computational models, recent studies have focused on developing statistical descriptions of nucleation probabilities. Laboratory experiments have demonstrated the stochastic nature of heterogeneous nucleation. When repeated crystal growth experiments are performed on (macroscopically) identical substrates, the positions of the nuclei vary each time, and the effect that crystallization has on fluid flow also varies (133, 52). The stochastic nature of heterogeneous nucleation can be captured by probabilistic models, in which each



point in space is associated with a probability of forming a nucleus. Various probabilistic models exist, all estimating the probability of nucleation based on CNT (61, 247, 278, 161, 133). These probabilistic models have clear advantages compared to purely deterministic models, in which nucleation is assumed to occur simultaneously everywhere and at all macroscopically identical substrates at the same temperature and supersaturation. Probabilistic models, however, add additional computational cost. Building on this trade-off, probabilistic models become essential when fluid flow is spatially focused, such as in fracture networks or other geological heterogeneities that restrict flow to one or two dimensions, and when crystal growth rates dominate over nucleation with sufficient time for pore clogging to significantly alter fluid flow (33). In such systems, stochastic modeling reveals the uncertainty inherent in the relationship between porosity clogging and permeability, information a deterministic model cannot provide. Deciding whether a probabilistic approach should be used requires estimating the relative rates of nucleation and growth, as well as the relative time of interest (induction time vs. simulation time).

This time dependence is well illustrated by rapid, evaporation-driven salt precipitation, a regime in which nucleation dominates over growth. On short timescales, spatial distribution of salt appears stochastic (52), but as more of the pore space or flow channels become filled over longer periods, the distribution becomes increasingly uniform and deterministic. The same pattern holds for induction times: they are inherently probabilistic on short timescales but converge toward a mean or median value as system size and observation time increase (161, 163). Because this convergence depends on the nucleation rate, the time required for a system to transition from stochastic to deterministic behavior can, in principle, be estimated — with some systems remaining stochastic for millions of years (6), while others become effectively deterministic within days (13).

The demonstration of the stochastic nature of heterogeneous nucleation in laboratory experiments requires repeated experiments with “identical” laboratory models. Such experiments are rare, but two recent examples illustrate this behavior. The first is a study by Ma et al. (133) that combines a microfluidic fracture network (each fracture is represented by a 1D channel), and stochastic numerical modeling at the pore- and Darcy scale, to demonstrate how flow rate and fluid mixing affect the stochasticity of secondary crystallization. The paper clearly illustrates how more dispersed mixing and larger regions with lower supersaturations lead to greater variation in the spatial distribution of crystal growth and to an overall reduction in permeability (Fig. 4b, c). Dąbrowski et al. (52) similarly show in a two-dimensional (2D) microfluidic porous medium that evaporation-driven salt precipitation is stochastic and that salt aggregates form at different locations during repeated runs (Fig. 4a). If the boundary of this model had allowed capillary backflow and feeding of more brine into the model, it may have resulted in a complete “uniform” clogging, but this assumption remains to be confirmed.

2.3. Challenges in using laboratory experiments to study heterogeneous nucleation of minerals in natural systems

Geological observations of crystal assemblages, combined with theoretical frameworks such as CNT, provide direct constraints to the conditions under which crystals form in nature. Finely dispersed micron-sized crystals may suggest elevated supersaturations, while the giant crystals seen in Figure 1a, b indicate low supersaturations maintained over very long periods. Geological observations, however, can only inform us to a limited extent about the physical and chemical conditions that operated during nucleation, making it hard to extract fundamental knowledge of the nucleation process from geological data alone, as it starts at the scale of solid-solution interfaces (266). Laboratory experiments thus complement geological observations by providing well-controlled reactors in which the specific factors affecting nucleation rates can be isolated and studied, yielding more fundamental insight at spatiotemporal scales inaccessible from field observations.

However, studying heterogeneous and confined nucleation in a laboratory poses specific challenges related to the temporal and spatial constraints. The time during which experiments can be carried out in a laboratory differs enormously from the timescales of the processes in geological systems they aim to represent. For example, the time required for CO₂ mineralization in the subsurface can vary from a few years to hundreds of years (286, 239), something rarely accessible in laboratory experiments. Strict time constraints force researchers to use high temperatures or extreme supersaturations (>100x) to accelerate the kinetics of reactions. However, the nucleation mechanism and crystal growth dynamics under such conditions often differ from the processes occurring in natural geological systems, where the characteristics of porous matrices often evolve as reactions progress (266). Nucleation can dominate over growth, precipitates become highly dispersed, and the least stable polymorphs or amorphous hydrated phases preferentially form (179). If the aim is instead to study the stochasticity of nucleation, or the nucleation rate of a specific stable polymorph, supersaturation must be lowered, but this inevitably requires unrealistically long experimental times to observe nucleation and growth.

The length scale of the experimental system, or the spatial resolution of the detector used, limits what we can observe, and this length scale is tightly coupled to the achievable experimental time scale. Atomic force microscopy (AFM) offers near-perfect nanoscale resolution, making it well suited for capturing the earliest stages of heterogeneous nucleation and fine details of local growth patterns (256). However, its typical field of view is limited to a square area of only 10–1000 μm², which makes it challenging to gather meaningful statistics on nucleation or precipitation in the bulk of a sample. This spatial constraint also imposes a practical requirement on supersaturation: it must be high enough to ensure that at least one nucleus forms within the small field of view during the available experimental time.

Optical microscopy offers a much wider field of view, but its lower resolution means that nucleation events themselves are usually overlooked; observations are instead limited to later-stage crystal growth or counts of already-visible crystals. White-light interferometry occupies an intermediate position, combining a large field of view with excellent vertical resolution, but its lateral spatial resolution (200–300 nm) remains insufficient to resolve the geometry or shape of individual growing nuclei.

Because of these trade-offs, AFM or other atomistic or nanoscopic techniques and optical microscopy are best used together rather than in isolation: AFM can be used to probe local nanoscale variation and catch the earliest moments of nucleus formation and growth, and optical microscopy, ideally complemented by X-ray diffraction (XRD) or scanning electron microscopy (SEM), serves to provide a broader, bird's-eye view of the sample that enables proper statistical sampling across many nucleation events. This complementarity also has consequences for induction time measurements: since induction time is defined as the time required to detect a nucleus, its measured value depends on the resolution of the detection method itself. Atomic force microscopy therefore reports shorter induction times than optical microscopy, simply because it can detect nuclei at a much earlier and smaller stage of growth. In addition, recent instrumental advances now allow AFM observations to be coupled with chemical and mineralogical information by incorporating in-situ spectroscopic methods into AFM (276), enabling a more complete picture of nucleation and early-stage growth processes.

3. CRYSTAL GROWTH AND RECRYSTALLIZATION

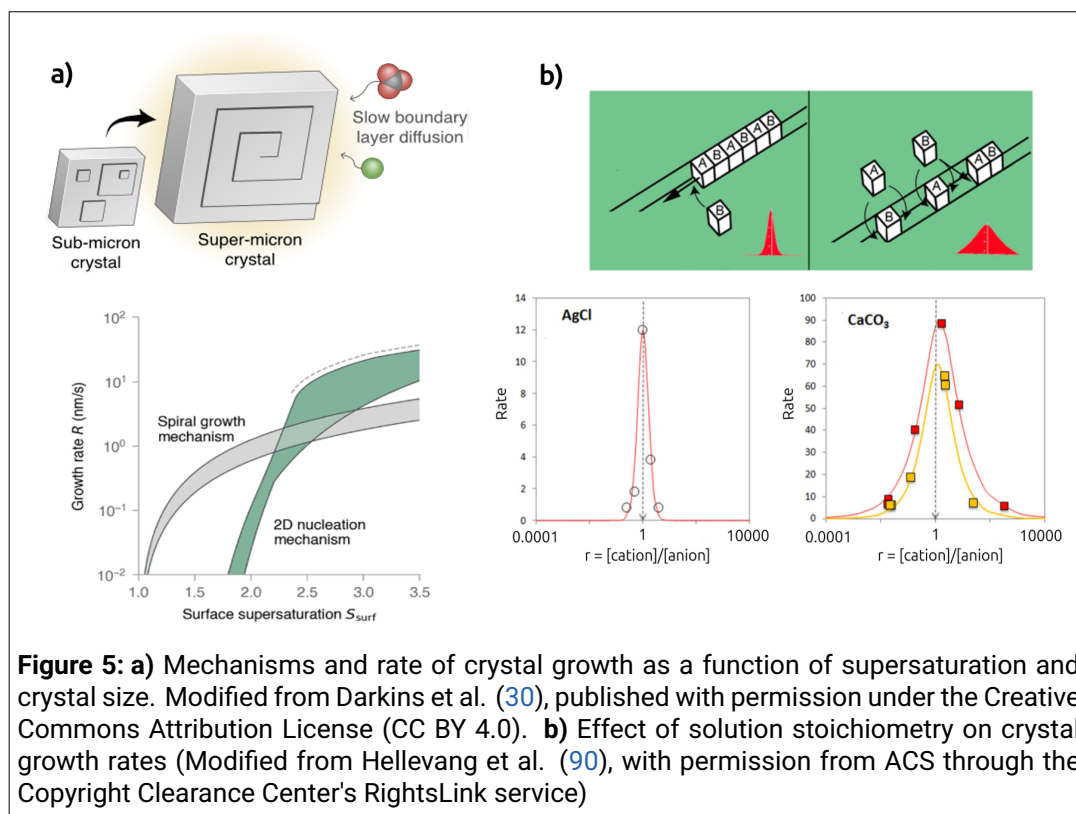
After the nucleus has reached its critical size, typically on the order of several tens of nanometers, it can continue to grow spontaneously as long as supersaturation persists. If the nucleus is a thermodynamically unstable polymorph or an amorphous phase, it may also undergo recrystallization to the more stable polymorph. A good example of such behavior is calcite, which is commonly first formed as the less stable vaterite, or even as amorphous calcium carbonate (207, 244).

In porous media, crystal growth is spatially restricted in confined volumes, affecting crystal shape compared to free-surface growth, and the rates of crystal growth are severely modified by complex transport phenomena and thus the amount of the material that is available for reaction (266). Crystal growth in porous media is affected by substrate properties, the pore size distribution, and spatially variable flow and transport that affects local geochemical conditions (33). This section summarizes what is known about rates of crystal growth and recrystallization and growth of crystals in confinement and the resulting force of crystallization.

3.1. Rates of crystal growth

The fundamental mechanisms of crystal growth have been investigated for more than a century, culminating in the seminal paper by Burton, Cabrera and Frank (BCF) in 1951 (17). While research prior to 1950 explained how “perfect” crystal surfaces at low temperature could not grow without elevated supersaturations and 2D surface nucleation, the BCF model demonstrated how crystals, even at infinitely low supersaturations, can grow by the advancement of steps at screw dislocations, leading to the so-called spiral growth mechanism. Spiral growth was first confirmed with optical microscopy in 1950–1951 (76, 261), and has later been demonstrated for a number of minerals, also at atomic and nanoscopic scales using AFM (75, 182, 183, 256).

The mathematics of crystal growth is now well established through the BCF-framework and growth by 2D-nucleation (17, 256, 30), providing relations between crystal growth rates, crystal size, supersaturation and temperature, and also explaining the effects of chemical additives that modify the growth along certain crystallographic directions (Fig. 5a). The shape of the growing crystal reflects

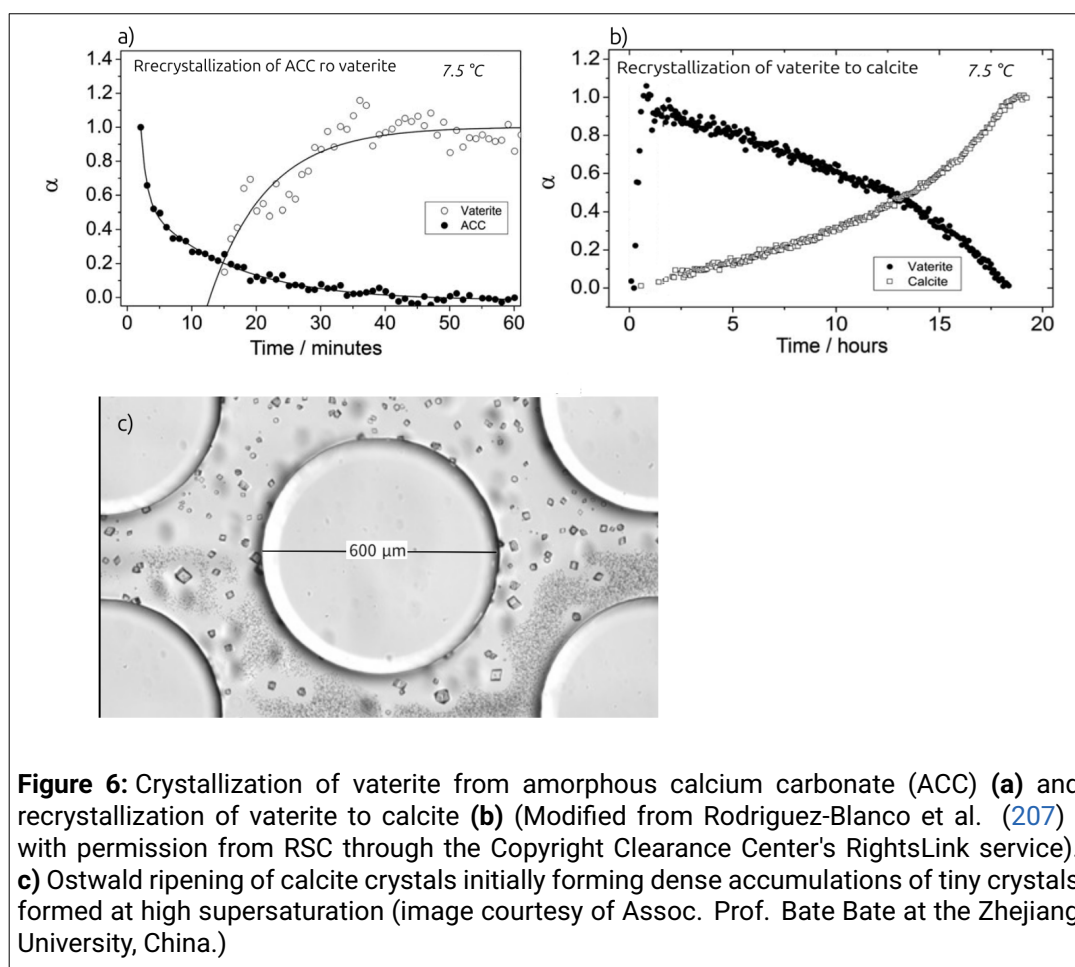


the thermodynamic stability of its different faces, as preferential growth occurs along those faces that maximize the reduction in free energy.

