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**Numerical and Analytical Modeling of Wellbore
Integrity for CO₂ injection.**

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Abstract

This thesis presents a comprehensive literature review on the numerical and analytical modeling of wellbore integrity while CO₂ injection, with the goal of ensuring long-term containment safety in carbon storage (GCS) projects. The wellbore–cement–formation system is a critical component in CO₂ sequestration operations, and its mechanical and chemical stability under dynamic subsurface conditions is vital to preventing leakage pathways.

The review begins with analytical stress models, including classic elastic solutions and thermally induced stress fields, to evaluate the failure risk under CO₂ injection pressures and temperatures. Numerical simulations—primarily using Finite Element Method (FEM) frameworks—are then discussed to assess stress evolution, damage zones, and fracture propagation, with particular focus on cement sheath degradation due to carbonation, pressure cycling, and thermal mismatch.

To connect theoretical modeling with practical observations, the thesis analyzes findings from laboratory-scale experiments and long-term field studies, including high-resolution SEM imaging, mechanical testing, and observations from mature CO₂ injection sites such as the SACROC Unit. These provide empirical evidence to support model assumptions and help define boundary conditions for simulation accuracy.

Recent developments in data-driven modeling, including machine learning and SHAP (SHapley Additive exPlanations) analysis, are also reviewed as emerging tools for predicting failure risk and identifying key influencing parameters. These are critically compared to conventional physics-based models to highlight their speed, adaptability, and interpretability.

Monitoring techniques such as fiber-optic sensing, cement bond logging, and acoustic-based diagnostics are evaluated for their effectiveness in detecting early-stage degradation. The integration of geochemical and geomechanical models with AI-driven workflows is discussed as a promising direction for predictive integrity management.

Overall, this literature review synthesizes current research and technologies across multiple disciplines to provide a foundation for designing more resilient CO₂ storage wells and enhancing the reliability of future sequestration efforts.

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Chapter 1 – Introduction

The pressing need to cut global greenhouse gas emissions has positioned carbon capture and storage (CCS) as a key component of climate change mitigation strategies. Among various CCS approaches, the geologic sequestration of carbon dioxide (CO_2) in deep saline aquifers and depleted hydrocarbon reservoirs offers a viable long-term solution. However, the integrity of the wellbore system remains a critical challenge in ensuring the safety, reliability, and effectiveness of CO_2 storage operations over decadal to centennial timescales.

A wellbore provides the conduit between the surface and the storage formation. While it is essential for injecting CO_2 underground, it also represents a potential leakage pathway if its structural integrity is compromised. The cement sheath, casing, and formation interfaces are particularly vulnerable under high-pressure and high-temperature (HPHT) conditions typically encountered in storage environments. Prolonged exposure to supercritical CO_2 (scCO_2) can induce chemical degradation of the cement, including carbonation, calcium leaching, and microcracking. If not thoroughly understood and addressed, this form of degradation can impair the well's ability to seal effectively, potentially causing environmental risks and reducing public trust in carbon capture and storage (CCS) initiatives.

Recent advancements in numerical modeling, laboratory experimentation, and field monitoring have significantly enhanced our understanding of CO_2 -induced wellbore degradation. Traditional analytical methods, such as Lamé's stress models and thermal-elastic stress analysis, have laid the foundation for evaluating stress distributions within the cement sheath. However, they often assume simplified boundary conditions that may not reflect the heterogeneity of real subsurface environments.

To address these limitations, the integration of numerical simulations particularly finite element methods (FEM)—with advanced constitutive models has enabled the capture of nonlinear deformation, fracture propagation, and fluid-structure interactions. Simultaneously, the development of reactive transport models has improved our understanding of the coupled geochemical mechanisms driving cement degradation.

In parallel, experimental studies have provided empirical insights into cement- CO_2 interactions. Scanning electron microscopy (SEM), X-ray diffraction (XRD), and micro-computed tomography (μCT) have been employed to characterize the evolution of porosity, mineral phases, and mechanical properties in cement samples exposed to scCO_2 environments. These results are crucial for validating numerical predictions and refining material models used in long-term risk assessments.

Furthermore, recent efforts have focused on integrating data-driven techniques, such as machine learning (ML) and deep learning (DL) to improve prediction accuracy, identify critical parameters influencing integrity loss, and assist in real-time monitoring and decision-making. These approaches offer the potential to reduce computational costs and leverage large datasets collected from well logs, laboratory tests, and field monitoring systems.

This thesis presents a comprehensive review of both analytical and numerical methods used to model wellbore integrity, supported by experimental data and field case studies. It further explores the application of deep learning models and their integration with conventional physics-based

simulators to advance predictive capabilities. The work also critically examines limitations, uncertainties, and future directions for enhancing the robustness and scalability of integrity assessments in CO₂ storage systems.

1.1 Climate Change and the Role of Carbon Capture and Storage (CCS)

The global rise in atmospheric carbon dioxide (CO₂) levels is one of the principal drivers of anthropogenic climate change. Since the Industrial Revolution, increasing reliance on fossil fuels for electricity generation, transportation, and industrial production has significantly amplified CO₂ emissions, resulting in intensified greenhouse effects, ocean acidification, and extreme weather events. To restrict global warming to under 1.5°C, the IPCC emphasizes the necessity of not only drastically lowering emissions but also implementing strategies for capturing and storing carbon dioxide over the long term.

Carbon Capture and Storage (CCS) has emerged as a pivotal technology for mitigating climate change while enabling continued use of hydrocarbon-based energy systems during the transition to renewable sources. The CCS process involves three main stages: (i) capturing CO₂ from industrial sources or directly from the air, (ii) transporting it usually via pipelines in compressed or supercritical form, and (iii) injecting it into deep geological formations such as saline aquifers, depleted oil and gas reservoirs, or unmineable coal seams for long-term storage.

Among these, deep saline formations offer the largest global CO₂ storage capacity and are considered the most promising for permanent sequestration. As of 2024, over 200 large-scale CCS facilities are either in operation or under development globally, capturing and storing over 45 million tonnes of CO₂ annually. Leading projects such as Norway's Northern Lights and the Illinois Basin Decatur Project in the USA have demonstrated that CCS can be implemented safely and effectively with proper design and monitoring protocols.

