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Research Paper

Integrated Study of Geochemical, Geomechanical, and Mineralogy Leak Potential on Caprocks with Shale: A Review

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Abstract
This study presents an integrated analysis of the geochemical, geomechanical, and mineralogical properties of shale caprocks in Asian sedimentary basins to evaluate their potential for leakage in carbon sequestration and petroleum extraction applications. Caprocks play a critical role in trapping subsurface fluids, ensuring both environmental protection and operational efficiency. The geochemical analysis involved detailed mineralogical characterization using X-ray diffraction (XRD) and evaluation of formation water chemistry, highlighting interactions with injected CO_2-rich fluids. Variations in mineral content—such as clay, quartz, and carbonate—significantly influence the sealing capabilities and chemical stability of shale formations.
Geomechanical properties were thoroughly investigated, focusing on strength, porosity, permeability, elastic and acoustic characteristics, and reactive surface area. Laboratory experiments and numerical modeling have demonstrated that shales exhibit remarkably low permeability, generally less than that of microfacies to nanodevices, paired with limited porosity, typically below 10%. Elastic parameters indicated significant variability related to mineralogical differences; quartz- and carbonate-rich shales were stiffer and more brittle, increasing fracture risks, whereas clay-rich shales were more ductile, better accommodating deformation without fracturing. Furthermore, the reactive surface area of clays, particularly smectite and illite, has a significant impact on geochemical reactions, influencing the long-term integrity of the caprock.
The novelty of this study lies in its comprehensive integration of multiple disciplinary analyses, specifically targeting shale caprocks, where diverse geological conditions prevail. Findings reveal critical correlations between mineralogical composition, geomechanical behavior, and sealing capacity, enabling more reliable prediction of leak risks associated with carbon sequestration and petroleum extraction. The outcomes provide essential guidance for reservoir management practices, significantly contributing to the safe and sustainable development of energy and supporting regional and global efforts to reduce greenhouse gas emissions.

Keywords: *shale caprocks, geochemical, geomechanical, mineralogy, leak potential*

INTRODUCTION

Caprocks are essential geological formations that act as barriers, preventing fluids from migrating out of subsurface reservoirs (Ali et al., 2021). Due to their low permeability and favorable mineral composition, shale formations commonly serve as effective caprocks for petroleum reservoirs and carbon sequestration projects. Understanding caprock behavior in potentially reactive fluids is critical to the safe and predictable long-term storage of CO2 within geological media. Injection of CO2 for storage into saline aquifers and/or depleted hydrocarbon reservoirs will alter the in-situ geochemical environment (Worden & Smith, 2004), potentially leading to reactions with the caprock that holds the injected gas in place. An integrated approach that considers geochemical properties, geomechanical behavior, and mineralogical characteristics is crucial to understanding their potential to prevent leaks (Dewhurst et al., 2018).

Geochemically, Asian shale caprocks typically consist of clay minerals, quartz, carbonates,

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and feldspar. Clay minerals such as smectite, illite, chlorite, and kaolinite dominate, significantly impacting the sealing capacity through their swelling properties and reactive nature. Quartz and carbonate minerals contribute to the strength and brittleness of shales, influencing their susceptibility to fractures and leakage under stress (Baines & Worden, 2004a).

Geomechanical analyses measure properties like strength, porosity, permeability, elastic, and acoustic parameters. Asian shale caprocks exhibit low permeability, often ranging from microdarcy to nanodarcy levels, with limited porosity typically less than 10%. Elastic properties, indicated by Young's modulus and Poisson's ratio, reveal significant variations depending on mineral composition. Higher quartz and carbonate content correlate with brittleness, whereas clay-rich shales are typically more ductile, making them less susceptible to fracturing. This, in turn, may alter the geomechanical and petrophysical properties of the caprock, possibly increasing the risk of migration out of the host reservoir (Baines & Worden, 2004b).

Mineralogical studies, utilizing X-ray diffraction (XRD) and Scanning Electron Microscopy (SEM), reveal a direct relationship between mineral composition and caprock integrity. Clay-rich shales usually offer high sealing capability and potential for self-healing, while carbonate-rich shales can undergo transient permeability changes upon interaction with CO_2-charged fluids. Depending on the formation's specific mineralogy and fluid chemistry, these interactions either enhance or impair the caprock integrity.