Contrary to heterogeneous nucleation which, at least at low supersaturation levels and low temperatures, should be treated with probabilistic models, crystal growth in macroscopic systems can in principal be estimated with deterministic models, provided sufficient experimental data exist to support them. This lack of supporting data is a central concern in this field. While several comprehensive databases exist for mineral dissolution rates (175, 92), no comparable databases exist for rates of crystal growth.

This asymmetry partly reflects a broader failure to recognize that growth and dissolution are not simply mirror-image processes governed by the same rate law. Transition State Theory (TST)-based models are commonly used to describe both dissolution and growth, and underpin existing rate databases (33), yet they cannot accurately predict growth rates (181, 88). Saldi et al. demonstrated this directly by comparing the dissolution (219) and growth (218) rates of magnesite (MgCO_3), showing that the growth rate constant is orders of magnitude smaller than predicted by the TST model, indicating that the mechanisms that govern the dissolution and growth of magnesite cannot be the same. The apparent reversibility of dissolution and growth, where both appear to follow the same rate constant, holds only for a short time immediately after the dissolution rate experiment is switched to a supersaturated condition. As the experiment proceeds, consumption of high-reactive sites during growth, and generation of the same high reactive sites during dissolution, drives two rate constants apart by the orders of magnitude, exactly as was found by Saldi et al. (219, 218).

Another phenomena that has been largely overlooked in the porous-media community is the strong effect solution stoichiometry has on the growth rate of ionic salts (barium sulfate, calcium carbonate, silver chloride, etc.). Because of the ordered structures of these minerals, incorporation of cations and anions must occur in an ordered way, and this leads to a statistical dependency of the growth rate on the ratio of the cations and anions (284, 271, 90, 87). Growth rates of non-stoichiometric solutions may be many orders of magnitude lower than those "ideal" solutions with



a near 1:1 ratio between the cation and anion (90) (Fig. 5b). Taking into account the stoichiometry effect may be especially important when dealing with carbonate growth at acidic conditions, which is usually the case for CO₂ storage in clastic reservoirs or before pH-buffering in basaltic reservoirs. In this case, the very low concentrations of carbonate (CO₃²⁻) compared to the cation may slow down the entire carbonatization process by orders of magnitude (89), or even arrest the whole process if the dissolving silicates approach equilibrium. The effect of solution stoichiometry can be added on the top of other kinetic models by an empirical relation that has been shown to provide good estimates for various ionic salts (90).

3.2. Evolution of crystals with time – Recrystallization

Evolution of minerals with time, most commonly driven by fluid-induced mineral re-equilibration, exerts a key control on how fluid-rock interactions modify the rock reactivity, pore structure, connectivity, and transport properties. These changes can involve replacement crystallization via coupled dissolution and precipitation, recrystallization of metastable phases, as well as coarsening and recrystallization by Ostwald ripening.

Whenever percolating fluids encounter minerals that are thermodynamically unstable with respect to the fluid composition, the mineral phase assemblage undergo changes toward a new equilibrium state. This evolution often proceeds via replacement crystallization through interface-coupled dissolution–precipitation (ICDP) reactions (212, 205), in which the original phase dissolves at the mineral-fluid interface while a more stable phase precipitates from the locally modified solution. Interface-coupled dissolution–precipitation mechanisms are widely observed in weathering, diagenetic, hydrothermal, and metamorphic environments, as well as in geological fluid storage operations (e.g. 194, 72, 211, 274, 63, 184, 70, 185, 242), where they often lead to the formation

of entirely new mineral assemblages. The timescales of ICDP reactions are primarily controlled by interfacial kinetics at the unstable mineral surface. Because dissolution and precipitation are closely linked at the advancing interface, these reactions are often strongly spatially coupled and controlled by chemical gradients that develop around the dissolving surface. In addition, replacement crystallization may proceed pseudomorphically, whereby one unstable mineral is replaced by a different, more stable phase that preserves the external shape of the original crystal. As such, the replacement crystallization can substantially alter the mechanical properties of porous media through associated changes in porosity and in the available reactive surface area (195). Because of that, there is a need to incorporate this process into reactive transport models, as demonstrated in recent studies (34, 265).

A related but mechanistically distinct process is the sequential recrystallization of polymorphs, in which particles of the same chemical composition but with different thermodynamic stabilities transform into progressively more stable forms. Unlike mineral replacement, this process does not involve a change in bulk chemistry between fluid and precipitating phases; however, as in replacement reactions, each step requires nucleation and growth of the new, more stable mineral phase (168, 180). One central question is the kinetic stability of these metastable polymorphs and amorphous phases. How long do they persist after nucleation and initial growth? This depends critically on the nucleation and growth rates of the more stable compounds, which in turn are controlled by temperature, supersaturation, and interfacial properties. Some minerals, such as magnesite, cannot precipitate directly from solution at low temperatures because the rate of anhydrous carbonate nucleation is too sluggish. Instead metastable hydrous carbonates tend to form first. These transient intermediates subsequently convert to more thermodynamically stable mineral assemblages. Understanding their transformation pathways is important in many low-temperature geological settings, not only for defining mineral stability fields, but also for assessing long-term changes in porosity and permeability. For example, formation of magnesian carbonates during CO_2 storage in basalt depends on the initial formation and later recrystallization of metastable carbonate phases (198).

Kinetic contrasts between Ca- and Mg- carbonates further illustrate the wide range of timescales involved. While dehydration of ACC and the formation of vaterite, and the recrystallization of vaterite to calcite may take minutes to hours at temperatures as low as 7.5°C (Fig. 6) (207), the step-wise recrystallization of hydrous magnesian carbonates (nesquehonite ($\text{MgCO}_3 \cdot 3\text{H}_2\text{O}$) $\rightarrow$ dypingite ($\text{Mg}_5(\text{CO}_3)_4(\text{OH})_2 \cdot 5\text{H}_2\text{O}$) $\rightarrow$ hydromagnesite ($\text{Mg}_5(\text{CO}_3)_4(\text{OH})_2 \cdot 4\text{H}_2\text{O}$) $\rightarrow$ magnesite) may take orders of magnitude longer (285, 94, 83, 187, 189). The final transformation from hydromagnesite to magnesite is particularly sluggish. Zhang et al. (285) estimated that the half-life of hydromagnesite during recrystallization to magnesite is on the order of 4.7 to 73 years at 25°C , but recrystallization first requires an induction time of 18 to 200 years, associated with magnesite nucleation (285). Together, these examples show that the kinetic stability of metastable phases can span from minutes to hundreds of years and must be considered when evaluating recrystallization processes and their impact on porous media.

Ostwald ripening refers to crystal coarsening and is mechanistically distinct from both replacement and polymorphic recrystallization; it involves larger particles of the same phase growing at the expense of smaller ones, driven primarily by size-dependent solubility (The Gibbs-Thomson effect), and thus does not require nucleation of a new phase or associated induction time. In many systems, Ostwald ripening proceeds more rapidly than the recrystallization chains described above, with rates controlled either by solute diffusion (for rapidly growing minerals) or by the growth kinetics at the surfaces of larger crystals. In microfluidic experiments conducted at high CaCO_3 supersaturation (exact supersaturation not known), Zhou et al. (290) initially observed dense CaCO_3 precipitation, while “shadows” surrounding the larger calcite crystals that were consum-

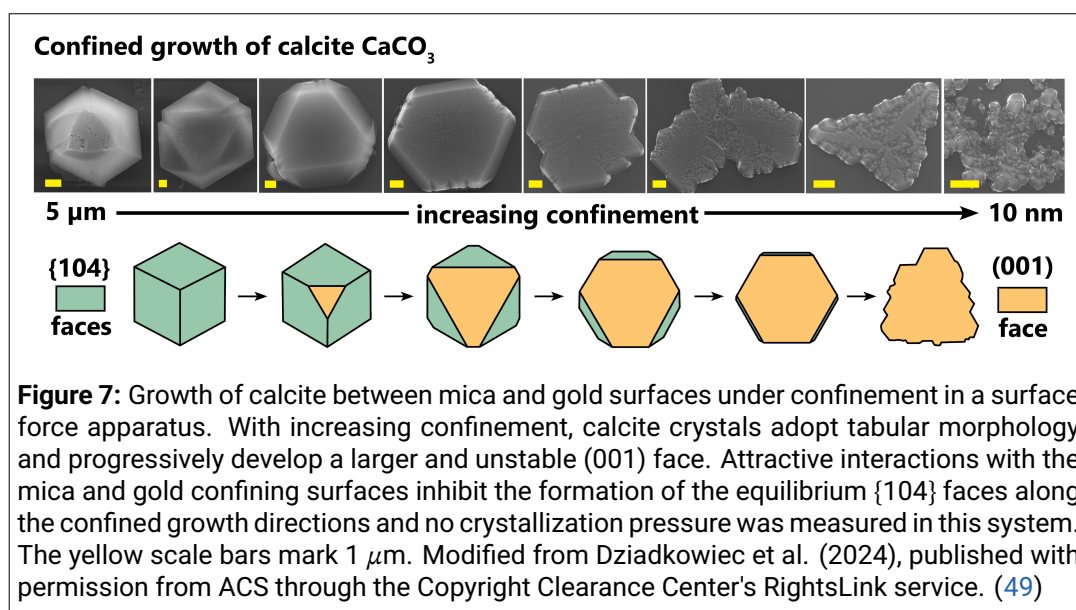
ing the small crystallites were clearly seen after 1-3 days (**Fig. 6c**). This example illustrates how ripening and competitive growth can reorganize pore-scale flow paths. Ostwald ripening slows and may eventually cease as crystals coarsen and curvature-driven solubility differences diminish, such that the solubility of individual crystals approaches the bulk solubility (260).

3.3. Crystal growth under confinement and the force of crystallization

In natural settings, crystal nucleation and growth rarely occur homogeneously in bulk solutions in the absence of surfaces. Instead, crystallization commonly proceeds in restricted volumes, under spatial confinement imposed by porous matrices in rocks, building stones, materials, soils, or within biological compartments, as in biomineralization. Confinement in a porous medium modifies crystallization outcomes relative to bulk-solution conditions, and crystal growth in pores can significantly alter the host medium by changing its mechanical, petrophysical, reservoir, and transport properties (35, 164, 1). The effects of confinement on nucleation and crystallization are numerous and have been summarized in several comprehensive review articles on the subject (140, 62, 101). In short, crystallization in confinement occurs in the presence of abundant solid surfaces, which influences crystal morphology and orientation (as exemplified in **Fig. 7**), kinetic and thermodynamic stability of crystalline polymorphs and amorphous phases, nucleation rates, and mass transport. One of the key questions is how high supersaturation is achieved and maintained inside pores (64). Recent advances in experimental and computational methods, particularly high-resolution 4D synchrotron-based imaging (155, 24), have substantially improved our understanding of how confined crystallization affects the properties of host porous media. These advances help address key questions about preferred crystallization sites within the pore space, the evolution of porosity and permeability, the capacity of growing crystals to deform a porous matrix, and the often difficult-to-predict rates of crystallization in porous media. Here, we focus on how nanoscale confinement and interfacial phenomena control crystallization pressure and, consequently, the deformation of porous media.

One particularly important aspect of crystal growth under confinement is the ability of certain crystals to exert mechanical stress on the confining pore wall that is in direct contact with the growing crystal face. This phenomenon, known as the force of crystallization or crystallization pressure, was first identified in experiments showing that a crystal could lift its own weight or the weight placed on top of it while growing in a supersaturated solution (121, 7, 8, 252). Since then, sustained interest in crystallization pressure has been driven by the fact that the mechanical stress locally exerted by a growing crystal can induce damage and deformation in the host porous medium, often manifested as brittle fracturing of its mineral constituents. This effect has been most extensively documented in salt-induced damage to cultural heritage objects, where subflorescence precipitation of salt crystals is driven by fluctuations in environmental conditions (41). Considering that the tensile strength of most common building stones is typically below 20 MPa (233, 241), this provides a rough indication of the potential magnitude of crystallization pressure effects.