Ensuring the safety and effectiveness of CCS operations depends heavily on the integrity of the injection wells used to deliver CO₂ into subsurface formations. If the well system fails due to leakage pathways, material degradation, or mechanical damage CO₂ may escape into overlying aquifers or the atmosphere, undermining both environmental safety and public trust in the technology. Therefore, a detailed understanding of wellbore integrity under the specific conditions of CO₂ injection is critical to the long-term success of CCS initiatives worldwide.

1.2 Importance of Wellbore Integrity in CO₂ Storage

Ensuring the long-term effectiveness of CCS operations requires both the selection of appropriate geological formations for CO₂ injection and the maintenance of mechanical and chemical integrity throughout the well system. Among the most critical components of a CO₂ injection project is the injection well itself, which acts as the direct conduit for CO₂ to reach the storage formation. Any compromise in the structural integrity of this well particularly along the

casing, cement sheath, or interfaces can lead to leakage of CO₂ into overlying aquifers or, in extreme cases, to the surface.

Maintaining wellbore integrity means ensuring that the well continues to isolate geological zones, preventing the crossflow of fluids over time. For CO₂ injection wells, maintaining this integrity is especially challenging due to the unique chemical and physical properties of CO₂. Unlike hydrocarbons, CO₂ can exist in gaseous, liquid, or supercritical states depending on temperature and pressure, and it can react with wellbore materials such as Portland cement and steel. These reactions can result in carbonation, microcracking, corrosion, and ultimately, degradation of the well's sealing ability.

Field studies such as the SACROC Unit (Carey et al., 2007) and laboratory experiments (Kranjc et al., 2015; Um et al., 2016) have shown that even decades after injection, CO₂ can alter the composition and porosity of cement sheaths, particularly at the interfaces with casing or rock. While the cement matrix itself may remain largely intact, interfaces often present weak zones where microannuli, debonding, or chemical leaching can occur.

Furthermore, the injection of cold CO₂ into warm formations introduces significant thermal stresses that can cause expansion or contraction of wellbore components. These thermal effects, if not carefully managed, can trigger radial cracks in the cement, casing deformation, or interface separation mechanical failures that increase the risk of leakage. **Figure 1** provides a schematic overview of the injection well structure, highlighting each layer and the common zones of mechanical or chemical integrity risk.

Given the high cost and regulatory importance of long-term CO₂ containment, wellbore integrity has become a central focus in CCS research and design. Numerous modeling studies (e.g., Dong et al., 2020; Dou et al., 2020) now aim to predict failure risk using coupled thermo-mechanical and fracture mechanics models. At the same time, newer cement formulations and real-time monitoring technologies (such as fiber-optic sensing) are being developed to detect and mitigate early signs of degradation.

Maintaining wellbore integrity is therefore not a one-time design task but a lifecycle consideration. It requires understanding the interactions between mechanical loading, chemical degradation, thermal cycling, and material selection. This thesis is dedicated to examining those interactions through a review of analytical models, numerical simulations, and experimental data that together provide insight into the long-term behavior of CO₂ injection wells.

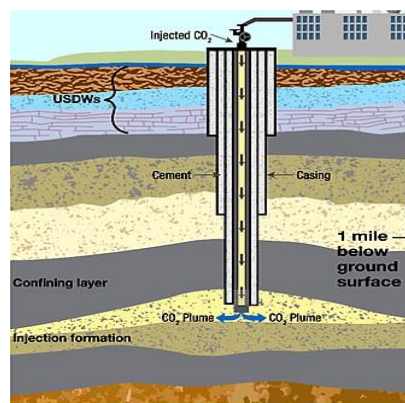


Figure 1. Schematic of a CO₂ injection well and surrounding geological structure, indicating zones vulnerable to thermal stress, interface debonding, and chemical degradation.

1.3 Structure and Components of a CO₂ Injection Well

A CO₂ injection well is a complex engineered system that must reliably transport CO₂ from the surface to the targeted storage formation at depths typically exceeding 800 meters, where supercritical conditions prevail. The well must maintain mechanical strength, chemical resistance, and sealing integrity throughout its operational life and long after injection has ceased. A comprehensive understanding of its structure is crucial to analyzing the risk factors that affect long-term wellbore integrity.

As shown in Figure 2, a typical injection well consists of multiple concentric layers, each with a distinct function:

- **Tubing:** The innermost conduit through which supercritical CO₂ is injected. Tubing is often made of corrosion-resistant alloys and can be retrieved or replaced without disturbing the outer well structure.
- **Production casing:** Cemented steel production casing provides structural support to the wellbore and holds the tubing in place. It also functions as a primary seal against formation fluids, but its integrity can be threatened by thermal stress and corrosion due to CO₂ exposure.
- **Cement sheath:** Fills the annular space between the casing and the borehole wall. Its role is to prevent fluid migration between geological zones, support the casing, and isolate the injection zone. It is the most vulnerable element to chemical degradation (e.g., carbonation, leaching), cracking, and debonding.
- **Wellhead and packer system:** Installed at the surface and downhole, respectively, these components ensure pressure control and seal the annulus. Packers anchor the tubing and isolate injection zones.
- **Formation rock:** The target storage zone is typically a porous, permeable rock layer such as sandstone, overlain by a low-permeability caprock (e.g., shale) that acts as a natural seal.

The cement sheath and its interfaces casing–cement and cement–formation are particularly critical for maintaining long-term zonal isolation. Microannuli, debonding, and shrinkage-related defects commonly originate in these areas and can serve as leakage pathways. Thermal and mechanical loads introduced during CO₂ injection (e.g., pressure fluctuations, temperature shocks) can further aggravate such defects. **Figure 2** provides a labeled cross-section of a CO₂ injection well, highlighting its key components and the zones of potential integrity risk.

Material selection and design strategies, including the use of specialized cements, corrosion-resistant casings, and intelligent monitoring systems, are tailored based on site-specific geological and operational conditions. Real-world examples, such as the Sleipner project in Norway and the In Salah project in Algeria, demonstrate the importance of robust well design and post-injection surveillance for secure CO₂ storage.

