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Perspective

Numerical simulation and optimization design of complex underground fracture network

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Abstract:
Understanding the complex behavior of fractured rock systems is critical for applications in energy development, geological sequestration, and tunnel construction. Microscale fracture surface morphology influences flow and mechanical behaviors, while upscaling frameworks. Despite progress in hydro-mechanical and thermo-hydro-mechanical coupling models, two-way mechanical-chemical interactions remain underexplored. Discrete fracture networks offer a robust statistical framework for modeling subsurface fracture systems. Advances in machine learning have accelerated the simulation and optimization of fractured geothermal systems, addressing the computational limitations of high-fidelity models. These methods support multi-objective design, enhance life cycle assessments, and provide insights into optimal geothermal management strategies. Fractured rocks serve as preferential pathways for fluid flow and heat transport, significantly influencing permeability and mechanical stability. However, the inherent complexity of coupled thermo-hydro-mechanical-chemical processes in these systems presents major challenges. Nonlinear fracture mechanics, stress perturbations, and chemical interactions drive dynamic changes in fracture connectivity and permeability, further complicated by recursive feedback mechanisms. By integrating numerical tools, machine learning techniques, and advanced discrete fracture network models, the fractured rock system could be optimized and clearly analyzed.

1. Introduction

Fractured rock systems play a pivotal role in subsurface processes, influencing fluid flow, heat transfer, and mechanical stability across geoengineering applications such as geothermal energy, geological sequestration, and tunnel construction. The complexity of these systems arises from the coupled thermo-hydro-mechanical-chemical (THMC) processes, which govern fracture behavior and connectivity. Stress perturbations, chemical interactions, and feedback mechanisms further complicate the dynamics, challenging accurate modeling and prediction.

Discrete fracture networks (DFNs) offer a practical statistical framework for representing these systems, enabling efficient characterization of fracture geometries and connectivity. Machine learning (ML) methods, which is extensively used to provide accurate predictions (Wood, 2023), have advanced the simulation of fractured systems, overcoming computational constraints of traditional high-fidelity models.

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This perspective aims to explore the mechanisms governing connectivity in complex fractured networks and its evolution over time. By integrating DFN modeling, ML approaches, and upscaling frameworks, the research seeks to provide novel insights into optimizing energy systems and addressing environmental challenges in a sustainable and decarbonized future (Feng et al., 2024).

2. Complexity and challenges of THMC coupling in fractured rock masses

The mechanical, mass/heat transport, and THMC coupling mechanisms in fractured rocks are crucial for geoengineering and geoscience applications, such as tunnel construction, energy development, and geological sequestration (Xia et al., 2024). However, THMC coupling processes in fractured rocks are inherently complex. First, the mechanical behaviors of fractures present significant complexities involving nonlinear normal closure, shear slip and dilatancy, matrix damage, and fracture propagation. Shear behaviors of fractures are further controlled by intricate mechanisms such as slip weakening and rate-and-state friction, foundational to understanding rapid, sudden slip during fault reactivation and earthquake triggering (Xia et al., 2024Ikari et al., 2013). Stress perturbations-arising from hydraulic poroelastic or thermoelastic effects—disrupt fracture mechanical equilibrium, altering normal closure, dilatancy, and fracture connectivity. These stress changes also impact permeability, fluid flow, and heat transfer, forming the fully coupled thermal-hydraulic-mechanical effect. Introducing chemical processes, particularly water-rock interactions (i.e., dissolution/precipitation), further complicates these coupling mechanisms. Geomechanical deformations influence fracture aperture changes caused by water-rock interactions, affecting fluid flow and reactive transport. Conversely, water-rock interactions modify fracture morphology, altering local stiffness and redistributing stress along fracture surfaces (Ameli et al., 2014). When THMC coupling mechanisms combine various fracture networks and boundary conditions, complex higher-order effects emerge. For instance, stress-induced fracture propagation may significantly alter flow networks, impacting the transport properties (Wang et al., 2023a) and capture capacity of upscaling models (Jiang et al., 2024). Therefore, systematic numerical simulation is an effective approach to understanding the THMC coupling mechanisms, starting with simplified models to incrementally incorporate complexity and dissect interactions.