Integrating geochemical, geomechanical, and mineralogical evaluations is critical for accurately assessing leak potential in Asian shale caprocks. Such comprehensive studies guide the development of reliable strategies for long-term carbon sequestration and sustainable petroleum extraction, minimizing environmental risks and ensuring reservoir integrity.

LITERATURE REVIEW

The Significance of Shale Caprock Integrity

Shale caprock plays a crucial role as a geological barrier, preventing subsurface fluid migration to the surface. The effectiveness of shale formations as caprock in maintaining their integrity is critical for various subsurface applications (Soldal, 2008). The fundamental capacity of shale formations as caprock lies in their physical properties, namely, low permeability and porosity. The low permeability of shale is generally attributed to its composition, which is typically dominated by fine-grained materials, particularly clay minerals, and a complex, tortuous pore network. In the context of growing concerns about greenhouse gases, geological carbon dioxide storage (GCS) has emerged as a promising technology to reduce atmospheric CO_2 concentrations. Similarly, the increasing subsurface storage of hydrogen as a key component of sustainable energy highlights the essential role of the long-term integrity and sealing capacity of caprock formations in ensuring the durability and safety of these vital solutions. Therefore, a comprehensive understanding of the intricate interactions among geochemical reactions within shale, the geomechanical stresses acting upon it, and its mineralogical composition is crucial for improving accuracy in predicting potential fluid leakage from subsurface reservoirs and other applications that rely on the sealing capacity of shale caprocks (Murugesu et al., 2024).

Interplay of Geochemical, Geomechanical, and Mineralogical Aspects in Shale Caprocks: A Theoretical Framework

The integrity of shale caprocks arises from the intricate interplay among geochemical, geomechanical, and mineralogical processes. Perturbations in any one of these domains invariably influence the others, thereby modifying the formation's sealing capacity. Geochemical interactions between injected fluids and shale minerals may alter the rock's composition, with subsequent effects on its mechanical strength, elasticity, and permeability (Dilshan et al., 2024). Geomechanical perturbations, such as elevated pore pressure induced by fluid injection or tectonic activity, can generate or reactivate fractures, establishing potential pathways for fluid migration and simultaneously accelerating geochemical reactions. The mineralogical composition, particularly the clay content, influences both geochemical reactivity and geomechanical response. For example, clay swelling upon hydration can diminish permeability while concurrently inducing internal stresses, underscoring the coupled and interdependent nature of these processes (Kolawole et al., 2021).

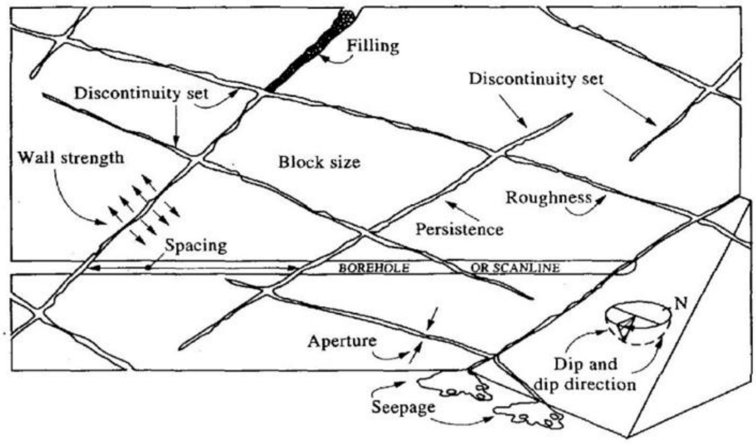

Figure 1. Geometric Properties of Discontinuities (Hudson & Priest, 1979)

Interactions among geochemical, geomechanical, and mineralogical processes in shale caprocks occur across multiple scales, ranging from nanometer-sized pores to large fracture systems. Fluid migration may proceed slowly through fine pore networks or rapidly along fractures. Geochemical reactions at the mineral grain scale can alter the shale's microstructure, thereby influencing its overall strength and permeability. These processes are inherently time-dependent. Reactive minerals, such as carbonates, may dissolve rapidly in acidic solutions, whereas silicate transformations may occur over thousands of years. Mechanical responses, such as creep under sustained stress, introduce additional long-term complications for the sealing integrity of caprocks. Accurate prediction of caprock behavior thus necessitates a comprehensive understanding of these complex, scale-dependent, and time-dependent interactions (Shi et al., 2024).