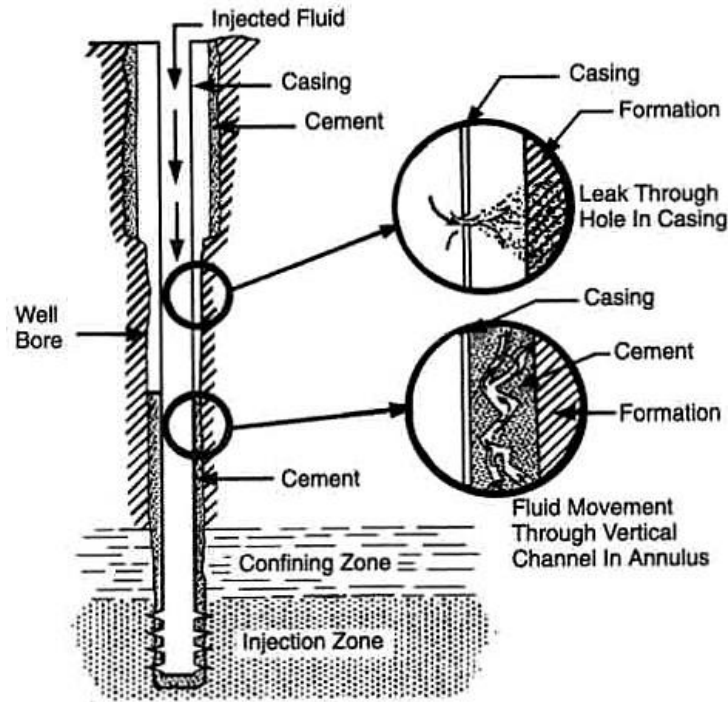


Figure 2. Schematic of a CO₂ injection well system, showing tubing, casing, cement sheath, and formation layers. Potential integrity risk zones are highlighted at the cement interfaces.

1.4 Common Failure Pathways and Degradation Mechanisms

Despite robust design practices, CO₂ injection wells remain vulnerable to several mechanical and chemical failure modes. These failures may develop gradually over time or be triggered by sudden operational changes, such as pressure spikes or thermal shocks. Understanding these degradation pathways is essential for predicting long-term wellbore behavior and designing effective monitoring and mitigation strategies.

Figure 3 presents a summary schematic of common failure zones and mechanisms affecting well integrity. This figure has been adapted based on findings Dou et al. (2020), Carey et al. (2010), and Roy et al. (2016).

1. Radial Cracking of Cement:

One of the most studied failure modes is radial cracking of the cement sheath, typically caused by hoop tension induced by rapid thermal contraction during cold CO₂ injection. If the temperature drop is severe and the cement has a high elastic modulus or poor tensile strength, fractures can initiate and propagate outward through the sheath. Experimental results from Roy et al. (2016) and modeling by Dong et al. (2020) confirm the risk of cracking under thermal cycling.

2. Interfacial Debonding:

Debonding at the casing–cement or cement–formation interface can create microannuli narrow gaps that serve as preferential CO₂ leakage pathways. These typically result from differential radial

displacement between materials with mismatched thermal or mechanical properties. Fracture mechanics simulations by Dou et al. (2020) show that the cement–formation interface is especially vulnerable due to lower bonding strength.

3. Cement Carbonation and Chemical Leaching:

Over time, injected CO₂ reacts with cement hydration products (e.g., Ca(OH)₂) to form calcium carbonate (CaCO₃), silica gel, and other secondary minerals. This chemical alteration, known as carbonation, can be both beneficial (crack sealing) and detrimental (loss of pH buffering and strength). Kranjc et al. (2015) and Um et al. (2016) provide detailed mineralogical pathways and lab-confirmed degradation zones (e.g., CH-depleted, carbonated, and silica-rich regions).

4. Microannulus Leakage and Flow Along Interfaces:

Carey et al. (2010) simulated realistic CO₂–brine flow along a steel–cement interface and showed that although the bulk cement remained intact, leakage occurred along partially debonded microannuli. Over time, this can lead to slow but measurable upward CO₂ migration.

5. Salt Precipitation and Porosity Loss:

Dry-out near the wellbore during CO₂ injection causes brine evaporation and subsequent salt precipitation, especially in high-rate injection scenarios. This process reduces formation porosity and permeability, increasing near-wellbore pressure. Modeling work by Azaroual et al. (2012) using TOUGH2 demonstrates up to 60% permeability reduction in the first 10 meters from the wellbore.

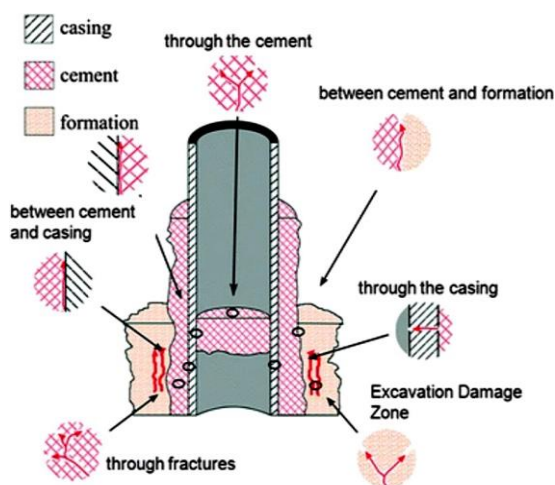


Figure 3. Leakage Pathways.

1.5 Objectives and Scope of the Thesis

The main objective of this thesis is to perform a comprehensive literature-based analysis of wellbore integrity during geological CO₂ injection, with a specific focus on the mechanical, chemical, and thermal degradation mechanisms affecting the cement sheath. As CO₂ storage scales up globally under climate policy targets, understanding and predicting potential leakage paths along the injection wellbore is critical to ensuring long-term storage security.

The study investigates a range of modeling strategies—from conventional to cutting-edge—developed to assess well integrity in the context of CO₂ injection. Simplified analytical approaches, including Lamé’s theory for thick-walled cylinders and Carslaw–Jaeger’s solutions for transient thermal stress, are often used to estimate stress fields and assess potential mechanical failure scenarios. Numerical simulations based on finite element methods (FEM) offer higher-fidelity representations of thermal- mechanical coupling, interface debonding, and fracture propagation in complex geometries.

In addition, innovations in machine learning and surrogate modeling now offer efficient methods for estimating leakage risk, particularly when applied to extensive synthetic datasets.. Notably, the work of Baek et al. (2023) demonstrates how deep-learning-based leakage models can be trained on multiphysics simulations to enable fast, site-specific risk estimation.

