Multi-scale numerical simulation of the viscoplastic behavior of rock salt

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Abstract

The global energy landscape is undergoing a significant transformation driven by the urgent need to mitigate climate change and reduce carbon emissions. Hydrogen stands out as a highly promising alternative among the various energy storage methods under investigation, offering the potential to decarbonize multiple sectors-ranging from transportation to industrial processes-and acting as a versatile fuel for energy systems. As a green energy carrier, hydrogen's role in future energy systems could be transformative. However, one of the major hurdles for the widespread deployment of hydrogen-based systems is the challenge of storing hydrogen safely and efficiently. Hydrogen's low density, combined with its high reactivity, presents significant challenges in terms of storage volume and containment safety, necessitating the development of innovative storage solutions.
Underground geological formations, such as depleted oil and gas reservoirs, aquifers, and salt caverns, have been considered for large-scale hydrogen storage. Among these, rock salt formations are especially attractive due to their unique physical and mechanical properties. One of rock salt's most critical properties is its viscoplastic behavior, which allows it to deform slowly under pressure while maintaining structural integrity. This viscoplasticity enables the formation of stable cavities in rock salt, which can accommodate high-pressure conditions over extended periods. Additionally, rock salt possesses a self-healing capability, where cracks generated by stress naturally seal over time, making it highly reliable for containing gases like hydrogen. These self-healing properties, coupled with the absence of permeability, reduce the risk of leakage, thereby enhancing safety. Unlike other geological formations that may require significant engineering interventions to ensure containment, rock salt's inherent characteristics provide a naturally stable and secure environment for hydrogen storage.

The primary objective of this research is to advance the numerical modeling of rock salt's viscoplastic behavior, focusing specifically on its application in hydrogen storage. Previous studies have explored the viscoplastic properties of rock salt, highlighting the importance of crystal slip plasticity observed at the level of individual grains. However, there is a need to go beyond conventional models by incorporating additional deformation mechanisms-namely, inter- and intra-granular cracking. Experimental evidence has shown that the opening and sliding of grain boundaries occur concomitantly with the viscoplastic deformation observed by formation of glide planes on the grain surfaces. These phenomena, often overlooked in traditional models, are significant because grain boundary sliding and opening can account for up to half of the total strain experienced by the rock salt, depending on the size of the

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grain aggregate. Although crystal slip plasticity remains the dominant deformation mechanism, accurately modeling the behavior of grain boundaries is essential for predicting the overall mechanical response of rock salt.

This research seeks to address the gap in the current understanding of grain boundary behavior by developing a more comprehensive model that integrates these cracking mechanisms. Specifically, the study aims to formulate a thermodynamically consistent relationship between the traction and separation which governs the material behavior at grain boundaries. Additionally, since rock salt exhibits rate-dependent behavior, the model must account for this rate dependency at the grain boundaries by incorporating a rate-dependent traction-separation law. This will allow for a more accurate prediction of how the material behaves under different loading rates, which is key for ensuring long-term stability and safety in hydrogen storage applications. This traction separation law is also tailored for rock salt in both mode I and mode II of fracture, accommodating for the co-dependency of the opening and sliding.

The methodology employed in this research involves the use of multi-scale numerical simulations to capture the complex deformation mechanisms of rock salt. These simulations are performed using finite element analysis within the MOOSE (Multiphysics Object-Oriented Simulation Environment) framework, an open-source platform widely used for modeling complex physical systems. The multi-scale approach allows for the integration of deformation behaviors observed at different length scales, from the microstructural level of individual grains to the macroscopic level of the polycrystalline rock. By capturing the behavior of cracks at grain boundaries, as well as within the grains themselves, this study aims to provide a more accurate and detailed prediction of the mechanical response of rock salt highlighting the interplay between cracking and the crystal slip plasticity.
By developing a constitutive model that incorporates the experimentally observed deformation mechanisms (the crystal slip plasticity and grain boundary cracking), this study will contribute to more accurate predictions of how rock salt behaves under the conditions imposed by hydrogen storage and will be compared to experimental results conducted at different observation scales within the framework of the ANR RockStoryHy project (Multiscale investigation of ROCKsalt flow for underground STORage of Hydrogen) by other collaborators. The coupling of all these mechanisms, made possible by the MOOSE advanced framework, will allow us to investigate numerically the competition and interaction between intergranular and transgranular deformation mechanisms and fracture. These insights will be invaluable for the operation of underground hydrogen storage facilities, which are critical for the large-scale deployment of hydrogen as a green energy carrier.