Geochemical Controls on Leak Potential

a. Diffusion and Advection in Shale Caprocks

Fluid migration within shale caprocks is governed predominantly by two mechanisms: diffusion and advection. Diffusion is driven by concentration differences, whereby fluids such as CO2 migrate from regions of higher concentration to regions of lower concentration. In the context of geological CO2 storage, diffusion becomes the dominant transport process under low-pressure gradients, allowing dissolved CO2 to permeate the caprock over extended timescales. Advection, in contrast, refers to the bulk displacement of fluids induced by pressure gradients, which may arise from buoyant forces associated with CO2 or from elevated injection pressures. This mechanism is typically more rapid and efficient, particularly in the presence of fractures or faults that provide preferential pathways with high permeability. The microstructural characteristics of shale, including porosity and tortuosity, exert a primary control on diffusive transport. Elevated tortuosity reduces diffusion efficiency by imposing complex and elongated pathways for fluid movement. Furthermore, the inherent anisotropy of shale results in directional variability in diffusion rates, with transport occurring more readily along bedding planes than across them. Consequently, robust long-term prediction of CO2 migration necessitates a comprehensive understanding of the coupled dynamics of diffusion and advection in anisotropic, heterogeneous caprock systems (Al-Yaseri et al., 2023; Jia et al., 2023).

b. Fluid-Rock Interactions: Dissolution, Precipitation, and Transformation Processes

When injected fluids, such as CO_2-rich brine, interact with shale minerals, a suite of complex geochemical processes is initiated, including dissolution, mineral transformations, and secondary mineral precipitation.

- **Dissolution:** Acidic CO_2-rich brine can dissolve carbonate minerals (e.g., calcite, dolomite), resulting in increased porosity and permeability but potentially weakening the rock framework if the dissolved phases function as cements.
- **Clay mineral transformations:** Under certain conditions, clay minerals may transform (e.g., illite to kaolinite). Moreover, clay swelling upon hydration can reduce permeability by constricting pore throats, while simultaneously generating internal stresses that can induce new microfractures.
- **Precipitation:** The supersaturation of formation fluids can promote the precipitation of secondary minerals (e.g., calcite, barite, silica), which may decrease permeability through pore and fracture occlusion or alter porosity depending on the locus of deposition.

These fluid–rock interactions can either enhance or compromise the sealing capacity of shale caprocks. Precipitation processes may contribute to improved sealing, whereas dissolution and clay swelling can create or exacerbate potential leakage pathways. The overall impact is contingent upon the mineralogical composition of the shale and the geochemical characteristics of the interacting fluids (Dilshan et al., 2024; Shi et al., 2024; Shukla et al., 2010).

c. The Role of Secondary Mineral Formation on Seal Integrity

The formation of secondary minerals as a consequence of fluid–rock interactions exerts a critical influence on the long-term sealing capacity of shale caprocks:

- **Positive effects:** The precipitation of carbonate minerals (e.g., calcite, dolomite, siderite) and sulfate minerals (e.g., barite, gypsum) can decrease permeability by occluding pore throats and sealing fractures, thereby enhancing the caprock's ability to retain fluids. Such processes are particularly advantageous in the context of CO2 sequestration, where stable mineral trapping provides a long-term storage mechanism for carbon dioxide.
- **Negative effects:** Conversely, mineral precipitation within the shale matrix may modify the pore network in ways that either increase or decrease permeability. Additionally, volumetric expansion associated with mineral growth may induce mechanical stresses, potentially generating new fractures or reactivating pre-existing ones, which can compromise seal integrity.
- **Reversibility:** Certain mineral reactions, such as the dissolution–precipitation dynamics of calcite, are reversible and sensitive to evolving geochemical conditions. As a result, sealing effectiveness may fluctuate over time.