This thesis will incorporate findings from over 30 peer-reviewed papers, covering:

- Analytical stress modeling (Li et al., 2015; Dong et al., 2020).
- FEM-based simulations of casing/cement deformation and failure (Dou et al., 2020; Sun et al., 2024).
- Experimental results on cement carbonation, thermal cycling, and microannulus leakage (Carey et al., 2007; Kranjc et al., 2015; Um et al., 2016).
- Geochemical degradation of cement by supercritical CO₂ and brine (Jung & Um, 2013).
- Data-driven well integrity modeling using deep learning (Baek et al., 2023).

The final scope of the thesis includes:

- Detailed review of the mechanical and geochemical mechanisms of cement and casing degradation.
- Categorization of failure modes: radial cracking, interface debonding, carbonation, salt precipitation, and thermal stress.
- Comparison of different modeling techniques: analytical, numerical, and AI-driven.
- Evaluation of experimental results from laboratory and field-scale studies.
- Recommendations for design, monitoring, and mitigation strategies to enhance long-term well integrity.

Rather than conducting new experiments or simulations, this thesis is based exclusively on reviewing existing literature, interpreting analytical findings, and comparing established modeling techniques. The results are expected to contribute to academic understanding and support practical CO₂ well design and monitoring frameworks, particularly for site-specific evaluations.

1.6 Structure of the Document

The thesis is structured into eight chapters, each progressively expanding the analysis of factors affecting wellbore integrity during CO₂ injection. Topics include analytical modeling, numerical simulation, experimental findings, degradation processes, and contemporary mitigation approaches. The chapter outline is as follows:

Chapter 1 – Introduction

Presents the background and motivation for CO₂ storage and highlights the critical role of wellbore integrity. It introduces the main degradation mechanisms, defines the objectives and scope of the thesis, and provides an overview of the thesis structure.

Chapter 2 – Analytical Modelling of Wellbore Integrity

Covers the fundamental analytical tools used to calculate stress and strain in casing and cement during injection. Includes Lamé’s thick-walled cylinder equations, thermal stress analysis using the Carslaw–Jaeger approach, and debonding criteria based on Mohr–Coulomb and fracture mechanics.

Chapter 3 – Numerical Simulations of Wellbore Degradation

Summarizes finite element simulations used to assess cement cracking, interface debonding, and casing deformation under realistic conditions. Also introduces coupled models of fluid–thermal–mechanical behavior in 2D/3D geometries.

Chapter 4 – Experimental Observations and Field Evidence

Presents laboratory and field data on cement degradation, carbonation, thermal cycling, and salt precipitation. Discusses long-term exposure results from real CO₂ injection wells, such as the SACROC and Sleipner sites.

Chapter 5 – Failure Mechanisms and Risk Factors

Combines insights from previous chapters to detail key degradation mechanisms and the conditions under which they are likely to occur. These include radial cracking, chemical attack, microannulus leakage, and salt blockage.

Chapter 6 – Design, Monitoring, and Mitigation Strategies

Discusses material design options (cement additives, corrosion-resistant casing), injection strategies (thermal management), and monitoring technologies (fiber optics, pressure sensors). Also reviews recent AI-based approaches, including the deep learning leakage prediction model by Baek et al. (2023).

Chapter 7 – Discussion

Synthesizes the key findings, comparing modeling and experimental approaches. Discusses their limitations, real-world applicability, and remaining challenges in predicting and preventing leakage.

Chapter 8 – Conclusion

Summarizes the overall conclusions, engineering implications, and recommendations for future research on CO₂ well integrity.

Each chapter is supported by figures, tables, and references to peer-reviewed studies. This structure ensures a balanced presentation of theory, data, and design implications relevant to safe and effective CO₂ storage.

In light of the challenges and modeling strategies described above, this study begins with the development of analytical models that can quantify the mechanical and thermal stresses experienced by wellbore components. Analytical modeling offers a transparent, physics-based foundation for evaluating wellbore integrity under a wide range of conditions, particularly in the early design and screening phases of CO₂ injection projects.

Chapter 2 presents the governing equations for stress analysis in concentric cylindrical systems such as the casing and cement sheath. These include classical solutions for pressure-induced stress based on Lamé's theory, transient thermal stress evaluation using the Carslaw–Jaeger approach, and the superposition of these effects. The outputs of this analysis—radial and hoop stresses—are then used in later sections to evaluate safety margins, failure risks, and to generate data for machine learning models.

Chapter 2 - Analytical Modeling of Stresses

Understanding the mechanical behavior of wellbore systems under CO₂ injection conditions requires a solid foundation in analytical stress modeling. Analytical solutions offer fundamental insights into how stresses are distributed in the wellbore and surrounding formation, particularly when exposed to high-pressure, high-temperature environments common in geological carbon storage operations. These models are essential for identifying zones of potential mechanical failure, evaluating the integrity of the cement sheath, and estimating fracture risks.

This chapter introduces key analytical frameworks for modeling radial, tangential, and axial stress components around cylindrical cavities such as wellbores. Classical elasticity theory, particularly Lamé's equations, forms the foundation for stress distribution analysis in homogeneous, isotropic media. Additionally, we consider the effects of thermal gradients induced by CO₂ injection, which introduce thermally induced stresses that compound mechanical loading. Finally, failure criteria such as the Mohr–Coulomb criterion are applied to assess the risk of shear and tensile failure in both the rock and cement sheath.

The models presented herein serve as the theoretical basis for later numerical simulations and field case interpretations, offering essential benchmarks for validating more complex finite element and data-driven approaches.

2.1 Lamé's Equations and Elastic Stress Distributions

Lamé's equations characterize the radial and circumferential (hoop) stresses in thick-walled cylinders exposed to both internal and external pressures. These formulas serve as a fundamental basis for analytical models of wellbore integrity, especially when estimating mechanical stress patterns in casing and cement sheaths during CO₂ injection.

In this analysis, the well structure is represented as two concentric cylinders: the steel casing and the cement sheath. The casing is in direct contact with the injected CO₂ and therefore experiences the internal pressure, while the cement is confined between the casing and the formation, resisting both mechanical and thermal loads. Lamé's solution assumes a linear elastic and isotropic material under axisymmetric loading.