It is extremely difficult to precisely quantify the magnitude of crystallization pressure and to understand its governing processes across different systems. Repulsive crystallization pressures measured in laboratory experiments range from a few MPa to several hundred MPa (56, 42, 153, 115, 230, 125, 48, 51, 259, 206, 225, 120, 82). Similarly, pressures inferred for crystallization reactions in geological systems can induce rock deformation at values of only a few MPa (74), but may also reach hundreds of MPa and approach GPa levels (186, 106), far exceeding the typical tensile and even compressive strength of rocks (103). The thermodynamic expression for crystallization pressure, ΔP_C , sets an upper bound on its magnitude and is proportional to solution supersaturation, Ω , with respect to the growing crystal, and thus to the change in chemical potential, $\Delta\mu$, associated with the transition of the crystallizing species from the liquid to the solid state:



$\Delta P_C = \Omega k T V_m^{-1} = \Delta \mu V_m^{-1}$, where V_m is the molar volume of the crystal, and kT is the Boltzmann constant times temperature (27, 66, 41, 125). This equation links the force per unit area exerted by a crystal to the free energy stored in a supersaturated solution. More detailed expressions for the thermodynamic limit of crystallization pressure, accounting for the activities of the crystallizing ionic species and crystal-solution interfacial energies, as well as formulations incorporating the geometric and material properties of the porous medium, are provided in (249, 56, 223, 224, 65). Crystallization pressure observed in experimental and natural systems span over three orders of magnitude and frequently remains below its thermodynamic limit, as demonstrated by laboratory studies (125, 42). These two observations have motivated further research to better define the observable limits of crystallization pressure and have highlighted the importance of nanoscale controls on this phenomenon.

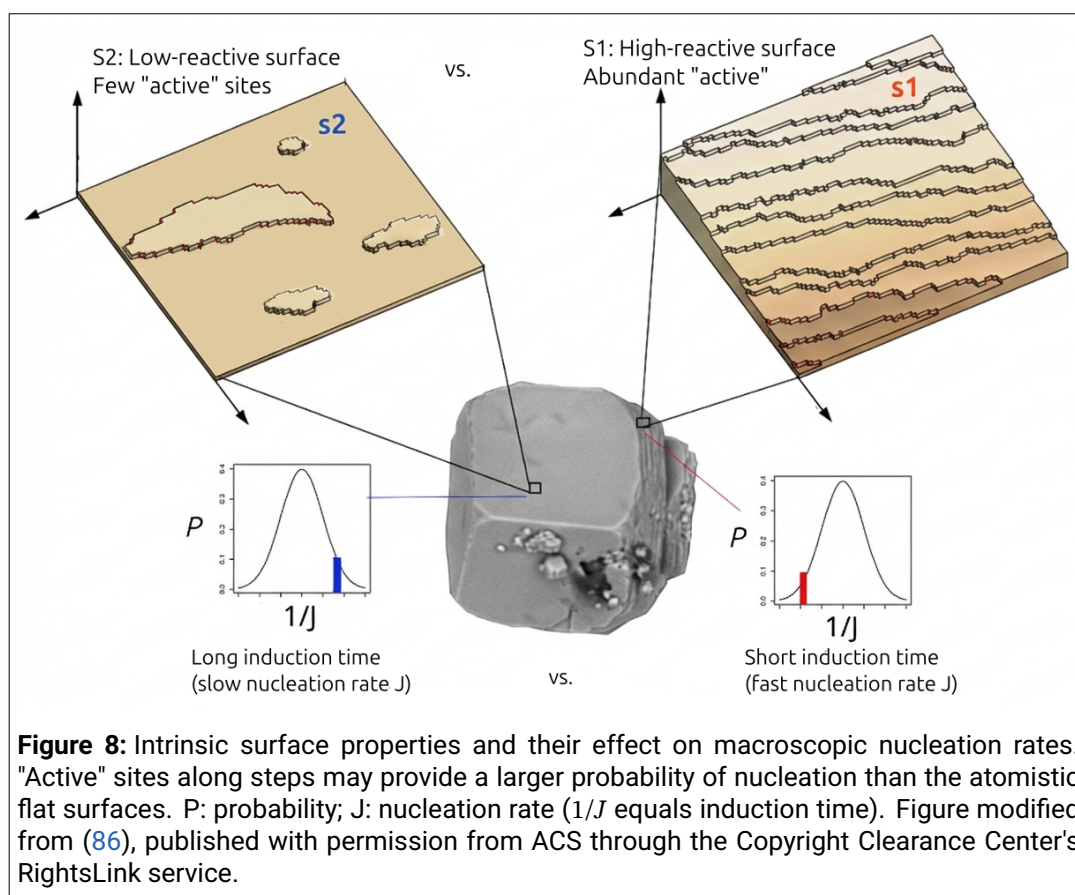
At the nanoscale, growth of a crystal face against a confining pore wall requires a continuous supply of growth units to the crystal-solid contact. This is facilitated by a nm-thick solution film that separates the loaded crystal face from the confining surface and transmits the stress between them, allowing the crystal to exert a local outward force on the pore wall. Although this concept was recognized in early works (252, 27, 66, 223, 57), only recent advances in experimental and computational techniques have provided a more detailed understanding of the critical role of such films. The thickness and stability of a confined water film, which are characterized by disjoining pressure, are thought to directly control the effective magnitude of the crystallization pressure. Disjoining pressure reflects the net repulsive or attractive surface forces acting across the confined liquid film and is defined as the difference between the pressure in the confined water film and the hydrostatic pressure in the surrounding bulk liquid. Positive disjoining pressure usually indicates that repulsive interactions dominate, resisting film thinning and making it energetically costly to displace water from the gap. Negative disjoining pressure indicates that attractive interactions prevail, favoring film thinning, possible dewetting, and migration of water into the bulk (20, 267, 213, 204, 50). Equivalently, in terms of wettability and interfacial energy, if the sum of the solid-liquid interfacial energies of the two surfaces exceeds the solid-solid interfacial energy, the water film separating the solids is energetically unfavorable, and the two solid surfaces tend make direct contact. In this case, repulsive forces across the water film can no longer balance the applied load, the unstable water film collapses, and no further crystallization pressure can be transmitted between the growing crystal and the confining wall (97). This situation can occur for hydrophobic pore walls, where little or no crystallization pressure develops (42, 259). In contrast, it is often very difficult to completely remove the water film from a contact between two hydrophilic mineral sur-

faces. Computational studies indicate that such films persist at high applied pressures and fully collapse only above hundreds of MPa (15, 81, 78).

Recent experimental observations indicate that system-specific behavior of crystallization pressure can often be explained by the complex dependence of disjoining pressure on surface separation, local solution composition, and physicochemical properties of the solid surfaces. The magnitude of the disjoining pressure varies with the thickness of the confined water (electrolyte) film and, for film thicknesses below a few nanometers, can exhibit a sequence of local repulsive maxima and attractive minima, reflecting the oscillatory nature of surface forces between solids in aqueous solutions (97, 45, 15, 281, 139). Li et al. (125) proposed that a rough crystal face growing under confinement at constant bulk supersaturation can locally experience such an attractive minimum in surface forces (i.e., a local negative disjoining pressure), leading to adhesive contact with the confining wall. This contact arrests further growth at relatively low confining pressures, even though a nm-thick solution film remains at the interface. Desarnaud et al. (42, 41) showed that a salt solution film stabilized by repulsive surface forces can be maintained between growing alkali salt crystals and a confining glass surface, even at high supersaturation during solution evaporation, and estimated its thickness to be approximately 1.5 nm. The authors concluded that crystallization ceases once the crystallization pressure exceeds the repulsive disjoining pressure, causing the film to collapse locally and the crystal to make direct contact with the confining wall. Naillon et al. (153) emphasized that the magnitude of crystallization pressure is transient and highly sensitive to the local supersaturation at the interface between the confined solution and the growing crystal. Tuluk et al. (259) further extended this framework by demonstrating that the generated crystallization pressure varies when different crystallographic faces of an alum salt crystal grow under confinement, highlighting the role of interfacial energy in controlling the disjoining pressure. Consequently, the magnitude of disjoining pressure is highly sensitive to local and evolving composition of the confined solution (238, 169), to the surface chemistry of the crystal and pore walls, to the applied load, and to mass transport within the confined water film. Mass transport in such thin films is often kinetically restricted, leading to experimentally observed rim topographies in confined crystals (259, 42, 125, 214, 113) and makes the true contact area of a loaded crystal face difficult to assess, which can result in underestimation of crystallization pressure.

At a macroscopic scale, crystallization pressure often manifests as deformation of porous media driven by local pressure gradients around growing crystals. These gradients generate tensile stress in the solid host, ultimately causing fracturing once the material's tensile strength is exceeded (156, 40). This phenomenon is observed across many different systems, particularly in salt-induced weathering (41, 208) and recrystallization-driven decay of concrete (117, 123, 202), and it has been proposed as a key mechanism in reaction-induced fracturing and hydration reactions (215, 289, 106, 185, 231), displacive growth (262), and vein formation (74) in rocks. Recently, crystallization pressure has become especially important in geotechnical engineering in the context of large-scale mineralization of CO₂ in porous rock reservoirs (28, 58, 136, 142, 159, 172). Nooraiepour et al. (164) reported major deterioration of sandstone samples undergoing CO₂-induced salt precipitation: as a CO₂ stream invades a brine-saturated porous matrix, it creates a dry-out zone and promotes evaporation of brine trapped in the pore space, resulting in intense salt precipitation and a concomitant build-up of crystallization pressure.

So far, the relationship between crystallization pressure and disjoining pressure has been treated mostly at a qualitative level. It is generally assumed that crystallization pressure can develop whenever the disjoining pressure is positive and the surface forces between the growing crystal and the confining wall are repulsive. However, a more robust quantitative link between nanoscale measurements of surface separation-dependent surface forces (i.e. the repulsive and attractive components of disjoining pressure) and crystallization pressure is needed to better



understand and quantify the extent of resulting macroscale deformation processes discussed above. Establishing such a connection would provide more reliable constraints on the magnitude of crystallization pressure effects and clarify its coupling to associated fluid-induced deformation mechanisms, including those driven by variations in hydrostatic pressure related to crystallization in pores and solid volume-changing reactions.

4. THE ROLE OF THE INTERFACE FOR CRYSTAL NUCLEATION AND GROWTH

Solid-liquid, solid-vapor and liquid-vapor interfaces give rise to condensation reactions, heterogeneous nucleation of minerals and crystal growth. Without the interface, neither crystal nucleation under low temperature and supersaturation nor crystal dissolution and growth would be possible. How do nanoscopic surface features, such as steps, kinks and pits, influence interfacial reactions, and how well can current macroscopic models account for these tiny features that are intrinsic to the surface? How can we characterize the supersaturation that develops at the brine-vapor interface during evaporation, and how does it affect the diverse crystal morphologies that form at this interface? Growth rates are proportional to the size of a solid-liquid interface, but how well can we quantify the reactive surface area, and how meaningful is the term "reactive surface area" itself? Here, we provide our perspective on these questions.

4.1. The intrinsic properties of the solid surface and how they affect crystal nucleation and growth

Crystal surfaces are structurally and chemically heterogeneous, even at the atomic scale. This heterogeneity leads to local differences in the chemical reactivity of a crystal surface or nucleation substrate that arise solely from the properties of solid material itself, even when its overall chemical composition and external conditions (e.g., temperature, solution chemistry, pH) are held

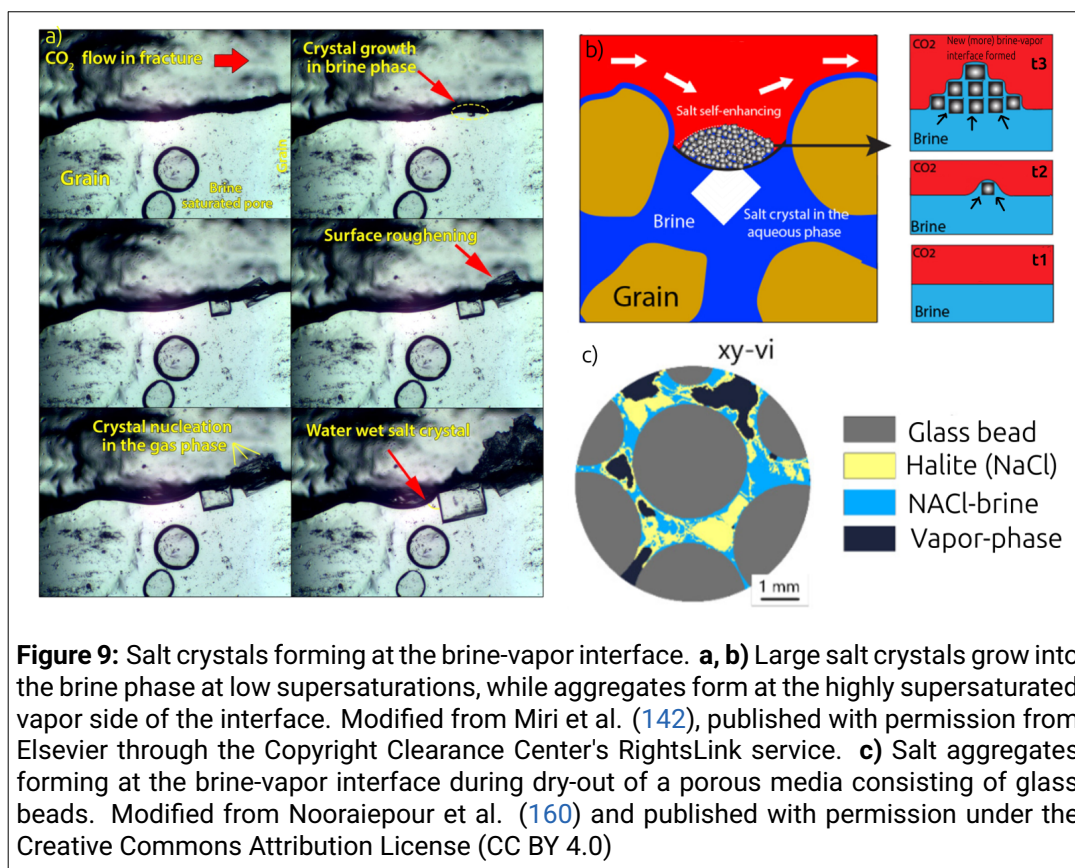
identical. The terms “reactive surface area” and “active site” are widely used to explain reactivity, but what actually defines a certain surface site as active (or reactive) and why do different macroscopic surfaces exhibit distinct degrees of reactivity?

