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Ensuring reliability in CO₂ leakage risk assessment through AI-driven uncertainty quantification across scales

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CO₂ storage in subsurface formations, such as saline aquifers, has emerged as a promising alternative to reduce greenhouse gas emissions and mitigate their impacts on global warming [1]. Ensuring the reliability of CO₂ leakage risk assessment remains critical in the context of carbon capture and storage (CCS) technologies and raises significant concerns for predicting long-term behaviours. Various potential sources of leakage, such as geological faults and fractures or mineralogical changes of the rock matrix due to the acidification of the medium, may compromise the integrity of the seal and caprock. On the one hand, fault damage zones characterized by a fracture network can become high-conductive flow pathways, where the permeability needs to be investigated to assess fault-related leakage rates [2]. On the other hand, the mineral reactivity of the reservoir structure with the injected CO₂ may result in mainly carbonate dissolution under acidic conditions, locally impacting the flow paths, porosity and permeability [3].

Investigating the effects of these two phenomena is, therefore, crucial to ensure reliable management of CCS facilities. However, several uncertainties are associated with modelling these geochemical and structural mechanisms at the reservoir scale. Subsurface uncertainties arise from missing geological features and data sparsity regarding macro-properties distributions such as permeability and porosity. This necessitates sensitivity analyses in terms of the macroscopic description of the porous structures to ensure reliable management of CO₂ storage in natural reservoirs. However, the parametrization of geological distributions is often left to the user's discretion [4].

At the same time, laboratory studies and pore-scale modelling of reactive processes and fluid transport within complex fracture geometries provide insights into the local interactions of these processes, enabling the analysis of a Representative Elementary Volume of an extracted rock core. At this scale, the 3D porous geometry is explicitly described through X-ray microtomography (X-ray μ CT) experiments, a non-destructive imaging technique that can subsequently be combined with pore-scale modelling and direct numerical simulations [3]. This renders pore-scale analyses an interesting interplay between laboratory experiments and mathematical modelling, providing valuable insights for upscaling reliable characteristics. However, uncertainties also arise at the small scales both from the imaging and modelling sides. X-ray μ CT reconstruction suffers from artefacts such as noise and unresolved morphological features, which disrupt the description of the pore space. Capturing the heterogeneous features that are below the characteristic voxel size, especially sub-resolved porosity, and assessing their impact on pore-scale modelling remains challenging and requires imaging uncertainty quantification (UQ) [5, 6]. Moreover, modelling uncertainty plays an important role in the calibration of reactive pore-scale models, regarding the estimation of mineral reactivities and kinetic parameters that can suffer from wide discrepancies or be difficult to estimate from laboratory measurements [7].

Therefore, incorporating uncertainty quantification in pore-scale modelling is crucial for applications to CO₂ leakage risk assessment. In particular, the knowledge gained from understanding the uncertainties at the pore scale can be upscaled, enabling a propagation of uncertainty quantification across the scales to provide macro-properties distributions based on pore scale estimations of the uncertainties. Our ongoing research will explore these uncertainty considerations regarding the potential sources of leakage identified by fault damage zones and carbonate dissolution in CSS facilities.

A robust deep learning data assimilation framework for uncertainty quantification

Incorporating UQ into pore scale modelling requires dedicated and robust deep learning approaches embedded within a Bayesian inference framework. A Bayesian Physics-Informed Neural Networks

(BPINNs) paradigm provides the opportunity to simultaneously evaluate prediction confidence, measurement uncertainty, and model adequacy through posterior distributions of neural network predictions [8]. To achieve this, the Hamiltonian Monte Carlo process is commonly used to sample from a target posterior distribution in high dimension, involving the laboratory data and model constraints as different objectives or tasks. The sampling approach thus introduces a weighted multi-task posterior distribution, whose weights reflect uncertainties across the tasks; however, they mostly remain hand tuned. Unsuitable choices of these weighting parameters can lead to biased predictions, vanishing tasks behaviour or instabilities, rendering the sampling inoperative, as in the PINNs framework [9].