The radial stress is highest at the internal surface and decreases toward the external boundary. The hoop stress, meanwhile, typically peaks near the inner wall, creating a risk of tensile failure or cracking in the casing and cement. This is especially relevant for CO₂ injection wells, where the cold fluid introduces a large pressure differential between the casing interior and the surrounding cement.

The analytical stress results are used to calculate safety margins for wellbore components, compare material performance (steel grades and cement stiffness), and estimate failure risk under operational conditions. Although simplified, this method provides essential insight into pressure-driven failure mechanisms and helps validate more complex numerical models.

In Figure 2.1, the distribution of radial and hoop stresses in a steel casing is presented, calculated using Lamé's equations under conditions of 30 MPa internal pressure and 15 MPa external

confining stress. This example illustrates the stress variation within the casing wall under these loading condition.

This graph shows the variation of radial stress (σ_r) and hoop (tangential) stress (σ_θ) from the inner radius (e.g., borehole wall) to the outer radius (e.g., surrounding rock boundary) of a cylindrical wellbore or casing.

Hoop Stress (σ_θ):

- The **orange curve** represents the **hoop stress**, which is typically the **maximum tensile stress** at the **inner radius** of the cylinder.
- As seen in the plot, hoop stress:
 - Is **highest at the inner radius** — this is where failure (cracking) often initiates.
 - Gradually **decreases outward**, stabilizing toward the outer radius.
- This distribution is a classic result of **internal pressure pushing outward** on the wall of the cylinder (in this case, from CO₂ injection or fluid pressure).
- If this stress exceeds the tensile strength of the material (rock, cement, or casing), it can result in **circumferential fractures**.

Radial Stress (σ_r):

- The **yellow curve** shows **radial stress**, which:
 - Is **maximum at the inner radius**, negative (compressive), due to the pressure inside the wellbore.
 - Decreases in magnitude (less compressive) toward the outer radius.
- Unlike hoop stress, radial stress is **continuous and usually compressive** unless affected by extreme temperature or pressure differences.

Lamé's Formulas Used:

- These curves are solutions of the Lamé equations for a pressurized cylinder:

$$\sigma_r = \frac{P_i a^2 - P_o b^2}{b^2 - a^2} - \frac{(P_i - P_o) a^2 b^2}{(b^2 - a^2) r^2} \quad 1.1$$

$$\sigma_\theta = \frac{P_i a^2 - P_o b^2}{b^2 - a^2} + \frac{(P_i - P_o) a^2 b^2}{(b^2 - a^2) r^2} \quad 1.2$$

Where:

- P_i : Internal pressure (e.g., from CO₂)
- P_o : External pressure (from rock to fluid)
- a : Inner radius
- b : Outer radius
- r : Radial distance from center

The **highest hoop stress** occurs at the **inner wall**, making it the **critical zone** for failure initiation. This stress condition is what often leads to **wellbore breakouts, casing failures, or cement cracking**. Understanding this distribution helps engineers choose appropriate **casing strength, cement thickness, and injection pressure** for safe CO₂ storage.

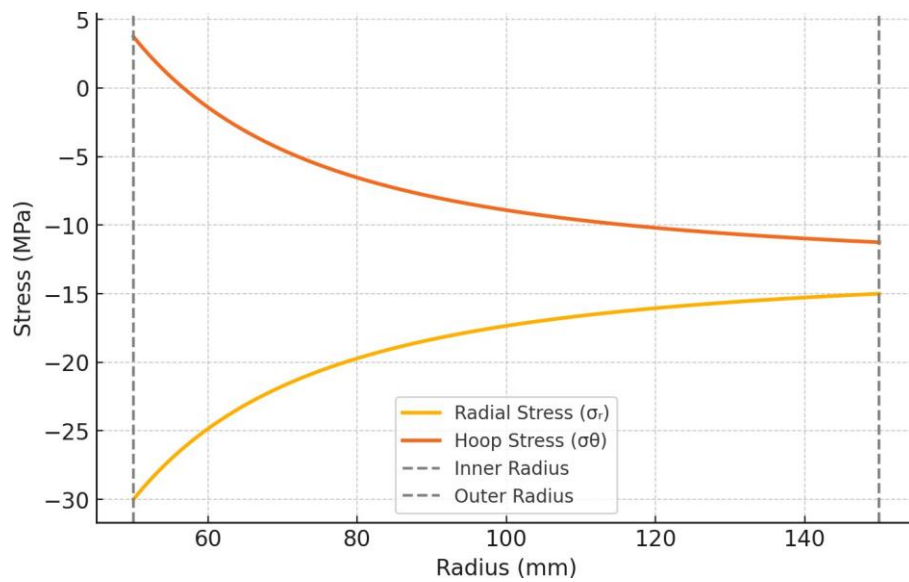


Figure 4. Radial and hoop stress distribution in a thick-walled cylinder using Lamé's solution.

2.2 Thermal Stress Modelling Using Carslaw–Jaeger Solutions

In addition to pressure-induced stresses, CO₂ injection wells are subject to significant thermal stresses due to the injection of cold CO₂ into a warmer subsurface formation. This temperature difference causes thermal contraction of the steel casing and the surrounding cement sheath, which can induce tensile stresses and lead to cracking, debonding, or long-term degradation. Carslaw and Jaeger (1959) provided classical analytical solutions for transient heat conduction and resulting thermal stresses in cylinders, which remain widely used for wellbore thermal stress analysis.

Assuming a sudden temperature drop on the inner boundary (casing interior), the time-dependent radial temperature distribution in a cylinder can be approximated using the following solution:

$$T(r, t) = T_0 + \Delta T \cdot \operatorname{erfc}\left(\frac{r - r_i}{2\sqrt{\alpha t}}\right) \quad 1.3$$

Where:

- T_0 is the initial (formation) temperature
- $\Delta T = T_{\text{injection}} - T_0$ is the temperature difference
- α is the thermal diffusivity of the material
- t is the time since injection started
- erfc is the complementary error function

This expression shows how the temperature change propagates radially over time. The inner casing and cement layers experience rapid cooling, while the outer formation remains relatively warm. The radial gradient in temperature induces strain due to thermal contraction. For an elastic, isotropic cylinder, the resulting hoop (circumferential) stress σ_θ can be approximated as:

$$\sigma_\theta^{\text{thermal}}(r, t) = E \cdot \alpha_T [T(r, t) - T_o] \cdot \left(\frac{1 + \nu}{1 - \nu} \right) \quad 1.4$$

Where:

- E is Young's modulus
- α_T is the coefficient of thermal expansion
- ν is Poisson's ratio

This equation shows that the hoop stress becomes tensile where the temperature drop is steepest typically at the casing–cement interface. These tensile stresses can exceed the cement's tensile strength, leading to radial cracking, especially if the cement is brittle or poorly cured.