The concept of active surface sites stems from relative differences in reactivity, where some sites provide substantially faster reaction rates than others, such that it is useful to divide them into “active” and “passive” (although they are all reactive!). The same principle applies for crystal dissolution and growth. The reactive surface area is defined as the fraction of the total surface that dominantly contributes to macroscopic reactivity (**Fig. 8**).

Nucleation of ice crystals on feldspar surfaces offers a well-studied example of active sites for heterogeneous nucleation. Mineral dust particles originating from wind-blown soils are recognized as efficient ice-nucleating particles in the atmosphere and are thought to play an important role in the formation of mixed-phase clouds containing both liquid and frozen water. Feldspars are proposed to be the most efficient ice nucleators among the mineral components commonly present in atmospheric mineral dust (79, 112). Harrison et al. (79) concluded that feldspars possess a range of active site types with varying stability and activity, and that different feldspar samples show a significant variation in their ability to nucleate ice crystals. Kisilev et al. (112) later demonstrated that the basal plane of hexagonal ice crystals exhibits a particularly good lattice match to the high energy (100) surface of K-feldspar, which is exposed at defects of the most stable (001) and (010) surfaces. The large variation in nucleation rates among K-feldspar samples can thus be attributed to differences in the proportion of (100) surfaces exposed at surface defects such as steps, kinks, and pits, and it highlights the important role of interfacial energies and possible epitaxy in heterogeneous nucleation.

In a new perspective, Hellevang et al. (86) suggest a new multi-site, multi-polymorph probabilistic nucleation model taking into account the active sites. The new model replaces the classical use of a single averaged interfacial free energy with an explicit sum over site types, substrates, and polymorphs, each characterized by its own nucleation probability and site density, thus grounding macroscopic nucleation-rate predictions in physically meaningful, measurable surface properties rather than abstract probability distributions. Conceptually similar to multi-site sorption models, it assumes that macroscopic variability in heterogeneous nucleation arises mainly from differences in the density and spatial distribution of reactive surface features (steps, kinks, pits, etc.) and explicitly accounts for competition between multiple amorphous and crystalline phases across all such sites, so that the total number of nuclei is obtained by summing contributions from all phase-site-substrate combinations. Once the distributions of site types and their polymorph-selective nucleation probabilities are characterized, macroscopic nucleation rates can in principle be derived deterministically, and the observed “stochastic” spread in rates is reinterpreted as a consequence of real, resolvable surface heterogeneity rather than intrinsic randomness. The main challenge is the large parameter space for many polymorph-site-substrate triplets—which makes direct calibration difficult, but this may become tractable through carefully designed experiments, high-throughput imaging, and artificial intelligence (AI) and machine learning (ML) tools that can extract nucleation statistics, constrain parameters efficiently, and accelerate reactive-transport simulations, thereby enabling practical application of the multi-site framework in realistic, multiscale geological systems.

While differences in heterogeneous nucleation rates can be connected to specific surface features here termed “active sites” (86), extending this concept to macroscopic crystal growth by defining an effective reactive surface area is considerably more challenging. At low supersaturations, growth is mainly constrained by the advancement of growth spirals at dislocations, and these constitute permanent features that can, in principle, be quantified. At high supersaturations, 2D nucleation dominates, and this could likewise be linked to certain intrinsic surface properties, or



be treated as essentially random, reflecting stochastic nucleation on a surface. However, as Zhou and Fischer (291) showed, reactive surface areas may be highly dynamic and exhibit both temporal and spatial variations for the same material because of continuous surface restructuring and changes in the population of active sites. Moreover, for rapidly growing crystals at high temperature and/or high supersaturations, growth may be transport (diffusion) controlled, leading to the formation of nucleation-dominated aggregates, or dendritic crystals with complex solid-solution interfaces that are difficult to quantify. From a modeling standpoint, it is, however, necessary to normalize experimental rates to mass or surface area. Established sorption techniques based on Brunauer-Emmett-Teller theory (BET) (16) and novel methods such as the use of Positron emission tomography (PET) for sorption of radioactive tracers (229) can, to some extent, provide useful information on the density of specific reactive surface sites.

4.2. Salt formation at the brine-vapor interface

Salt precipitation in porous media is a complex phenomenon in which nucleation and growth processes are strongly influenced and constrained by the structure and properties of the porous matrix. Injection of dry CO₂ during geological storage is known to cause evaporation of the formation water, and potential precipitation of salt in the near-well region (191, 67, 141). This may impair permeability and much research has been done to predict the different factors that impact salt formation (192, 111, 171, 142, 141, 232, 172, 160, 99, 282). Still, little is known about how the salt growth is initiated at the brine-vapor interface (except that it is nucleating there), and how the salt precipitation itself affects the dynamic development of the brine-vapor interface and rates of evaporation.

Laboratory experiments distinguish two types of crystals that may grow at the brine-vapor interface: porous aggregates of sub-micron to micron-sized crystals, which dominate, and larger mm-sized crystals, which occur less frequently (Fig. 9). Salt crystals composed of aggregates appear to nucleate directly at the interface, where removal of water molecules from a saturated

solution may produce high supersaturations (160). Once a first crystallite has formed, new crystals nucleate in the same location, forming an aggregate. The high interfacial energy of the salt pulls in additional water and creates more interfacial area for evaporation and new salt growth (Fig. 9b). As the evaporation-salt growth process proceeds, the salt crystal and the increasing brine-vapor interfaces move into the vapor phase where salt precipitation may clog the flow pathway (142). The large isolated crystals grow in the opposite direction, away from the brine-vapor interface, and their growth is constrained by comparatively low supersaturation in this region (142). The large crystals are limited in volume compared to the aggregates, and are not expected to have a significant impact on CO₂ transport.

The salt aggregates affect brine transport to the evaporation front by enhancing capillarity, thereby drawing in more water, and increasing the brine-vapor interfacial area. Both effects lead to accelerated evaporation and a self-enhanced salt growth mechanism (142, 160). There are indications that solution trapped within the salt aggregates may also be supersaturated and that the salt aggregates develop a denser structure with time (160). The effect of this on capillarity and enhanced evaporation is not yet known, but it is possible that the flow of brine to the evaporation interface is cut off and the evaporation continues elsewhere along the vapor channel. This process may explain the formation of multiple salt aggregates in experiments by Miri et al. (142). Furthermore, we still do not know how pore-size distribution and interfaces between lithologies with very large capillarity contrasts will affect these salt growth patterns. To our knowledge, all experiments to date have been conducted with fairly coarse materials.

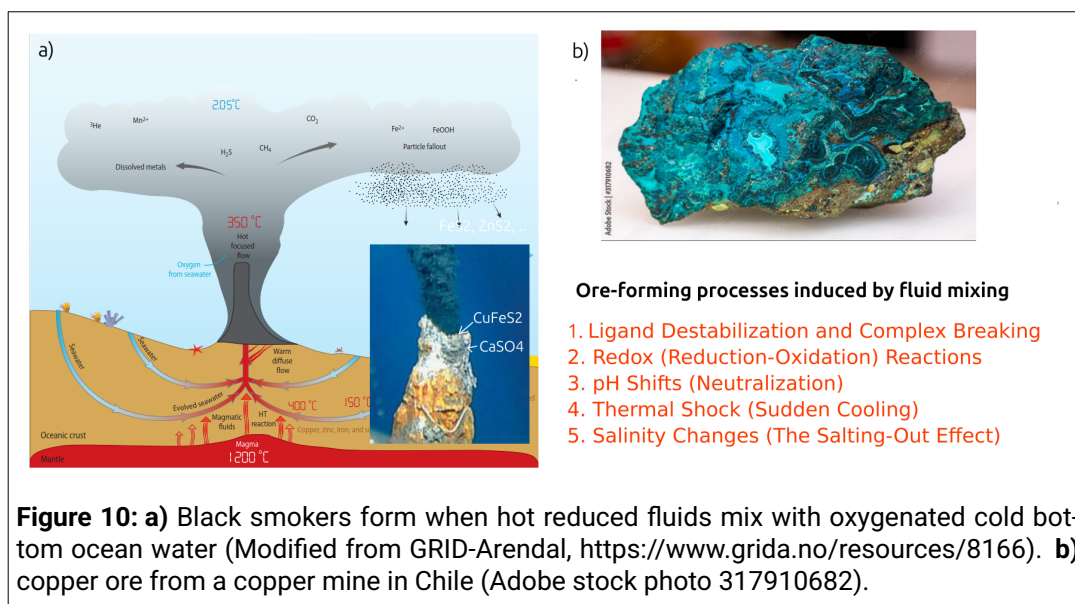
5. ROLE OF FLUID FLOW AND FLUID MIXING ON CRYSTAL NUCLEATION AND GROWTH

Fluid flow and mixing may lead to sharp solute concentration gradients, inducing crystal nucleation and growth, often directly at the mixing front. Examples include natural systems such as hydrothermal circulation at mid-ocean ridges, which gives rise to white and black smokers, and the formation of hydrothermal ore deposits. In addition, engineering solutions, such as geological storage of acidic CO₂-laden waters within alkaline pore waters in basalt, create important subsurface environments for fluid mixing and crystal growth. Fluid flow in porous media and the associated processes of transport and mixing of solutes constitute a complex topic, especially during multi-phase flow (254, 283, 36, 122, 188, 279, 129, 33). In this work, fluid dynamics and solute mixing are not the primary focus, but instead we concentrate on the role of mixing in crystal nucleation and growth, and on the feedback from crystal growth on mixing, which sometimes leads to re-dissolution.

5.1. Examples from nature - "Black smokers" and hydrothermal ore deposits

Examples of crystallization in hydrothermal systems illustrate how steep chemical and thermal gradients, fluid circulation, and fluid-rock interaction combine to drive rapid mineral precipitation and metal concentration in porous hosts.

"Black smokers" form at mid-ocean ridges where divergent plate boundaries and magmatic heat give rise to large-scale convection cells bringing seawater down to depths at which it becomes heated to hundreds of degrees and interacts with mafic and ultramafic rocks before circulating back to the surface where the dissolved mineral load is released (255) (Fig. 10). The hydrothermal circulation acts as a major sink for magnesium and sulfate, removing about 10-40% of the total riverine input of magnesium (147), and is a major source of elements such as iron, lithium, and manganese to the world deep oceans (29). When hot acidic reduced fluids are emitted in focused flow at the seafloor, they mix with cold alkaline oxygenated waters and sharp redox and temperature gradients develop. This leads to very high supersaturations in the water column and rapid nucleation of pyrite and marcasite (FeS₂ polymorphs), which results in the black color of the mix-



ing plume. The hydrothermal plume may extend hundreds of meters up from the seafloor until reaching neutral buoyancy, and fine crystallites may be carried far by ocean currents before sedimenting at the seafloor. The chimney itself forms a porous medium with a sequence of mineral zones controlled by the thermal gradient from the hot interior to the cold exterior. The inner part consists of CuFe-sulfides, the cooler middle part of Zn-sulfides, and the outermost zone consists of anhydrite (CaSO_4), with amorphous silica cementing the outer part of the structures and providing mechanical strength (83). It is of interest to understand the formation of these deposits because the rich metal content of the black-smoker systems makes them primary targets for seafloor metal mining.

Hydrothermal ore deposits are the primary source of most of the world's metals. They provide nearly 100% of global lead, zinc, molybdenum, and silver, and supply between 60% and 90% of global copper, gold, and uranium (3). These metals are commonly transported by hydrothermal solutions until mixing with other fluids in the subsurface occurs, leading to either focused or dispersed precipitation of the metals (91, 11). Supersaturation of dissolved metal species in the mixed fluids results from one or more of the following four processes: **(1)** breakdown of metal-ligand complexes, **(2)** changes in redox conditions, **(3)** pH shifts, and **(4)** thermal shock. Gold and base metals such as copper, lead, and zinc, do not migrate through water as free ions; instead, they are transported as complexes bound to ligands, primarily sulfide and chloride. Mixing a hydrothermal fluid with a second water mass can drastically reduce ligand concentrations through simple dilution or consume them via chemical reactions. The result is that the metal-ligand complexes break apart and dissociate, forcing the free metal atoms to bond together and precipitate. Hydrothermal fluids are commonly oxygen-depleted (strongly reducing) and acidic, both of which promote elevated solubilities of the base-metal species. When such fluids mix with shallow, oxidized meteoric water (groundwater), the fluid redox state may shift and ligands may also become oxidized and break apart from the base metals. Metals such as iron and manganese can be oxidized to form highly insoluble oxides and hydroxides, which also act to scavenge and co-precipitate more base metals. Finally, hot fluids can typically dissolve substantially more material than cold fluids, and sudden cooling may promote ore formation by decreasing mineral solubility. When a hot magmatic or metamorphic fluid ($>250^\circ\text{C}$) mixes with a body of cold groundwater or ocean water ($<10^\circ\text{C}$), the temperature of the metal-bearing fluid plummets in seconds. This rapid cooling (thermal shock) causes a catastrophic drop in the kinetic energy of the fluid, triggering rapid, widespread supersaturation and immediate crystalline precipitation.