The overall impact of secondary mineral formation is therefore highly context-dependent, governed by the type of mineral precipitated, its spatial distribution, and the dynamic geochemical environment in which it occurs. These factors interact in complex ways, such that the same process may either enhance or undermine sealing capacity. This underscores the necessity of evaluating mineralogical evolution in tandem with geochemical and geomechanical conditions when assessing the long-term performance of shale caprocks as sealing barriers (Al-Yaseri et al., 2023; Shukla et al., 2010).

Geomechanical Behavior and Leakage Pathways in Shale

a. Mechanical Strength and Failure Mechanisms of Shale under Stress

The mechanical properties of shale are governed by its mineralogical composition, porosity, fluid saturation, and prevailing stress conditions. Depending on the stress environment, shale may undergo brittle failure, ductile deformation, or exhibit semi-brittle behavior, with higher confining pressures generally promoting a transition from brittle to ductile responses. Failure mechanisms can manifest through tensile fracturing, shear failure along weakness planes, or slip along bedding planes, with stress orientation relative to bedding exerting a strong influence on the dominant mode of failure. The presence of water further complicates shale's mechanical behavior by reducing compressive strength and enhancing plasticity through the hydration of clay minerals, thereby increasing susceptibility to deformation and failure. Moreover, the inherent anisotropy of shale results in directional variability in strength and deformation characteristics, depending on the orientation of the applied stresses relative to the bedding structures. Collectively, shale's mechanical response reflects the coupled effects of mineralogy, stress state, fluid saturation, and anisotropy, all of which must be rigorously assessed to evaluate and predict the long-term integrity of shale caprocks (Kolawole et al., 2021; Shi et al., 2024).

b. Permeability Evolution in Shale: Influence of Stress and Fluid Interactions

Shale's inherently low permeability underpins its effectiveness as a caprock. However, its permeability is highly sensitive to variations in stress state and fluid–rock interactions. Increasing effective stress, defined as confining pressure minus pore pressure, generally reduces permeability by compacting the pore network and closing microfractures. In contrast, shear deformation can initially enhance permeability by forming or reactivating fractures. However, prolonged shear may ultimately reduce permeability due to the accumulation of wear products and clogging of fractures. Geochemical processes further modulate permeability: mineral dissolution can enlarge pore spaces and increase permeability, while weakening the rock framework; precipitation of secondary minerals, such as calcite or barite, can occlude flow pathways and decrease permeability; and clay swelling upon hydration can markedly reduce permeability by constricting pore throats. Consequently, shale permeability should be regarded as a dynamic property that evolves in response to coupled mechanical and geochemical processes, underscoring the necessity of integrated modeling approaches that incorporate stress, deformation, and fluid–rock interactions to accurately predict caprock performance (Dilshan et al., 2024; Shi et al., 2024).

c. Fracture Dynamics in Shale Caprocks: Initiation, Propagation, and Self-Sealing

Fractures, whether naturally occurring or induced, represent potential high-permeability pathways that can compromise the sealing capacity of shale caprocks. Such features may originate from tectonic stresses, diagenetic processes, overpressure, or uplift, and can also be induced by engineering activities including drilling, hydraulic fracturing, and fluid injection. Fracture initiation and propagation occur when the in-situ stress state, defined by principal stresses and pore pressure, exceeds the tensile strength of the shale. Bedding planes and pre-existing weaknesses exert a firm control on fracture orientation and growth. Importantly, fractures do not always persist as permanent conduits. Self-sealing mechanisms may operate through geochemical processes, such as mineral precipitation (e.g., calcite, barite) and clay swelling, or through geomechanical processes, including fracture closure under confining stress, particularly when dissolution has smoothed the fracture surfaces. The anisotropic nature of shale further influences fracture networks, creating directional variability in fluid flow. Faults, on the other hand, may function either as conduits or as barriers, depending on their structural characteristics and stress state. Consequently, fractures constitute a dynamic risk to seal integrity, and their capacity to self-seal under favorable conditions is critical for ensuring the long-term containment performance of shale caprocks (Alanazi et al., 2022; Khan et al., 2024; Kolawole et al., 2021; Paluszny et al., 2020).