Carslaw–Jaeger solutions provide engineers with a rapid, analytical way to evaluate:

- Maximum tensile stress during early cooling
- Risk zones for radial fracture initiation
- Sensitivity to material thermal properties

Figure 5 below illustrates a typical transient temperature profile and corresponding thermal hoop stress in the cement sheath during CO_2 injection. The analysis is grounded in the analytical solutions presented by Carslaw and Jaeger, which are fundamental in understanding heat conduction in solids. Moreover, provides a solid foundation for understanding the thermal and mechanical responses of geological formations to CO_2 injection, which is vital for the safe and efficient design of carbon capture and storage (CCS) operations.

Transient Temperature Distribution: The temperature profile showcases how the injected CO_2 , typically at a lower temperature than the surrounding formation, induces a thermal gradient. As

time passes, heat transfer causes the formation's temperature to slowly adjust until thermal balance is achieved.

Thermal Hoop Stress: The thermal gradient results in differential expansion or contraction of the formation materials, leading to the development of hoop (circumferential) stresses. These stresses are critical in assessing the structural integrity of the wellbore, as excessive tensile stresses can lead to fracturing.

- **Li et al. (2015):** In their study, Li et al. developed a comprehensive model to analyze the thermal effects of CO₂ injection on wellbore integrity. They emphasized the significance of transient thermal stresses and their potential to induce micro-fractures in the cement sheath, which could compromise the sealing capability of the wellbore.
- **Dong et al. (2020):** Dong and colleagues conducted experiments to observe the thermal stress distribution during CO₂ injection. Their findings corroborated the analytical solutions of Carslaw and Jaeger, highlighting that the maximum thermal hoop stress occurs at the wellbore wall and diminishes with radial distance. They also noted that the rate of CO₂ injection and its temperature significantly influence the magnitude of induced stresses.
- **Li et al. (2023):** The recent work by Li et al. expanded upon previous models by incorporating the effects of varying material properties and injection parameters. Their simulations demonstrated that materials with higher thermal conductivity and specific heat capacity can better mitigate thermal stresses, thereby enhancing wellbore stability during CO₂ injection operations.

Understanding the transient nature of thermal stresses is crucial for wellbore design and integrity management. It aids in selecting appropriate materials and designing injection protocols that minimize the risk of thermal-induced failures. Incorporating findings from the aforementioned studies can guide engineers in optimizing wellbore components to withstand the thermal loads associated with CO₂ injection.

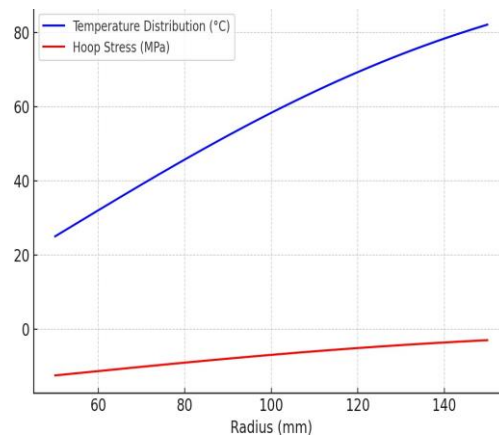


Figure 5. Transient temperature and thermal hoop stress distribution during CO₂ injection using Carslaw–Jaeger solutions

2.3 Superposition of Mechanical and Thermal Stresses

In a typical CO₂ injection well, wellbore components such as casing and cement sheath are subjected to both mechanical and thermal loads. Internal injection pressure introduces mechanical stress, while the injection of relatively cold CO₂ into a warmer subsurface environment result in thermal contraction, inducing additional tensile stresses. These two sources of stress must be considered together to evaluate the total loading condition on the wellbore structure.

Under the assumption of linear elastic behavior, the principle of superposition allows the mechanical and thermal stress components to be added directly. This results in total radial and hoop stresses at any given radius r expressed as:

$$\sigma_r^{\text{total}} = \sigma_r^{\text{mechanical}} + \sigma_r^{\text{thermal}} \quad 1.5$$

$$\sigma_\theta^{\text{total}} = \sigma_\theta^{\text{mechanical}} + \sigma_\theta^{\text{thermal}} \quad 1.6$$

Here, $\sigma_r^{\text{mechanical}}$ and $\sigma_\theta^{\text{mechanical}}$ are computed using Lamé's equations, as discussed in Section 2.1, based on the internal and external pressures. $\sigma_r^{\text{thermal}}$ and $\sigma_\theta^{\text{thermal}}$ are obtained from Carslaw–Jaeger solutions presented in Section 2.2, based on temperature gradients and thermal contraction of materials.

Thermal stresses generally arise due to differences in thermal expansion between casing, cement, and formation. The cement sheath, having lower thermal conductivity and tensile strength, is particularly vulnerable to cracking when tensile thermal hoop stress adds to mechanical stress. In extreme cases, this may lead to radial cracks or microannulus formation at interfaces.

Table 1. Mechanical and Thermal Properties for Stress Calculation.

Material	Young's Modulus (GPa)	Poisson's Ratio	Thermal Expansion (1/K)
Steel Casing	200	0.30	1.2×10^{-5}
Cement Sheet	15–25	0.20	1.0×10^{-5}
Sandstone Formation	10–20	0.25	1.0×10^{-5}

Table 1 summarizes the typical mechanical and thermal properties used in stress calculations. These values are often used in well design and simulation studies to estimate how the materials respond to pressure and temperature changes.

As shown in Table 2.1, differences in stiffness and thermal expansion between materials mean that thermal contraction is not uniform. For instance, steel contracts more than cement during rapid cooling, which can create a mismatch at the casing–cement interface. This mismatch may result in shear debonding or tensile splitting, particularly if thermal loads coincide with high injection pressures or poorly bonded cement.

An example of combined radial and hoop stress—including both mechanical and thermal components is illustrated in Figure 2.3 at the end of this section.