5.2. Feedback between fluid mixing and crystallization

Crystallization induced by fluid mixing may impact both fluid flow and fluid mixing through complex feedback loops (33). Clogging of pore space in mixing zones may reduce mixing, and redirect it to other zones. Loss of mixing and the associated supersaturation source may also cause re-dissolution of crystals, opening up the pore space for new or renewed mixing. Such feedbacks have been studied both numerically (280) and in laboratory settings using Hele-Shaw cell (254) and microfluidic experiments (283, 188, 279, 133).

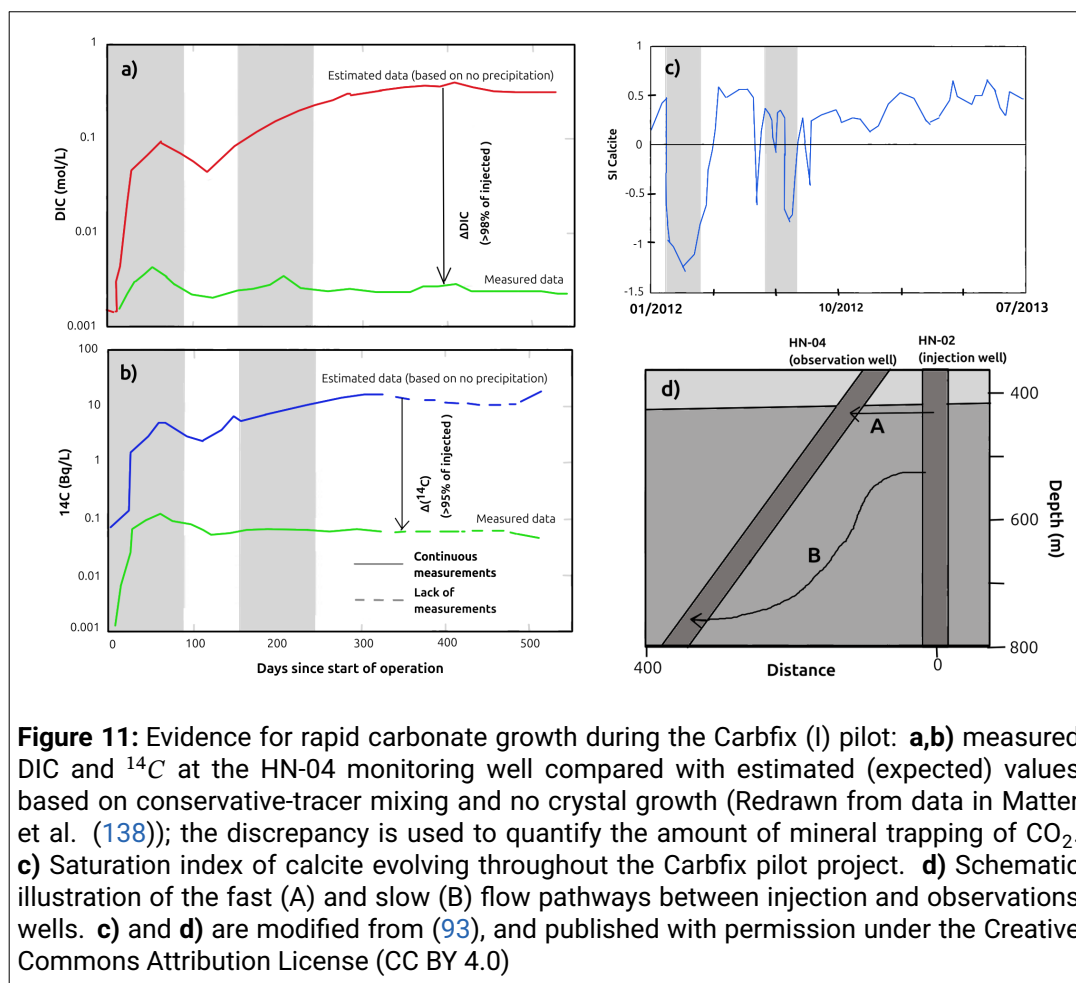
One common observation in systems where two solutions are mixed along (overall) parallel flow lines is the formation of a narrow mixing band that results from diffusive mixing in the direction transverse to the advective flow (254, 283, 133). A related observation is that, at a certain stage of mixing-induced crystal growth, diffusive mixing of the solutes becomes impeded. As a consequence, the solutions on both sides of the crystal barrier become undersaturated with respect to the precipitated phase, and crystals forming the barrier start to dissolve (188). A further, initially counterintuitive finding, by Zhang et al. (283) is that as precipitation rates increase, the total amount of precipitates decreases despite an increasing injected concentration and saturation states in the mixing bands. This behavior has been attributed to occlusion of the pore space by precipitates along the transverse mixing zone, which substantially reduces porosity and permeability and thereby limits diffusive mixing.

Yang et al. (279) studied the effects of flow rate and the channel width-to-depth ratio on fluid mixing and mixing-induced barite (BaSO_4) precipitation in a microfluidic system comprised of two intersecting channels. They observed that increasing Reynolds numbers led to enhanced precipitation and more pronounced local clogging. In addition, they found that decreasing the channel width-to-depth ratio induced inertial effects on solute mixing, which led to more severe precipitation and clogging.

The microfluidic cell used by Ma et al. (133), consisting of a 2D fracture network of 1D-channels, enabled investigation of how fluid flow rate and elapsed time (expressed as the local Reynolds number (Re)) control the feedback between fluid mixing and crystallization (see Fig. 4b, c). Their results indicate a strong feedback: high flow rates (high Re) produced a narrow mixing band with dense precipitation, whereas lower flow rates (low Re) resulted in a wider mixing band and more spatially dispersed crystallization. This more condensed precipitation at higher flow rates had a relatively larger impact on local fluid flow and the associated flow reorganization. The authors also found that flow-controlled mixing regulates which Ca-carbonate phases (ACC or crystalline polymorphs) nucleate and persist, with precipitation-induced reductions in mixing lowering supersaturation, thereby causing unstable phases to transform more rapidly into the more thermodynamically stable crystalline CaCO_3 polymorphs.

5.3. Potential role of fluid mixing during CO_2 storage in basalt

Understanding of the potential role of fluid mixing in complex porous reservoirs is essential for constraining the rates of engineered carbon mineralization, in which large volumes of carbon-rich fluids are continuously injected into the subsurface, yet direct monitoring of the rates and extent of carbonate precipitation remains extremely challenging. The Wallula (US) and Carbfix (Iceland) are two pioneering pilot-scale CO_2 storage projects, in which CO_2 was injected into basaltic reservoirs. Monitoring data from these sites indicate that 60-95% of injected CO_2 precipitated as solid carbonates within less than two years (138, 268) as inferred from numerical simulations at the Wallula site (268) and from analytical data on water samples at the Carbfix site (138). However, despite substantial monitoring efforts, mineral carbonatization at both pilot sites has not been directly observed. At Carbfix, estimates were derived by comparing reductions in the concentrations of conservative tracers (SF_6 and SF_5CF_3) and dissolved carbon (DIC and ^{14}C) resulting from dilution and mixing of



injected water with ambient formation water. In this approach, any excess loss of carbon relative to the conservative tracers was attributed to carbonate precipitation in the basaltic reservoir (**Fig. 11**). This raises questions about the actual rate of calcite growth in these pilot tests. The available data indicate nearly complete removal of DIC after just a few days. About 3% of the injected fluids migrated rapidly through low-volume horizontal fractures and reached the observation wells after a few days (93). Still, even over this short period, estimates suggest that nearly all carbon was removed from the injected fluids (**Fig. 11a,b**).

The crystal growth rate of calcite is relatively high (226) and may, in isolation, explain such rapid reactions, even at the moderate supersaturations inferred from the sampled Carbfix data (**Fig. 11c**). However, calcite formation requires a sustained supply of Ca^{2+} , originating from basalt dissolution and/or fluid mixing. It is insightful to carry out a back-of-the-envelope calculation to assess whether basalt dissolution alone is sufficient to provide a substantial amount of Ca^{2+} . We adopt a conservative rate estimate based on Oelkers and Gislason (167) and assume the formation of a mixed-phase carbonate that scavenge all divalent metal cations from basalt dissolution. The rate of basalt dissolution is approximately $10^{-10} \text{ moles/m}^2\text{s}$. Let us assume 50 days of reaction time, corresponding to 4.32×10^6 seconds. The total amount of dissolved basalt is then $4.32 \times 10^{-4} \text{ moles/m}^2$. The exemplary basalt composition, determined by Oelkers and Gislason is $\text{Ti}_{0.02}\text{Al}_{0.36}\text{Fe(III)}_{0.02}\text{Fe(II)}_{0.17}\text{Mg}_{0.28}\text{Ca}_{0.26}\text{Na}_{0.08}\text{K}_{0.008}\text{SiO}_{3.45}$ (167). One mole of basalt therefore contains $0.17 + 0.28 + 0.26 = 0.71$ moles of divalent metal cations. The total supply of these metal cations over 50 days is therefore $3.07 \times 10^{-4} \text{ moles/m}^2$. If the initial concentration of DIC is 0.5 moles/L (relevant for the later stages of injection), and all dissolved carbon is removed, such a rate would require a quantity of basalt, expressed as a reactive surface area, of $0.5 \text{ moles.L}^{-1} / 3.07 \times 10^{-4} \text{ moles.m}^{-2} = 1629 \text{ m}^2/\text{L}$ solution. If only pure calcite were to form, the required

reactive surface area of basalt would further increase to $6849 \text{ m}^2/\text{L}$ solution. Based on these calculations, it is unlikely that basalt dissolution rates alone can account for the observed rapid mineralization, and it is therefore necessary to consider the role of fluid mixing as an additional source of metal cations.

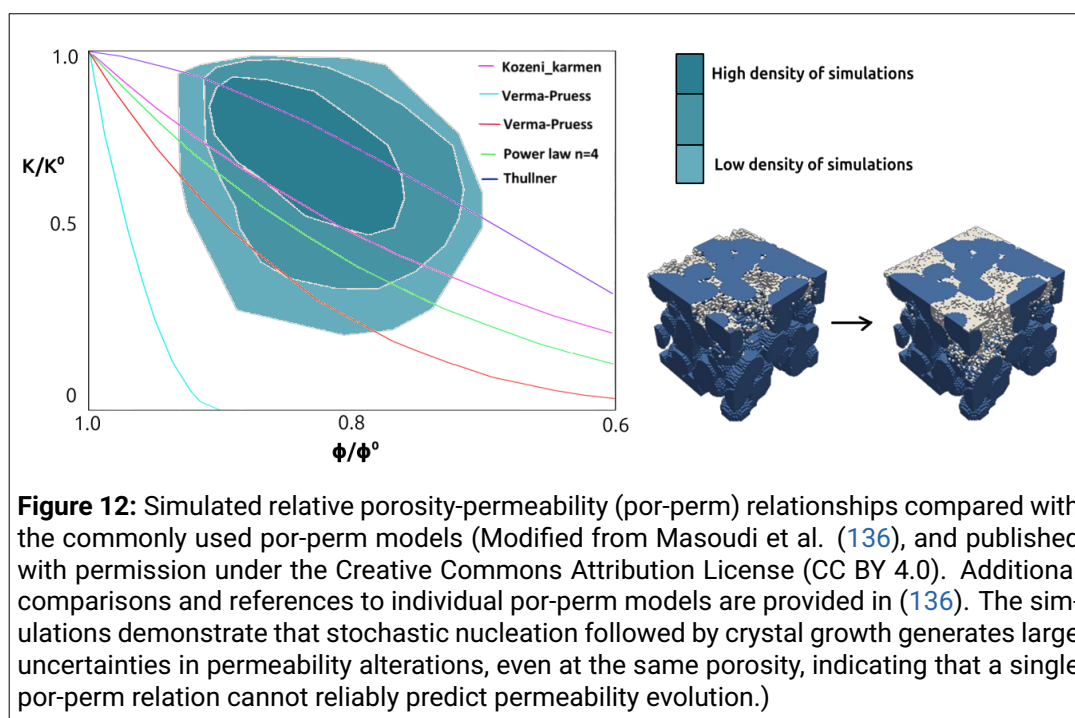
Fluid mixing between alkaline, high-pH pore water in the basalt and acidic, DIC-charged injected fluids may produce waters that are highly supersaturated with respect to carbonate minerals. Both advective mixing along intersecting flow lines and transverse diffusive mixing may occur within the fractured or porous basalt. Data on the differences in concentration between injected and sampled conservative tracers provide an estimate of the extent of mixing along the flow path. The first sampled solutions, arriving within the first 200 days at the Carbfix monitoring wells, suggest a 5 to 10-fold dilution of the injected waters, while later samples approach a 50/50 mix, corresponding to approximately 2-fold dilution of the injected solutions (240). However, fluid mixing alone cannot explain the observed massive CO_2 mineralization, as the initial pore water and the injected waters are chemically similar, with a total divalent metal cation concentration ($\text{Ca}^{2+} + \text{Mg}^{2+} + \text{Fe}^{2+}$) of about 0.42 millimoles/L (240). Differences in diffusion behavior between the conservative tracers and DIC may, however, provide an alternative explanation for the greater loss of DIC relative to the tracers. Although the diffusion coefficients of CO_2 and the SF_6 and SF_5CF_3 tracers are similar, the concentration gradients ∇C_i for these species may evolve very differently, leading to markedly different diffusive fluxes. The acidic, injected DIC-rich solutions are dominated by molecular CO_2 , which will speciate into bicarbonate and carbonate as soon as it diffuses into and mixes with the alkaline formation water. This behavior may maintain a substantial CO_2 flux driven by large concentration gradients, whereas the diffusive flux of the tracer flux will eventually approach zero.