RESEARCH METHOD

Integrating geochemical, geomechanical, and mineralogical analyses ensures the reliability of assessments of caprock integrity. In Indonesia, identifying optimal intervals within shale formations—balancing mechanical strength, geochemical stability, and low permeability—is essential for successful carbon sequestration projects and sustainable petroleum extraction. Continuous monitoring and adaptive management strategies, informed by integrated analyses, significantly enhance long-term reservoir safety and efficiency (Dewhurst et al., 2018).

Summary of Key Insights:

- Indonesian shale caprocks exhibit highly favorable sealing characteristics, characterized by low permeability and limited porosity.
- Geochemical stability largely depends on the mineralogical composition and the chemistry of the formation water, which impact the long-term integrity.
- Elastic and acoustic parameters guide geomechanical assessments to avoid fracturing risks.
- Reactive mineralogy can either strengthen or weaken sealing capacity depending on fluid-rock interactions, underscoring the importance of mineralogical and geochemical evaluations.

This integrated approach provides critical insights for managing leak potential and ensuring the integrity of caprocks in carbon sequestration and petroleum extraction operations.

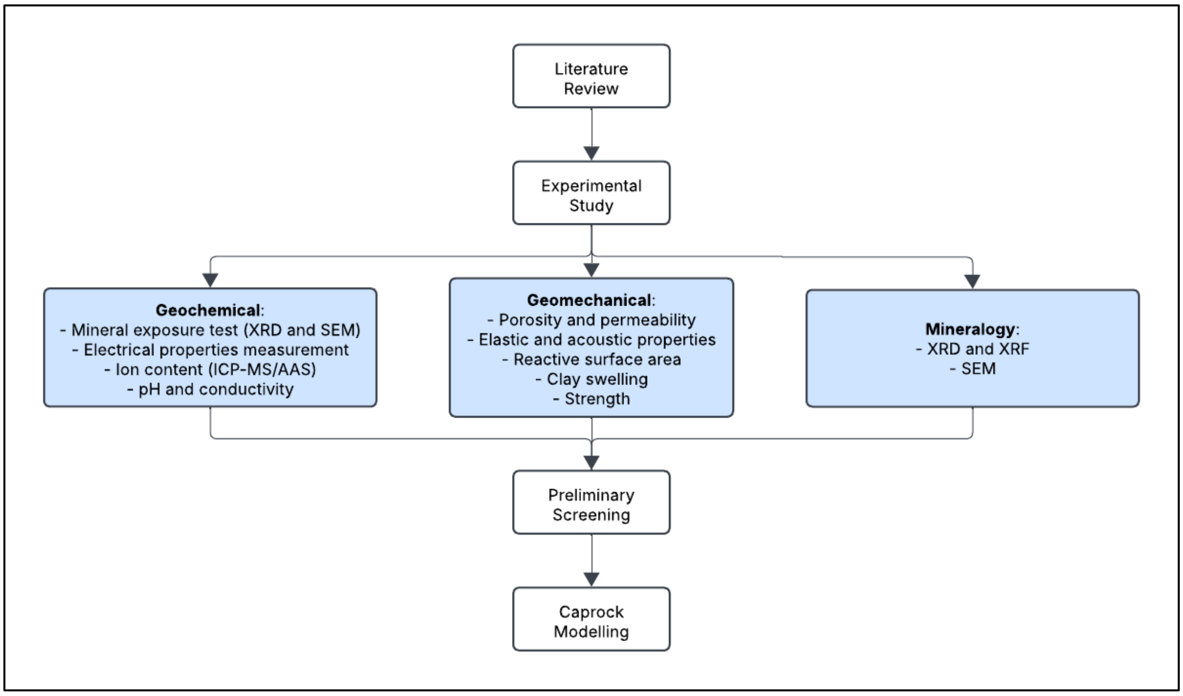

Figure 2. Research Flow Diagram

FINDINGS AND DISCUSSION

Integrating the Geochemical and Geomechanical Analysis with Mineralogy Study to Harness the Accuracy of Mitigation of Leakage in Caprock. Clay mineralogy exerts a profound influence on the geochemical reactivity, mechanical behaviour, and sealing capacity of shale caprocks. Different clay types—such as smectite, illite, kaolinite, and chlorite—exhibit distinct responses when exposed to CO_2-rich brine. Smectite is highly expansive upon hydration, leading to swelling that reduces permeability by constricting nanopores. Illite and kaolinite, in contrast, are more prone to dissolution or transformation into secondary mineral phases under acidic conditions. The surface charge of clay minerals also affects ion partitioning and transport, shaping reaction pathways and ultimately controlling fluid migration through the shale matrix. Moreover, certain clays act as catalysts, accelerating specific geochemical reactions that can alter mineral assemblages and influence the strength of rocks. Consequently, the type and proportion of clay minerals are critical in determining the extent of dissolution, precipitation, and overall permeability, underscoring their central role in predicting long-term caprock performance.

Mineralogical composition also dictates the geomechanical properties of shale. Substantial, brittle minerals such as quartz, feldspar, and carbonates contribute to higher compressive strength, stiffness, and brittleness, while high clay content reduces strength and increases ductility. This duality means that clay-rich shales are generally more resistant to fracturing but may deform plastically under stress. Permeability is likewise controlled by mineralogy and microstructure. Elevated clay content decreases permeability due to smaller pore sizes and greater tortuosity, whereas the arrangement of clay and non-clay minerals affects pore connectivity and fluid transport efficiency. The balance between brittle and ductile components, therefore, governs both fracture resistance and fluid flow, highlighting the importance of detailed mineralogical characterization for reliable assessment of sealing integrity.