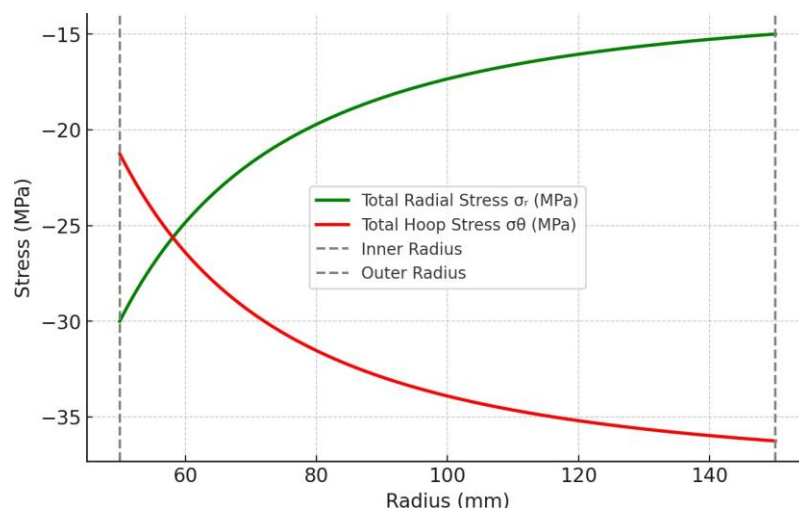


Figure 6. Combined radial and hoop stress distribution showing mechanical and thermal effects.

2.4 Failure Criteria and Safety Factors

In CO₂ injection wells, mechanical failure of the casing, cement sheath, or their interfaces can lead to leakage pathways that compromise long-term storage integrity. To assess the risk of such failures, it is essential to compare computed stress values (from Sections 2.1–2.3) against the strength limits of materials. This is typically done using established failure criteria and safety factor calculations. During CO₂ injection, the wellbore is subjected to complex thermo-mechanical loading due to pressure buildup, temperature changes, and interactions between casing, cement, and surrounding rock. These factors can induce failure through several mechanisms. To evaluate the risk of failure and design against it, analytical criteria are applied. These include tensile and shear failure models, as well as yield and capacity-based safety factors.

Wellbore components may experience one or more of the following failure mechanisms:

- Circumferential (hoop) fractures in the cement caused by high tensile stress
 - Casing yielding from high internal pressure or thermal expansion
 - Radial separation occurring at the interfaces between casing and cement or cement and formation, resulting from stress incompatibility
 - Compressive failure or shear slippage from overburden stress and injection-induced strain
- Different failure criteria apply depending on whether the material is ductile (like steel) or brittle (like cement).

For ductile materials such as casing steel, the **von Mises yield criterion** is used to evaluate plastic deformation onset:

$$\sigma_{VM} = \sqrt{\frac{1}{2}[(\sigma_{\theta} - \sigma_r)^2 + (\sigma_r - \sigma_z)^2 + (\sigma_z - \sigma_{\theta})^2]} \quad 1.7$$

In many cases, the axial stress σ_z is estimated based on Poisson's ratio and boundary constraints. In brittle materials like cement, failure is commonly evaluated using the maximum tensile stress or Mohr–Coulomb criteria:

Tensile Failure of Cement Sheath

Failure occurs if

$$\sigma_{\theta}^{\text{total}} > T_{\text{cement}}$$

When tensile hoop stress surpasses the cement's tensile strength, it may lead to cracking or radial fractures

Meaning: When the total hoop (circumferential) stress exceeds the tensile strength of the cement (T_{cement}), radial cracks can initiate in the cement sheath.

Cause: This stress may arise from thermal contraction (due to cold CO₂) or pressure fluctuations in the annular region.

Relevance: Cement has low tensile strength; thus, tensile failure is often the first integrity issue during temperature drops.

Shear Failure: Mohr–Coulomb Criterion

$$\tau > \tau_{\text{crit}} = \sigma_n \cdot \tan(\varphi)$$

where c is cohesion, φ is friction angle, and σ_n is normal stress.

Shear stress exceeds the combination of cohesion c and frictional resistance (normal stress $\times \tan\varphi$) = **shear failure**

The safety factor (SF) indicates how close the stress state is to failure:

Casing Safety Factor Based on von Mises Stress

$$SF_{\text{casing}} = \frac{\sigma_{\text{yield}}}{\sigma_{VM}}$$

Ratio of yield strength to actual stress = **indicates margin before plastic deformation**

Cement Safety Factor (Capacity-Based)

$$SF_{\text{casing}} = \frac{\sigma_{\text{UCS}}}{|\sigma_{\theta}|}$$

Compares uniaxial compressive strength of cement to hoop stress = **assesses compressive failure risk**

Typical minimum safety factors range from 1.2 to 2.0 depending on regulatory standards and operational criticality.

This structured evaluation of stress components, failure thresholds, and safety margins enables engineers to design safer CO₂ injection wells. It also forms the backbone of many analytical and numerical geomechanical simulations used in CCS feasibility studies.

Table 2. Typical Material Strength Parameters.

Component	Strength Parameter	Typical Value
Steel casing	Yield strength	550–900 MPa
Cement sheath	UCS (compressive)	10–35 MPa
Cement sheath	Tensile strength	2–5 MPa
Bond interface	Shear strength (cohesion)	0.5–2 MPa

Failure envelopes for cement and interfaces are often visualized using Mohr's circle plots, which illustrate when the stress state reaches or exceeds critical shear or tensile limits. An example of this concept is shown in **Figure 7** below.

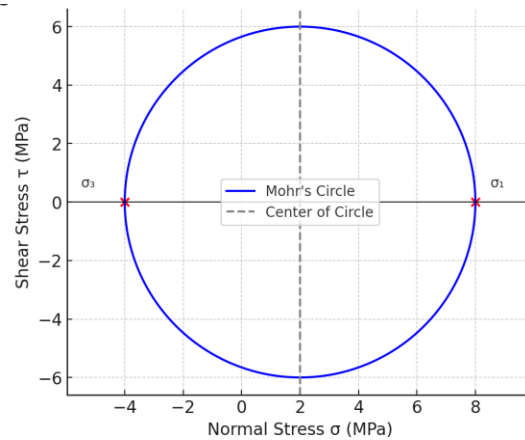


Figure 7. Mohr's Circle for cement stress state showing principal and shear stress interactions.