In natural settings, such as along mid-ocean ridges, carbonatization of basalt is typically extremely slow and may require millions of years (131), being severely constrained by the supply of metal cations from the dissolving basalt. This observation may call into question the comparatively rapid carbonatization rates reported for the engineered CO_2 storage sites and highlights the need for further research toward a more detailed and comprehensive understanding of fluid-rock interaction across different basaltic systems. There, rates of basalt dissolution, CO_2 mineralization, fluid mixing, and transport phenomena may collectively contribute to the rapid carbon mineralization reported at the Carbfix and Wallula pilot-scale basalt carbonatization sites, but the feedbacks among these processes are not yet fully understood.

6. IMPLEMENTATION OF CRYSTAL NUCLEATION AND GROWTH IN NUMERICAL MODELS

Nucleation and growth of crystals in porous media have been modelled for decades, but much work remains to develop truly predictive models of the coupled feedbacks between crystal growth and fluid flow, especially in extreme cases where systems approach complete pore-space clogging. The stochastic nature of heterogeneous nucleation may lead to strongly localized precipitation, making it difficult, and in some cases impossible, to derive robust estimates of the evolution of porosity-permeability relationships, so that one must instead rely on uncertainty quantification. In large-scale modeling of crystallization phenomena, for example CO_2 storage in siliciclastic reservoirs, complete clogging is generally not a concern; instead, the focus is on estimating the total mass of crystals formed over extended timescales. Uncertainty is also substantial in this case, as nucleation and growth typically occur at low supersaturation, with particularly large uncertainty in induction times. Here, the use of TST-based growth models overestimates reaction rates and consequently yields unrealistic results that are not comparable to natural diagenetic reactions (181, 88).

In this section we limit ourselves to present recent works on uncertainty quantification and modeling studies of evaporation-driven salt precipitation. For a comprehensive review of modeling



approaches related to conventional diagenesis, the reader is referred to the review by F.H. Nader (151). In addition, Steefel et al. (248) provide an overview of commonly used reactive transport codes and evaluate their ability to represent kinetic aspects of mineral nucleation, growth, and dissolution, thereby outlining the current capabilities and limitations of continuum-scale modeling tools for crystallization processes.

6.1. Uncertainty quantification for porosity-permeability evolution

Although numerous reactive transport models have examined porosity and permeability alteration in porous media, relatively few simulations have been performed to quantify the associated uncertainties. Stochastic simulations of dissolution and crystal growth and their associated permeability changes have been conducted using 3D pore network models based on real sandstones (9, 216), using 2D-3D pore-scale Lattice-Boltzmann models with synthetic geometries (136, 137), and using a combination of pore-scale (Comsol Multiphysics) and Darcy-scale (CrunchTope) models for 2D fractured media (133). In all cases, substantial simplifications were required to enable stochastic modeling.

Beckingham (9) and Sabo and Beckham (216) performed pore-network modeling to provide comprehensive analyses on the effects of solid dissolution and growth on porosity-permeability (por-perm) relations by systematically modifying pore and pore-throat radii to represent dissolution and precipitation reactions. Their work showed that the spatial distribution of dissolution and crystal growth, whether uniform, random, channelized, or pore size-dependent, strongly affects both the specific por-perm relationship and its spread (uncertainty). The por-perm relationship even reversed when dissolution occurred at the inlet while precipitation was focused at the outlet, leading to increased total porosity but reduced permeability (216). With random placement of dissolution and precipitation, permeability remained nearly constant over large intervals of porosity change, and none of the commonly used macroscopic models could reproduce the observed por-perm behavior (216). Moreover, permeability showed larger variability for randomly selected pore clogging than for uniform alteration of all pores and pore-throats (9). These studies concluded that commonly used por-perm relationships perform well for some reaction scenarios, but no single relationship can capture all cases, particularly systems with non-uniform patterns of dissolution and growth. These findings were further supported by Masoudi et al. (137) who simulated

crystal nucleation and growth using a probabilistic model and obtained a large spread in relative por-perm values that did not correlate with any common por-perm models, including power-law formulations (Fig. 12).

Other studies have further explored how stochastic nucleation and crystallization influence porosity-permeability evolution in fractured systems. Masoudi et al. (137) simulated the evolution of porosity and permeability in 2D systems relevant to crystal growth along, for example, fracture planes. This was done by varying a fixed number of growing crystals that were placed at random locations in each run. They suggested that a power-law function can be used to describe the relative changes in porosity and permeability, with the variance and mean (or median) of the power-law exponent strongly dependent on the number of growing crystals (i.e., the degree of uniform versus localized crystallization). Ma et al. (133) simulated clogging in 2D fracture networks, with separate simulations to assess flow fields, stochastic nucleation, and flow fields subsequently updated after crystallite formation. They demonstrated a clear connection between flow rates, solute mixing and nucleation, leading to stochastic and heterogeneous impacts on permeability, particularly at low flow rates. Since crystal growth was not included in the simulations, complete clogging of the fracture pathways was not observed. Together, these studies highlight that rigorous uncertainty quantification of porosity-permeability evolution requires stochastic nucleation models that account for spatially heterogeneous crystallization and its coupling to evolving flow fields, and that substantial further work is needed before such effects can be reliably represented in predictive models of crystallization in porous media.

6.2. Modeling evaporation-driven salt formation

Pruess and Müller (192) and later Kim et al. (111) simulated near-wellbore salt formation in homogeneous sandstone using TOUGH2 with the ECO2N equation of state (EOS)-based continuum models. They analyzed the effect of injection rate, salinity, and temperature and found that the relative dominance of viscous, capillary, and buoyancy forces controls the spatial distribution of salt precipitation. At low injection rates, capillary backflow causes salt to accumulate in the near-well region, reducing porosity and permeability. At higher injection rates, the zone of salt growth shifts away from the wellbore, and precipitation occurs at a characteristic distance from the well determined by gravitational segregation (111).

Nematollah et al. (282) also used TOUGH2, with model parameters adapted from Kim et al. (111). They extended the analysis by introducing three dimensionless numbers; the balance between viscous and capillary forces (Ca), the ratio of gravity to capillary forces (Bo), and the balance between the gravity and viscous forces (Gr). In their simplified geological model (homogeneous reservoir), they found that while both Ca and Gr influence the spatial distribution of salt, Bo does not control either near-wellbore salt precipitation or the development of localized salt precipitation away from the wellbore, and they identified a region in the Ca - Gr -space within which localized salt formation is expected (282). To assess salt formation in heterogeneous reservoirs, they found that cases with contrasts in capillarity and permeability yielded similar results to those with permeability contrasts alone. However, the contrasts considered were modest, with the fine layers having permeabilities and capillary properties comparable to very fine sand to silty sand (15 mD). Stronger contrasts are expected to reduce the gravitational segregation that controls the localized salt away from the well. Farajzadeh and Niasar (59) concluded that sharp contrasts in capillary-pressure gradients, such as those caused by lithofacies transitions and layering, can potentially drive intense capillary fluxes across boundaries, and that the effects of realistic reservoir heterogeneity require further investigation.

The capillary pressure is a key parameter for estimating the extent of near-well salt precipitation. As the complete dry-out may occur in the near-well region, conventional capillary pressure func-

tions must be modified, and several alternative formulations have been proposed (178, 165, 166, 59, 282). It is clear that the capillary backflow and the extent of salt precipitation and clogging are highly sensitive to the choice of relation between saturation and capillary pressure. Among these studies, only Parvin et al. (178) explicitly investigated the self-enhancing effect of salt precipitation, whereby the formation of salt aggregates increases capillarity and strengthens local water backflow (142). Incorporating this capillarity modification in the salt-rich zone led to substantially more salt formation compared with the unmodified case. However, the self-enhancement effect was implemented as a simple relation between salt saturation and capillary pressure that has not yet been experimentally verified.

It is now nearly 20 years since the first continuum-scale simulations of salt formation, and our understanding of the underlying mechanisms of salt formation has advanced substantially through microfluidics and core-scale experiments. Nevertheless, numerous questions remain regarding salt formation in real carbon capture and storage operations at the near-well scale. Observations at this scale are scarce, except for the notable exception of the study on the SaskPower's Boundary Dam Integrated Carbon Capture and Storage Demonstration project, which qualitatively confirms capillary backflow and extensive salt formation in and around the wellbore (253). Despite recognition of the critical role of capillary pressure, the dynamics of the capillary pressure within the dry-out zone and how the self-enhancing salt growth effect operates at scales larger than the laboratory are not yet well understood. Even though reservoir heterogeneity is acknowledged to play an important role for the salt formation, we still lack simulations and experimental data for salt formation in realistic geological media, where individual laminae and shale drapings span from millimeter to meter scales and exhibit strong contrasts in capillarity. Finally, the extent to which commonly used porosity-permeability relations remain valid for near-well processes, typically assuming uniform grain coatings or preferential precipitation in pore throats, is largely unknown (33).

7. MACHINE LEARNING AND SURROGATE MODELS

The preceding subsections have outlined the compounding limitations of current numerical approaches to modeling crystal nucleation and growth in porous media, specifically deterministic rate laws that bypass the nucleation barrier, TST-based growth models that diverge from experimental measurements by orders of magnitude, and continuum formulations that fail to resolve the nanoscale surface heterogeneity that governs reaction kinetics. These shortcomings share a common root: the physics that controls nucleation and growth operates at the scale of atoms, molecules, and nanometer-thick interfacial films, whereas engineering and reservoir-scale decisions must be made at scales of meters to kilometers and over years to decades. Directly resolving molecular-scale physics at reservoir scale is computationally intractable, so continuum models instead rely on simplified, effective rate laws, and it is precisely this simplification that introduces the biases discussed above. Machine learning and surrogate modeling approaches offer one promising way to close this gap between scales. Instead of replacing the underlying physics, these methods learn compact, fast-to-evaluate approximations of it, allowing predictions at scales where direct, physics-resolving simulation remains impractical. In the following subsections, we review these methods on a scale-by-scale basis, starting at the molecular level and moving up to field-scale reactive transport, and for each scale, we highlight the specific modeling gap that each method is intended to address.

7.1. Machine-learned interatomic potentials: Molecular scale

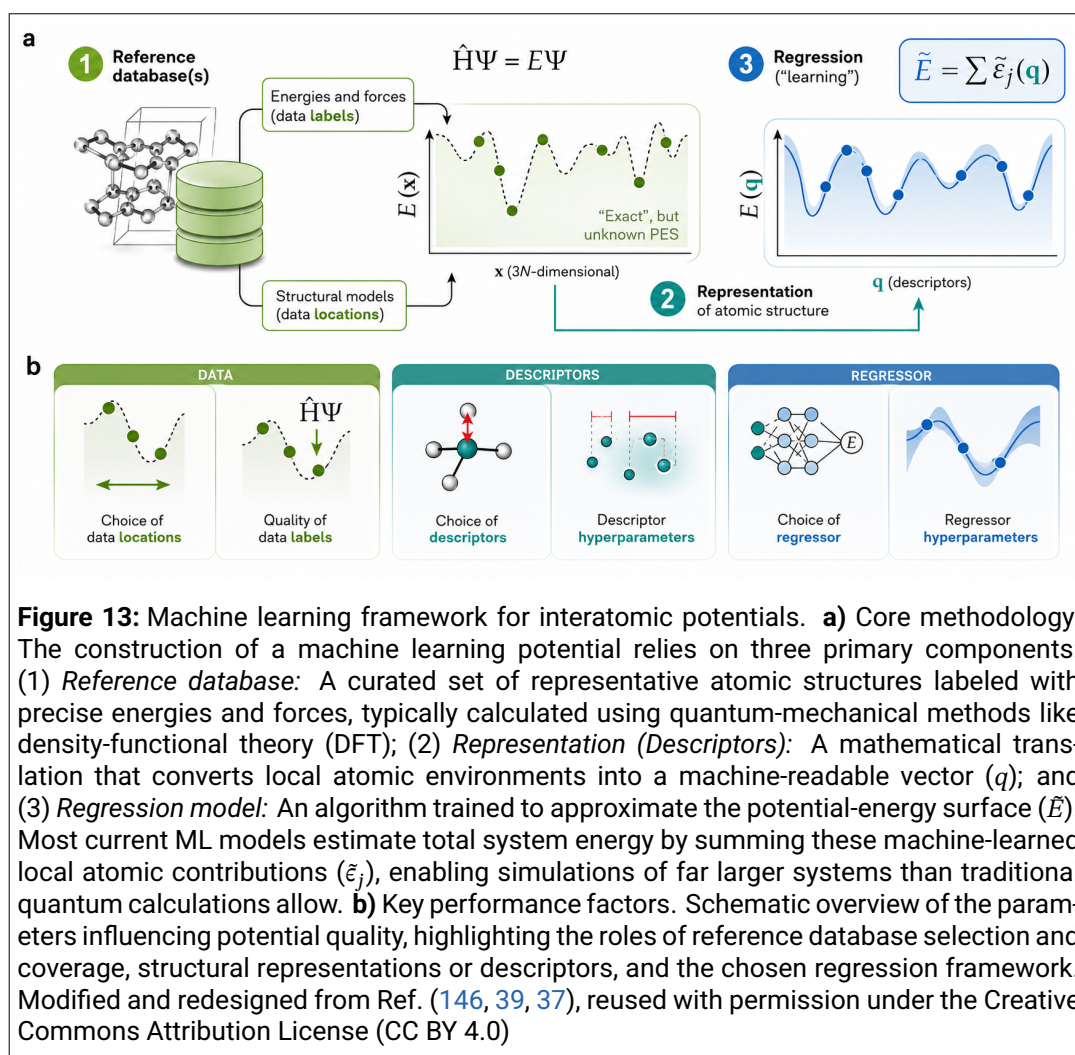
The most upstream challenge facing any nucleation model is the poor quantitative constraints on the molecular-scale parameters, most critically the interfacial free energy between the nucleus and the surrounding solution. As discussed in Section 2.1, the non-classical nucleation pathway

through hydrated amorphous intermediates means that the assumption of a single scalar interfacial free energy no longer holds. Because nucleation proceeds through a series of hydration states, no unique energy barrier can be assigned within the classical nucleation theory framework. Machine-learned interatomic potentials (MLIPs), neural networks trained on quantum-mechanical calculations to predict interatomic forces and energies at near-first-principles accuracy but at a fraction of the computational cost, are seen as a rigorous computational route to replace this approximation (236, 148, 2).