Transitioning from laboratory-scale phenomena to site- and regional-scale applications is essential for practical implementation. At the microscale, flow and geomechanics are controlled by fracture surface morphology and asperity contact, while at larger scales, an upscaling framework through the representative elementary volume concept implicitly captures the microscopic mechanisms via equivalent parameters (such as stiffness and hydraulic/mechanical aperture) and constitutive laws. Extensive site-scale studies based on DFN models within the upscaling framework have advanced understanding of hydro-mechanical and thermal-hydraulic-mechanical coupling. However, site-scale two-way mechanical-chemical coupling remains underexplored, with many models assuming constant fracture aperture and neglecting anisotropy and heterogeneity (Salimzadeh and Nick, 2019). Developing robust, fully coupled THMC models remains challenging, but careful simplifications and advancements in numerical tools will enable accurate, efficient simulations tailored to real-world scenarios.

3. ML-accelerated fracture network characterization and geothermal energy system optimization

As a sustainable and robust energy source instrumental in the cost-effective decarbonization of electrical systems, geothermal energy emerges as an essential technological asset capable of playing a pivotal role in a decarbonized future. Fractured rocks provide preferential fluid pathways within the geothermal systems due to the lower hydraulic resistance in comparison with the surrounding host rock and transport most of the solute and thermal energy. Understanding fracture distribution and heat transport in a fracture network are crucial to predict possible fluid dynamics and heat extraction (Wang et al., 2023b), optimize the heat extraction, and manage reservoir conditions with respect to dynamic changes. Consequently, fracture network characterization and design optimization hold profound significance for addressing earth, energy, and environmental challenges.

ML has emerged as a robust method for developing surrogate models, leading to significant advancements in various scientific and engineering fields (Bergen and Johnson, 2019), and promoting growth in geothermal energy and other related energy systems. Surrogate models, also referred to as metamodels or proxies, are cost-effective and analytically manageable mathematical models created from ML techniques to approximate the characteristics of complex systems (Karniadakis et al., 2021). Techniques such as Gaussian processes can effectively explore the objective landscapes and decipher multi-variable relationships. To mitigate the time-consuming nature of high-fidelity simulations, offline machine learning methods serve as surrogates for predicting fluid dynamics as described by partial differential equations. The construction of these surrogates enables parameter inversion and design optimization processes to become much more computationally efficient, thereby enhancing the speed of decision-making. However, these methods can experience significant approximation errors when the training dataset is limited, which may steer the evolutionary search in the wrong direction. Deep learning-based surrogate models have gained considerable recognition as alternatives to numerically evolving partial differential equations. Despite this, training globally accurate surrogates for complex systems often requires numerous simulation evaluations, which can be quite labour-intensive. GAN-based generative model is a considerable way to characterize the high-dimensional parameter fields (Chen et al., 2023, 2024), contributing insights into optimal geothermal well-control schemes and operational techniques for a decarbonized future.

4. Characterization and evolution of connectivity in complex fracture systems

DFNs offer a practical alternative for simulating complex fracture systems. These networks can be generated through various methods, including direct mapping from roadcuts, tunnels, and geomechanical simulations, as well as stochastically-generated fracture networks (Lei et al., 2017). The stochastically-generated fracture networks are computationally efficient and statistically robust, where different statistical distributions are used to describe essential fracture geometries. Connectivity is a fundamental characteristic of fracturing networks, directly influencing rock stability and hydraulic diffusivity. However, quantifying the impact of different geometries on connectivity is difficult. Natural fracture networks are composed of multiple clusters, which arise from compressive loads, mineral growth, and other factors. The quantification and evolution of connectivity can be addressed when the total connectivity of complex fracture networks consisting of multiple clusters is obtained (Zhu et al., 2021). Furthermore, the discrete element method and lattice Boltzmann method can be combined with the DFN approach, to investigate fracture initiation and propagation under significant stress disturbances (Zhu et al., 2024).

In summary, DFNs provide a practical framework for investigating complex fracture networks from a statistical perspective. While they may not provide a unique solution for actual subsurface structures, they offer valuable insights into essential influencing factors and the evolution of fracture networks. This approach helps us better understand the "black box" of subsurface fracture systems.

5. Conclusions

The perspective highlights the critical role of connectivity in complex fracture systems and its influence on fluid flow, heat transfer, and mechanical stability. Advanced modeling techniques, including DFNs, machine learning, and upscaling frameworks, enable efficient characterization and simulation of THMC coupling mechanisms. These approaches provide valuable insights into the evolution of fracture connectivity, offering practical solutions for optimizing energy systems and addressing potential challenges in a sustainable and decarbonized future.

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Conflict of interest

The authors declare no competing interest.

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