Developing an efficient data-assimilation framework to address multi-objective and multi-scale problems involving uncertainty quantification, therefore, remains challenging. We proposed a novel automatic and adaptive weighting strategy for the BPINNs, leveraging the gradient information of the different tasks to reach unbiased UQ. This ensures enhanced stability and convergence, reduces sampling bias and avoids hand-tuning of the weighting parameters [10]. We thus obtain reliable uncertainty estimates on the measurement data and the modelling constraints arising from potentially coupled and non-linear Partial Differential Equations (PDEs). This has extended the applicability of the BPINNs to more complex inference problems, such as multi-task and multi-scale reactive inverse problems of carbonate dissolution. The ongoing work thus relies on this newly developed framework to achieve robust Bayesian inference for CCS applications.

Quantifying uncertainties from reactive inverse problems at the pore scale

Reactive inverse problems of calcite dissolution offer the opportunity to investigate both imaging and modelling uncertainties at the pore scale. In this context, we proposed a data-assimilation framework combining dynamical μ CT data of calcite dissolution (Figure 1, on the left) along with physics-informed PDE system modelling the reaction-diffusion process for diffusive dominated regimes (with low Peclet numbers) [11]. This results in a multi-task formulation of the reactive inverse problems and enables us to simultaneously quantify morphological uncertainties in the micro-porosity field ε but also to estimate reliable ranges of the reactive parameters in the prescribed PDE model.

A Bayesian Model Average of the surrogate micro-porosity field ε_θ as well as its local uncertainty are obtained from sampling the posterior distribution with our adaptive weighting strategy for the BPINNs (Figure 1). This brings insights into the sub-resolved morphological features and provides an accurate description of the porous material initial state by observing its dissolution. We identified enhanced uncertainties on the calcite core edges, which confirm the challenges and discrepancies associated with estimating mineral reactivities through purely differential imaging techniques [7]. Finally, we ensure reliable calibration of the pore-scale PDE model parameters by identifying posterior distributions of the corresponding dimensionless numbers in the inverse problem formulation. Overall, combining data-driven and physics-based AI approaches allows to effectively address robust UQ at the pore-scale and to propagate the uncertainties for CO₂ leakage risk assessment due to carbonate dissolution in acidic fluids.

Propagating uncertainties on hydraulic conductivity based on fracture roughness

Fault conductivity in natural damage zones remains uncertain and sensitive to geometrical characteristics such as fracture aperture distributions and roughness. This queries the validity of the Cubic Law approximation for estimating fracture permeability, especially considering the discrepancies that roughness can induce between the mechanical and effective hydraulic apertures [12]. While assuming smooth fracture walls is a common assumption at the reservoir scale, uncertainties associated with such model mis-specification or falsification need to be investigated to support decision-making processes in fault-related leakage [13].

We propose an AI-driven propagation of the uncertainties on the hydraulic conductivity of fractures, accounting from their roughness at the pore and laboratory scales, by identifying the relevant hydraulic aperture through the combination of data-driven and physics-based formulations. This aims to mitigate the uncertainties associated with both, the Cubic Law modelling approximation and the measurement data of the mechanical aperture field obtained from X-ray μ CT. Permeability deviations due to the fracture roughness can then be upscaled to provide meaningful ranges of fault conductivities at the larger scales.