Machine-learned interatomic potentials (MLIPs) are typically implemented as neural networks that operate directly on atomic structure, and one particularly successful architectural class is the equivariant graph neural network, which represents atoms as nodes and their local bonding environment as a graph, and is constructed so that its predicted forces rotate and translate consistently with the underlying physical system. Equivariant graph neural network architectures, including NequIP, MACE, and the universal foundation potentials CHGNet and M3GNet, achieve near-DFT accuracy while exhibiting linear $\mathcal{O}(N)$ scaling with system size (107, 222, 25, 5, 32). Specifically, state-of-the-art MLIPs preserve energy errors and force errors low enough to enable large-scale molecular dynamics (MD) simulations comprising millions of atoms over nanosecond timescales. Nucleation itself is fundamentally a rare event: even in the classical picture, a stable nucleus forms only when a system crosses a single free-energy barrier through a chance fluctuation, which is why sufficiently long and large simulations are needed to observe it at all. Non-classical pathways compound this difficulty, since the system must instead traverse a sequence of intermediate, metastable states rather than a single barrier, which demands proportionally longer and larger simulations to sample without resorting to artificial overpressurization, a common shortcut that compromises the physical relevance of shorter simulations. Combined with free-energy sampling techniques such as metadynamics and umbrella sampling (118, 18, 19), MLIPs can enable the direct computation of orientation-resolved nucleation barriers and crystal growth velocities v_g across diverse crystallographic orientations and hydration states (221, 264, 26, 39). This methodology yields an orientation-resolved tensor of interfacial free energies that replaces the single empirical scalar of classical nucleation theory, providing the molecular-scale input required to parameterize non-classical nucleation models across various mineral systems. Although most published MLIP applications to nucleation have focused primarily on metallic and semiconductor systems, the emergence of universal potentials trained across broad regions of chemical space is progressively lowering the barrier to application at geologically relevant mineral-water interfaces.

Furthermore, because mineralization in porous media often occurs within sub-micron geometries, MLIPs offer a crucial advantage for capturing nanoconfinement effects. Classical empirical force fields fail to resolve the complex water structuring, local dielectric variations, and interfacial charge transfers that occur when fluid-solid boundaries are confined between narrow pore walls. By explicitly modeling these non-local interactions with near-quantum accuracy, MLIPs can map how spatial confinement systematically alters the orientation-resolved tensor of interfacial free energies, providing a direct physical link between molecular-scale geochemical simulations and macroscopic pore-scale behavior.

However, this potential remains only partially realized in practice due to several critical challenges. First, most contemporary MLIPs, including universal foundation models, are trained predominantly on bulk-phase or vacuum-interface configurations. Training datasets that explicitly represent confined, nanometer-thick water films between charged mineral surfaces remain scarce. Consequently, a potential may achieve near-density functional theory accuracy in bulk solutions yet remain poorly constrained under confinement if it lacks exposure to comparable local environments during training. Second, faithfully capturing long-range electrostatic screening and polarization effects, which amplify as opposing charged surfaces approach one another, remains



an active area of architectural development rather than a settled capability. Finally, even with linear-scaling algorithms, the computational timescales required for enhanced sampling methods like metadynamics to fully resolve nucleation and crystallization barriers under confinement remain prohibitive. Validated MLIP-predicted, confinement-dependent interfacial free energies against direct experimental measurements for geologically relevant mineral-water systems remain limited. Bridging this validation gap is necessary before these nanoconfinement frameworks can transition from qualitatively informative to quantitatively predictive across scales.

7.2. Data-driven rate prediction and active learning: Laboratory scale

As established in Section 3, no comprehensive database of crystal growth rate constants currently exists for geologically relevant minerals, and extrapolating dissolution rates to growth conditions using TST-based models is mechanistically unjustified. Supervised ML models (114, 234), including artificial neural networks and gradient-boosted regression trees such as XGBoost, can, in principle, map nonlinear relationships among solution chemistry (encompassing pH, ionic strength, and saturation index), temperature, and crystallographic orientation to experimentally measured growth rates. However, these approaches face a fundamental obstacle: the training datasets are scarce, inconsistently reported across laboratories, and heavily biased toward high-supersaturation conditions that are experimentally convenient but geologically unrepresentative.

Active learning frameworks built on Gaussian Process Regression (GPR) offer a principled solution to the data-scarcity constraint (105, 203, 21, 235). The GPR model can be leveraged to maintain a probabilistic estimate of the growth rate surface across the multi-dimensional parameter space

defined by temperature, supersaturation, and fluid composition (227, 38, 263). An acquisition function, such as the upper confidence bound or expected improvement, then identifies the region of the parameter space where predictive uncertainty is highest, indicating where a new experiment would provide the maximum reduction in model variance. Once this query is executed in the laboratory, the result is incorporated into the training database, and the cycle repeats. Consequently, the model autonomously guides the experimental design, targeting new measurements specifically at the conditions of highest uncertainty rather than distributing limited laboratory time arbitrarily. This focused approach efficiently populates the database for conditions most relevant to natural and engineered porous media systems.

However, standard GPR active learning loops face a secondary bottleneck: their computational complexity scales cubically with the number of data points, and purely data-driven kernels often struggle to resolve the highly localized, nonlinear discontinuities characteristic of crystal growth regimes, such as sharp transitions from step-pinning inhibition to rapid continuous growth. Left unconstrained, the acquisition function may prioritize sampling nonphysical or geologically irrelevant parameter spaces. To address this, recent frameworks build simple physical relationships directly into the model, such as equipping the GPR with an Arrhenius-like temperature dependence or a basic classical growth law as a baseline assumption. In practice, the model does not learn growth rates from scratch; instead, it trains on how real data deviate from a physically reasonable baseline. This constraint keeps predictions anchored to known thermodynamic behavior even when the model extrapolates into data-scarce regions. Extending this active learning loop to simultaneously vary substrate composition, surface roughness, and the concentration of foreign ions would directly address the effects on crystal growth discussed in Section 4, for which systematic experimental datasets are presently almost entirely absent.

7.3. Automated image analysis and experimental feedback: Pore scale

Automated image analysis refers to the use of computer vision and machine learning algorithms to detect, segment, and quantify events and features, such as crystal growth and geometry evolution, directly from microscopy or tomography images. This approach replaces slower, manual, human-annotated measurement with a reproducible, algorithmic pipeline. The observational bottleneck identified in Sections 2-3, specifically the challenge of distinguishing co-nucleation from regrowth and Ostwald ripening at low supersaturation, is increasingly manageable using such ML-assisted frameworks.

The active learning framework described in the preceding subsection requires both automated data generation and automated interpretation of the resulting experimental observations (246, 134, 257). Beyond semantic segmentation, which labels each pixel or voxel in an image frame as either crystal or background (69, 77, 143), the kinetic interpretation of nucleation experiments demands instance segmentation coupled with temporal tracking algorithms. Instance segmentation identifies each individual crystal in a frame as a distinct object. Temporal tracking algorithms, such as DeepSORT (270) or ByteTrack (287), were originally developed to track moving targets, such as pedestrians or vehicles, across video frames. When applied to crystallization time-lapse sequences, these algorithms link the identity of a specific crystal across successive frames. This pairing allows an algorithm to track a single crystal over time, distinguishing its continuous growth from the emergence of a separate, newly nucleated neighbor. This operational capability enables automated discrimination of events associated with the regrowth or recrystallization of existing crystal phases, resolving the central ambiguity that currently renders induction-time measurements highly dependent on instrumental spatial resolution.

Three-dimensional tracking within micro-CT volumes introduces additional complexity due to imaging artifacts and the limited temporal resolution achievable at high spatial resolutions.

Micro-CT provides non-destructive, volumetric images of pore spaces and mineral phases at micrometer-scale resolution. Consequently, it has become a preferred approach for observing fluid flow and reactive transport phenomena directly within intact porous media rather than on an open substrate. However, tracking is often hampered by low phase contrast and high signal-to-noise ratios. This issue is especially acute when the X-ray attenuation or optical refractive index of a precipitating phase closely matches the surrounding fluid matrix, or when sub-voxel crystallite formation is initially too small to resolve.

Classical thresholding methods routinely misclassify these features, introducing significant artifacts into the calculated kinetics. To overcome these limitations, modern workflows employ generative adversarial networks (GANs) and self-supervised denoising autoencoders to perform super-resolution and contrast enhancement prior to tracking. Furthermore, by embedding geometric and physical constraints, such as enforcing non-negative volume changes during independent crystal growth or maintaining mass balance constraints across frames, these deep learning architectures can filter out imaging noise and resolve topological features that fall below nominal instrumental detection limits. Three-dimensional convolutional long short-term memory networks (217, 95) can then be used to track temporal continuity across sequential scan volumes. Directly coupling these automated tracking pipelines to the active learning loop would establish a continuous pathway from raw experimental images to ready-to-use growth rate data. In principle, this could eliminate much of the manual, subjective image analysis that currently restricts experimental throughput and impedes consistent cross-laboratory reproducibility.

7.4. Surrogate models for pore-to-continuum upscaling

For modeling purposes, the experimental data generated and parameterized at the molecular-, pore-, and laboratory-scales must ultimately be translated into continuum-scale reactive transport predictions over engineering-relevant spatial and temporal domains. A surrogate model is a data-driven approximation of a computationally expensive function or simulation. Trained on a limited set of input-output pairs from direct numerical simulations or experiments, it rapidly predicts outcomes for new parameters, trading a negligible margin of exact physics-based accuracy for massive gains in computational speed. This upscaling step, identified in Section 1 as one primary outstanding challenge in porous media crystallization research, represents the domain where surrogate modeling methods offer their most immediate computational returns.

7.4.1. Geometric and structural surrogates

Convolutional neural networks (CNNs) (174, 128, 288) serve as a primary bridge between geometry and transport by directly mapping complex pore microstructures to macroscopic continuum parameters such as anisotropic permeability tensors, tortuosity factors, and evolving reactive surface areas (288, 220, 54, 272, 277, 135, 157, 292). Their core contribution lies in their ability to treat voxelized porous media images as direct spatial inputs. This allows the network to rapidly predict how morphological changes translate into evolving flow and transport properties without relying on computationally exhaustive direct numerical simulations.

However, standard CNN architectures are fundamentally constrained by local receptive fields. Because each layer of the network only examines a small, localized neighborhood of the image at a time, it can struggle to recognize structural features that span long distances across a sample, such as a single connected flow path running entirely through a pore network. To overcome this limitation, vision transformers (ViTs) are emerging as a powerful alternative. Instead of scanning small local neighborhoods, ViTs divide the pore volume into a grid of sub-blocks and use a mechanism called self-attention. This approach directly compares every sub-block against every other sub-block regardless of distance, allowing the network to capture long-range structural connectivity more robustly than localized convolutions (108, 154, 177).

Furthermore, physical porous media imaging techniques like micro-CT impose an implicit trade-off between macro-scale field of view and micro-scale spatial resolution. A single scan generally cannot capture both the full sample scale and its finest pore-throat details simultaneously. To address this, geometric inputs are increasingly preconditioned using generative latent diffusion models (22, 209, 152, 293, 132, 292). These generative frameworks perform cross-modal super-resolution by statistically reconstructing missing sub-micron pore-throat details within a larger, coarser-resolution, centimeter-scale core volume. This optimization ensures that downstream structural surrogates are supplied with the multi-scale geometric fidelity necessary to predict localized clogging.

7.4.2. Dynamic transport operators and topological discontinuities

Upscaling also requires capturing dynamic transport, which describes how fluid flow and solute transport evolve as pore geometry changes over time due to precipitation, alongside topological discontinuities, which occur when a pore throat narrows and disconnects entirely. Neural operators (NOs) are ML models built specifically for dynamic transport problems. Rather than mapping one fixed-resolution image to another as a CNN does, a NO learns a discretization-invariant solution rule that maps an input field, such as an initial pore geometry and its boundary conditions, to an output field, such as the resulting fluid velocity or solute concentration distribution. This trained rule can be evaluated on flow and transport data at any spatial resolution without retraining (116, 130, 4, 100, 127).

Fourier neural operators (FNOs) represent a common architecture that operates directly in the frequency domain via the fast Fourier transform, allowing a single trained model to be applied across grids of any resolution (127, 100, 47). Consequently, a single trained operator $\mathcal{G} : a \mapsto u$, where the input a encodes the initial pore geometry and boundary conditions and u represents the resulting velocity or concentration field, can solve the underlying partial differential equations (PDEs) across dynamically altering pore geometries (158, 127), varying supersaturation fields, and arbitrary flow boundary conditions.