Clay swelling introduces an additional layer of complexity. When hydrated, swelling can be beneficial by narrowing or blocking nanopores, thereby reducing permeability and enhancing sealing capacity. High-expansion clays such as smectite are particularly effective in this respect. However, swelling can also generate internal stresses that lead to the formation or widening of fractures, which may increase the risk of leakage. In operational contexts such as drilling, excessive swelling can compromise wellbore stability and reduce efficiency. The extent and direction of swelling effects depend on the type, content, and environmental factors of the clay, including water salinity, ionic strength, temperature, and pressure. In high-ionic-strength brines, for example, swelling may be suppressed or exacerbated depending on chemical compatibility with formation fluids. Thus, clay swelling is a context-dependent process that can either reinforce caprock integrity or undermine it by inducing structural weaknesses.

CONCLUSIONS

Complex interactions between geochemical, geomechanical, and mineralogical processes determine the integrity of shale caprocks in CO_2 storage systems. Geochemical reactions with CO_2-rich brine can dissolve carbonates, thereby increasing porosity but weakening rock strength. Conversely, secondary precipitation can either strengthen the rock or increase the risk of leakage. Geomechanical responses, such as injection stress or tectonic activity, have the potential to open or close fractures that serve as pathways for fluid migration. Mineralogy also plays a crucial role: quartz- and carbonate-rich lithologies tend to be brittle, while clays are more ductile but weaker; smectite can clog pores through swelling, but it also induces internal stresses. Thus, caprock performance cannot be assessed based on a single parameter, but requires an integrated approach to ensure the long-term safety of CO_2 storage.

Although this review provides an integrated understanding of geochemical, geomechanical, and mineralogical factors influencing shale caprock leakage potential, several limitations remain. First, regional datasets across Asian basins are uneven, limiting cross-basin comparison and standardization of results. Second, most analyses rely on laboratory-scale experiments that may not capture the full heterogeneity and stress–fluid interactions present in field conditions.

Third, current evaluations emphasize static properties, whereas the long-term, dynamic evolution of caprock integrity under CO_2 exposure remains insufficiently modeled. Coupled multiphysics approaches integrating geochemical reactions, stress response, and microstructural evolution are still limited. Moreover, existing mineralogical data from XRD and SEM lack nanoscale resolution needed to quantify reaction kinetics and pore-scale alteration. The influence of organic matter, micro-porosity, and surface roughness also warrants deeper investigation. Future research should therefore focus on reactive transport and THMC simulations, long-duration CO_2–shale interaction tests, and integration with real-time monitoring and probabilistic risk assessment frameworks. Such efforts will enhance predictive reliability for leakage potential and ensure safer, more sustainable carbon sequestration and petroleum operations.

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