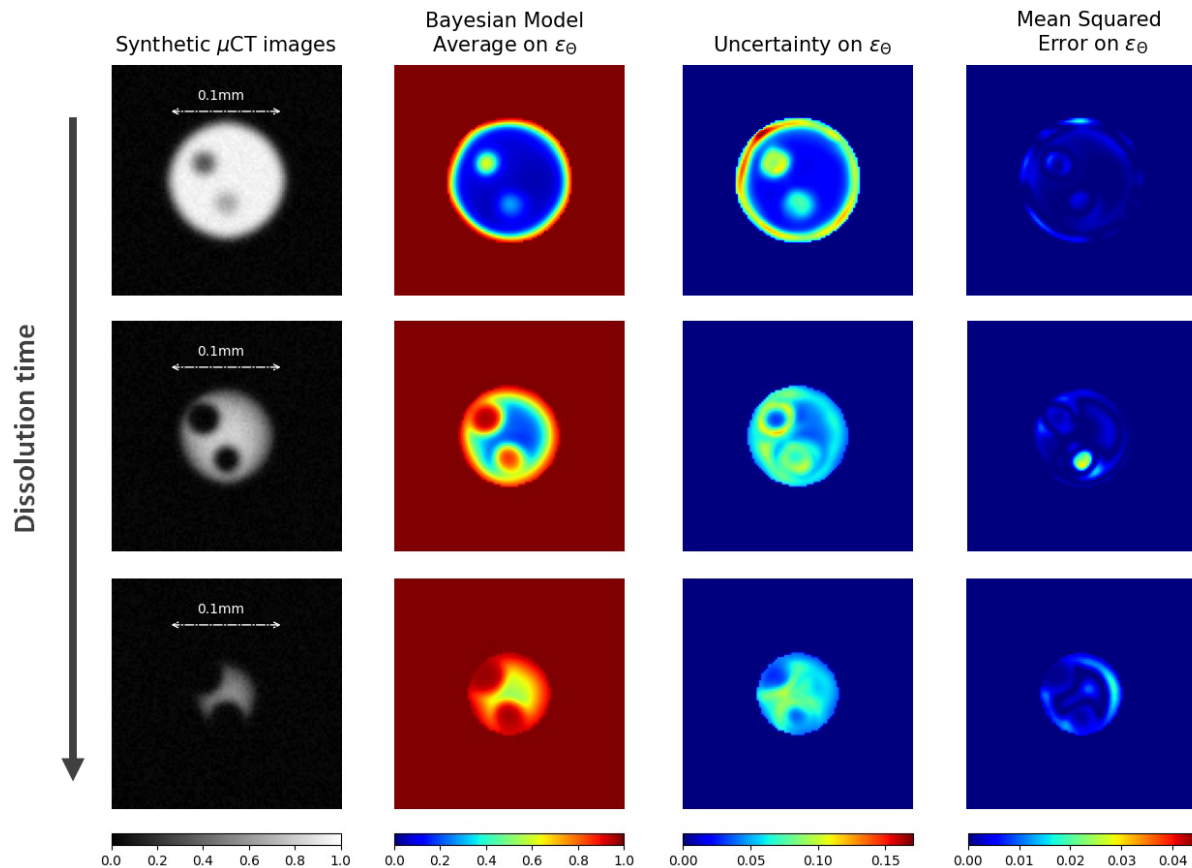


Figure 1 Predictions of the surrogate micro-porosity field ε_θ along the dissolution process of a calcite core using the AI-driven data assimilation framework developed in [10, 11]. Synthetic μ CT dynamical images, corrupted by strong noise, at the initial state and several dissolution times, on the left. The grey level intensities \mathcal{I}_m , depicting the material local attenuation, are related to the micro-porosity field by the mapping $\mathcal{I}_m = 1 - \varepsilon_\theta + \xi$, with ξ the measurement uncertainty arising from the noise. Bayesian Model Average predictions on ε_θ with the local uncertainties along the dissolution times, in the middle. Mean Squared errors between the micro-porosity ε and the surrogate field ε_θ , on the right.

Conclusions

Uncertainty quantification plays a crucial role in the sustainable management of CCS technologies and in the risk assessment of potential CO₂ leakage. The multi-scale considerations of the phenomena involved in CO₂ storage, either related to mineral reactivity or complex flow behaviours, affect the uncertainties at different levels. Investigating the propagation of uncertainties across the scales is therefore of great importance to achieve reliable predictions. AI approaches offer such a promising support to ensure reliable decision-making, especially when using experimental data and mathematical modelling through the combination of data-driven and physics-based approaches.

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