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On the generation of 3D Microstructural Models to Analyze Creep and Permeation Behavior through Digital Twin Simulations

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Abstract

This study presents the development of three-dimensional (3D) input datasets of natural rock salt at the laboratory scale, intended to support digital twin simulations of creep and permeation behavior. These simulations aim to improve the interpretation of experimental results and facilitate more reliable upscaling to reservoir-scale conditions. The 3D digital twin models introduced here account, for the first time, for internal grain size variations, providing a more realistic representation of sample heterogeneity to support advanced simulation workflows.

Natural rock salt exhibits significant heterogeneity in grain size and impurity content, further complicated by artifacts introduced during coring and laboratory preparation. Understanding how this heterogeneity influences deformation and fluid transport remains a key challenge.

Core samples from a Danish salt diapir were analyzed using multiscale imaging techniques, including reflected-light microscopy, slab-scale imaging in 2D, and 3D micro-computed tomography (CT). Grain sizes were quantified using semi-automated segmentation of thin sections and slab photographs, as well as a machine learning-based classification of CT data. A random forest classifier was trained on the basis of 2D data to segment CT volumes into distinct grain size classes and anhydrite-rich phases. Creep and permeation test results were linked to the internal grain size distributions of each sample.

Grain sizes measured from thin sections aligned well with creep rates predicted by established pressure solution creep laws, whereas coarser-grain estimates from CT and slab analyses underestimated deformation rates, likely due to unresolved fine grains or the passive role of large grains. In permeation tests, samples with larger grain sizes and mega-grain inclusions exhibited increased fluid transport, suggesting reduced healing efficiency and enhanced flow along coarse-grain boundaries.

Notably, discrepancies between 2D and 3D grain size estimates – particularly in samples exhibiting pronounced layering or coarse-grained facies with tabular-shaped grains – underscore the importance of considering spatial heterogeneity and directional textural variation when interpreting the mechanical and transport behavior of rock salt.

This study emphasizes the necessity of accurately capturing microstructural heterogeneity in digital models to better understand the mechanical and hydraulic response of rock salt. The generated 3D datasets serve as a foundational resource for future digital twin simulations, which will explore how internal grain size variation and structural anisotropy influence localized deformation and fluid flow.

Key words: rock salt, 3D digital twin models, digital rock physics, grain size facies, 3D anisotropy