By evaluating these velocity and concentration fields directly rather than operating on a fixed computational grid, NOs avoid a major bottleneck of traditional mesh-dependent solvers. When mineral precipitation changes the shape of pore walls, a conventional solver must repeatedly regenerate its computational mesh to match the updated geometry, which is a slow and numerically unstable step. Even so, capturing abrupt, discrete topological transitions, such as a pore throat narrowing to a critical zero-radius event that cuts off a flow pathway, remains a frontier challenge. Smooth, continuous operators struggle to represent locations where a previously continuous flow field suddenly splits into two disconnected segments. To resolve these discontinuous boundary movements, operators are increasingly paired with implicit neural representations, such as Neural Cellular Automata (245, 145) or deep signed distance fields (176). These methods track the pore wall as a continuous mathematical surface, or level set, that can move and pinch off smoothly while remaining natively differentiable within the ML architecture.

7.4.3. Uncertainty quantification and hybrid physics architectures

Deploying these surrogate models to make predictions at the field scale introduces two secondary requirements: uncertainty quantification (UQ) and hybrid physics architectures. Rather than producing a single deterministic value, a UQ-aware model reports a range of plausible outcomes alongside a calculated confidence level. A hybrid physics architecture integrates a trained neural network with explicit physical equations, ensuring that predictions remain physically plausible even when extrapolating beyond the training data.

Propagating upscaled parameters across spatial scales requires rigorous UQ frameworks that are structurally integrated into the surrogate pipeline (294, 250, 258). These uncertainties arise from both the inherently stochastic nature of the reactive transport process and the discretization errors introduced when converting continuous laboratory observations into the formatted inputs required by a surrogate model, such as approximating a smoothly varying concentration profile on a finite voxel grid. To prevent these errors from compounding catastrophically when propagated to macroscale equations, modern architectures deploy Bayesian neural networks (73, 102) or deep ensembles (119, 84) to output joint probability distributions rather than scalar values for target parameters. This integrated UQ layer converts deterministic predictions into stochastic fields, providing the mathematical variance needed to bound field-scale predictions of pore-clogging or structural evolution.

To maximize robustness, these operators are increasingly embedded within hybrid modeling frameworks (294, 269, 158). Rather than replacing the entire simulation with an unconstrained, black-box model, hybrid architectures preserve the governing physical equations. Depending on the framework, conservation laws for mass, momentum, or energy may be enforced as hard mathematical constraints within the neural network loss function. Alternatively, modular frameworks partition tasks between a classical numerical PDE solver, which handles well-understood macroscopic transport physics, and an embedded neural surrogate, which models highly nonlinear or poorly constrained sub-grid features (158).

For crystal nucleation and growth specifically, the surrogate architecture must capture both the stochastic induction period and the subsequent growth trajectory as coupled functions of supersaturation, temperature, substrate identity, and hydrodynamic conditions. Gaussian process regression surrogates are uniquely suited to this regime because they provide both deterministic predictions and calibrated uncertainty bounds that feed directly into the probabilistic porosity-permeability modeling frameworks discussed in Section 6.1, ensuring that the upscaled continuum framework remains physically anchored and mathematically closed. Specifically, traditional workflows alternate sequentially between chemical and fluid-flow updates, introducing operator-splitting errors that destabilize calculations near clogging thresholds. Hybrid neural surrogates evaluate these coupled source terms simultaneously, offering a numerically stable alternative for long-timescale simulations.

7.5. Physics-informed constraints and thermodynamic consistency

The surrogate and data-driven frameworks required for porous media upscaling share a fundamental vulnerability: purely data-driven architectures trained on finite datasets often yield physically infeasible predictions when forced to extrapolate beyond their training domain. In the context of crystallization, these anomalies could manifest as unrealistic precipitation rates, systemic violations of mass balance, or spontaneous phase growth below thermodynamic solubility thresholds. Because an unconstrained surrogate lacks intrinsic awareness of nonlinear nanoscale physics, such as the sharp exponential increase in effective solubility as the crystal radius approaches the critical nucleus threshold, it naturally minimizes computational loss by smoothing the nucleation barrier entirely. Consequently, such networks tend to erroneously predict the steady, continuous growth of subcritical nuclei under low supersaturation, invalidating the central physical mechanism underpinning the system's kinetics.

To remedy this, ML frameworks must structurally embed classical physics and thermodynamic consistency directly into the model's learning objective or network architecture. This integration operates along a design spectrum ranging from soft regularized constraints to hard invariant architectures. Soft constraints inject the residuals of the governing partial differential equations, such as the coupled advection-diffusion-reaction equations, directly into the optimization loss function,

penalizing predictions that violate mass, momentum, or charge conservation laws in the pore fluid. However, because soft penalties can be bypassed by the optimizer in highly nonlinear chemical regimes, stringent thermodynamic boundaries are increasingly enforced as hard constraints via custom neural network layers or analytical ansatzes.

By hard-coding core thermodynamic relations, such as the Gibbs free energy condition for spontaneous precipitation or the Ostwald-Freundlich size-solubility relationship, the surrogate is mathematically restricted to a physically valid prediction space. For instance, a hard constraint layer can project predicted precipitation rates directly to zero whenever the local saturation index falls below unity ($\Omega < 1$), or bound the effective surface area as a strict function of current mass to mathematically forbid the non-physical growth from zero-mass phases. Rather than letting the network produce unconstrained values, these custom layers alter how the final layer converts its internal computations into the output. This structural modification prevents unphysical growth predictions at the source rather than merely penalizing them via the loss function after they occur.

This enforcement is critical for long-timescale simulations, where even minor per-step errors can accumulate over thousands of iterations and eventually deviate into a macroscale trajectory that is qualitatively incorrect. The ultimate frontier for this domain lies in developing fully coupled, physics-informed architectures that simultaneously constrain fluid flow, solute transport, and interfacial geochemical reactions, thereby eliminating the numerical artifacts and temporal decoupling introduced by traditional operator-splitting approaches.

7.6. Data infrastructure, standardization, and outlook

Realizing the ML-integrated ecosystem described in the preceding subsections depends on a foundational requirement: a standardized, shared framework for storing and organizing data, enabling seamless integration of results from different laboratories and computational scales. At present, the data ecosystem remains severely fragmented. Transient microfluidic imagery, multi-scale structural tomography, MLIP training configurations, reactive transport surrogate weights, and macroscopic kinetic measurements are confined to isolated repositories governed by disparate, non-standardized metadata conventions. This fragmentation impedes the assembly of the large, heterogeneous, cross-mineral datasets required to train physically generalizable ML models. Overcoming this data sparsity requires a unified geochemical ML schema built on domain-specific ontologies and semantic web standards (68, 14, 193, 104, 251). By encoding dataset linkages via graph-based metadata and standardized serialization schemas (e.g., JSON-LD), such a framework would ensure that datasets generated across disparate laboratory and numerical platforms are natively Findable, Accessible, Interoperable, and Reusable (FAIR) (96, 199). Without this foundational infrastructure, the training sets required for robust, cross-scale models cannot be efficiently compiled, and the reproducibility of published computational results across the porous media sciences cannot be independently verified.

Looking forward, the convergence of multimodal foundation models with autonomous, self-driving laboratory platforms (257) represents the most transformative frontier for porous media crystallization research. Closed-loop systems that couple active learning algorithms with automated fluid-handling robotics and in-line spectroscopic monitoring, such as Raman or attenuated total reflectance infrared spectroscopy, can autonomously navigate complex experimental parameter spaces without human intervention. This automation holds the potential to rapidly characterize inhibitor effectiveness against pore-clogging mineral phases, map multi-component phase diagrams under geological conditions, and determine the kinetic stability of metastable polymorphs across wide temperature and supersaturation gradients. When seamlessly coupled with the surrogate modeling and upscaling frameworks described above, these autonomous experimental architectures complete a continuous data pipeline spanning from molecular-scale

interfacial interactions to field-scale reactive transport predictions, directly resolving the multi-scale upscaling constraint that remains the defining challenge in porous media crystallization research.

Depositing raw or lightly processed time-lapse images and micro-CT volumes, rather than only final, summarized growth curves, would allow automated tracking pipelines (Section 7.3) to be trained and tested on real experimental sequences rather than synthetic data alone. Finally, using consistent, machine-readable metadata formats when depositing these assets, following the FAIR principles, will ultimately enable a laboratory measurement, an MLIP output, and a segmented microfluidic image to serve as interoperable inputs to the same surrogate model. Until this connective layer is built and tested end-to-end, the multi-scale promise of ML for crystallization in porous media remains a well-motivated hypothesis rather than a validated capability. Closing even one of these specific handoffs, such as linking a molecular-scale interfacial energy calculation to an experimentally calibrated growth rate surrogate for a single mineral system like calcite or magnesite, would constitute a meaningful and tractable next step for the field.

8. SUMMARY AND CONCLUSIONS

This commentary offers a perspective on crystal formation in porous media, and feedbacks between crystal growth, fluid mixing and alteration of the porous media itself. We devoted extensive space for a review on developments in ML and how ML can be used to progress our understanding of crystal growth in porous media. The five computational layers discussed above in section 7 form one connected conceptual chain bridging the scales, from interatomic potentials to continuum modeling. Machine-learned interatomic potentials address the molecular-scale ambiguity of a single interfacial free energy raised in Section 2.1, active learning with Gaussian process regression targets the missing growth rate database discussed in Section 3.1, automated tracking addresses the induction time and resolution problem described in Section 2.3, and neural operators and hybrid surrogates confront the pore-to-continuum upscaling problem that motivates Section 7.4. However, the handoffs between these layers are largely aspirational rather than demonstrated. To our knowledge, no published study has used an MLIP-derived, orientation-resolved interfacial free energy directly as a prior or input feature for a GPR-based growth rate model, in which orientation-resolved energy barriers serve as structural descriptors alongside solution saturation indices. Nor has any automated tracking pipeline yet supplied training labels to a neural operator in a closed loop that spans from pore-scale imaging to continuum-scale prediction.

Closing these handoffs will depend as much on experimental practice as on model development, and laboratory scientists play a concrete, vital role in this process. Growth rate measurements are most useful for these models when reported alongside the full solution chemistry (encompassing pH, ionic strength, and the identities and concentrations of background or trace ions) rather than just temperature and supersaturation. This detailed compositional data is precisely what current rate databases lack, and it represents the exact space that active learning frameworks (Section 7.2) are designed to map efficiently. Furthermore, reporting crystallographic orientation alongside measured rates, rather than a single bulk rate per experiment, would allow laboratory data to directly test and calibrate the orientation-resolved interfacial energies that MLIPs are beginning to predict (Section 7.1).

The following conclusions have been reached:

- Crystal formation governs both natural processes, such as diagenesis, hydrothermal ore formation, and weathering, and engineered systems, including CO₂ storage, geothermal operations, and infrastructure durability. However, nucleation and growth kinetics for

most minerals remain poorly constrained, particularly at low supersaturation and over long timescales.

- Nucleation is a distinct, often rate-limiting step that cannot be bypassed without a serious loss of predictability. Ignoring nucleation when modeling the neo-formation of minerals, such as by assigning arbitrary surface area to phases with zero mass, produces unrealistic mineral assemblages, incorrect induction times, and misleading extrapolations of laboratory data. For key mineral systems such as carbonates and sulfates, non-classical pathways involving amorphous and metastable intermediates dominate. This behavior invalidates the use of a single, well-defined interfacial free energy and undermines rate laws based on classical nucleation theory, driving a critical need for pathway-specific nucleation parameters.
- Confinement, interfacial chemistry, and the disjoining pressure acting across nanometer-scale confined solution films jointly control whether a growing crystal can transmit sufficient crystallization pressure to fracture rock or a building stone, or instead forms an adhesive, low-stress contact. This behavior cannot be captured by bulk, supersaturation-based thermodynamic limits alone, highlighting the need for more quantitative links between the force of crystallization and surface separation-dependent disjoining pressure.
- Evaporation-driven salt crystallization and mixing-induced precipitation in flow systems, such as near-well CO₂ injection zones and microfluidic fracture networks, generate self-enhancing feedbacks among capillarity, flow reorganization, supersaturation, and clogging. These processes are highly stochastic at the pore scale, which makes single deterministic porosity-permeability relationships inadequate and calls for explicit uncertainty quantification.
- Continuum-scale reactive transport models face three coupled limitations: they often neglect nucleation and metastability, rely on oversimplified rate laws for growth and recrystallization, and impose overly rigid porosity-permeability relationships. Progress requires embracing stochastic nucleation alongside heterogeneous spatial patterns of precipitation and dissolution, using explicit uncertainty bands rather than single best-estimate curves.
- Machine learning and surrogate modeling offer a viable pathway to bridge scales, from molecular interfacial physics to pore-scale flow and field-scale predictions. However, this is only possible if these tools are tightly coupled to physical and thermodynamic constraints and supported by standardized, FAIR experimental and numerical datasets. Without this integration, data-driven models risk reproducing the same oversimplifications that limit current numerical approaches.
- Overall, crystal nucleation and growth in porous media must be treated as a multiscale, probabilistic, and interface-controlled phenomenon. Future work should prioritize four key objectives: **(i)** establishing kinetic databases for growth and recrystallization under geologically relevant conditions; **(ii)** quantifying crystallization pressure and deformation mechanisms from the nanoscale to the reservoir scale; **(iii)** developing physically informed, uncertainty-aware surrogate models; and **(iv)** designing experiments that directly test upscaled predictions in realistic heterogeneous media.

STATEMENTS AND DECLARATIONS

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H. Hellevang: Lead author. Concept and outline, drafting all sections except 7 and 3.3, all graphics except **Figures 7** and **13**, final review and editing, writing coordination. **M. Nooraiepour:** lead author section 7, **Figure 13**, review and editing. **A. Sednev-Lugovets:** co-authoring sections 1-3, review and editing. **J. Dziadkowiec:** lead author subsection 3.3, **Figure 7**, review and editing.

Conflicts of Interest

We declare no conflict of interest among the authors.

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