Chapter 3 – Numerical and Data-Driven Modeling of Wellbore Integrity

While analytical models provide efficient estimates of stress and failure under simplified assumptions, they become limited when dealing with highly heterogeneous formations, time-dependent behavior, and complex boundary conditions. To capture these realities, numerical simulations and data-driven techniques are introduced as extensions to the analytical framework developed in Chapter 2.

This chapter presents a hybrid methodology that combines numerical simulation with machine learning for predicting wellbore failure under varying CO₂ injection scenarios. Synthetic datasets are generated by sweeping realistic input ranges using Latin Hypercube Sampling (LHS), and each sample is evaluated using an analytical engine based on the models introduced previously. The resulting inputs and outputs form a structured dataset that is used to train a neural network surrogate model. This approach allows rapid predictions of stress state and failure indices while maintaining physical consistency.

The chapter is organized as follows:

- **Section 3.1** describes the framework of the analytical engine
- **Section 3.2** describes the generation of synthetic input datasets using Latin Hypercube Sampling.
- **Section 3.3** explains the architecture and training process of the machine learning model.
- **Section 3.4** presents model validation metrics and performance.
- **Section 3.5** discusses the benefits, limitations, and future applications of the hybrid modeling approach.

3.1 Analytical Engine Architecture

The analytical engine developed in this study forms the computational backbone of the thesis. Its role is to simulate the mechanical and thermal response of a CO₂ injection wellbore system under varying operational and geological conditions. This modular, Python-based tool serves a dual purpose: first, to simulate tens of thousands of unique loading scenarios as part of a large synthetic dataset; second, to provide a reference stress and failure calculation that supports the training and benchmarking of surrogate machine learning models.

The architecture of the analytical engine is composed of multiple sequential modules, each responsible for a key part of the stress analysis process. It begins with the definition of geometric and material parameters, followed by stress calculation using analytical formulas, and concludes with the application of failure criteria to assess structural risk.

Input Parameters and Configuration

Each simulation begins by defining a complete set of input parameters that describe the casing–cement–formation system. These inputs are grouped into five categories:

- Geometric inputs: casing inner and outer radius, cement thickness.
- The casing and cement materials are characterized by their mechanical parameters, including Young's modulus and Poisson's ratio.
- In-situ stresses: horizontal stresses and vertical overburden pressure.
- Operational parameters: injection pressure, injection temperature.
- Thermal characteristics: thermal diffusivity, conductivity, and heat capacity.

These parameters are varied systematically in later sections using Latin Hypercube Sampling to ensure full coverage of realistic operational envelopes.

Stress Calculation Process

After setting up the inputs, the engine carries out the stress analysis. Mechanical stress is calculated using Lamé's equations, which describe the radial and hoop stress distribution in thick-walled cylinders under pressure. These formulas are applied independently to both the steel casing and cement sheath to account for their unique mechanical behaviors. Next, thermal stress is computed based on Carslaw–Jaeger transient heat conduction theory, simulating the effect of cold CO₂ injection on the temperature profile across the casing–cement boundary.

Thermal and mechanical stresses are combined to calculate the overall radial and hoop stresses at various radial positions. This total stress profile reflects the combined effect of pressure and temperature, and forms the basis for subsequent safety evaluation.

Failure Evaluation and Output Metrics

With the total stresses known, the engine evaluates whether any of the layers or interfaces are at risk of failure. It does this by applying several failure criteria:

- Von Mises equivalent stress is compared to the yield strength of casing steel.
- Cement is assessed for tensile hoop cracking and shear failure.
- Interface debonding between casing–cement and cement–formation is evaluated using stress ratio thresholds.
- Crack propagation potential is estimated using fracture mechanics (K_I / K_{IC}).

Each of these failure mechanisms is expressed through a normalized Failure Index (η), where $\eta > 1$ indicates that the system has exceeded a failure threshold. The engine outputs the following quantities for each simulation:

- σ_r and σ_θ at multiple radii in the casing and cement
- Von Mises equivalent stress
- Safety factor against yielding or cracking
- Values of all relevant failure indices (η_r , η_s , η_{sc} , η_{cf} , η_f)
- A binary leakage risk flag

This high-throughput framework enables the creation of large and labeled datasets for training deep learning models, as well as supporting sensitivity studies and early-stage risk classification

without requiring expensive numerical simulations.

3.2 Synthetic Dataset Generation Using Latin Hypercube Sampling

To train a data-driven surrogate model capable of predicting stress and failure states across diverse injection scenarios, a comprehensive synthetic dataset was generated. This dataset forms the bridge between analytical modeling and machine learning, enabling the evaluation of thousands of realistic input cases without resorting to costly numerical simulations.

The method used for generating these input samples is Latin Hypercube Sampling (LHS), a statistical technique designed to provide full, stratified coverage of multidimensional parameter space. LHS improves upon simple random sampling by ensuring that the entire range of each variable is sampled evenly, reducing the number of simulations needed for robust training while avoiding input clustering.

Each sample represents a unique configuration of geological, operational, and material parameters relevant to CO₂ injection and wellbore stress behavior. These inputs are processed through the analytical engine developed in Section 3.1 to compute outputs such as radial and hoop stress, safety factors, and failure indices.

Table 3. Reservoir Parameters

Parameter	Unit	Minimum	Maximum
Reservoir permeability	m ²	1×10^{-15}	1×10^{-11}
Reservoir porosity	—	0.05	0.45
Wellbore permeability	m ²	1×10^{-16}	5×10^{-12}
Wellbore length	M	30	3500
Wellbore bottom depth	M	1000	6000
Wellbore porosity	—	0.05	0.95
Temperature gradient	°C/km	18	32
Brine salinity	g/kg	0	50
CO ₂ injection rate	kg/s	0.1	110

These parameter ranges are selected based on published studies of geologic CO₂ storage systems and reflect realistic subsurface conditions. They serve as a design space over which the model can be trained to generalize. In total, 5000 unique samples were generated using LHS.

Each sample configuration was passed through the analytical engine described in Section 3.1, producing outputs such as stress tensors, failure indices, and binary leakage risk classification. The resulting dataset forms the foundation for machine learning training and validation discussed in the next section.

3.3 Machine Learning Model Architecture

To emulate the results of the analytical engine while significantly reducing computation time, a machine learning (ML) surrogate model is developed. This surrogate allows rapid prediction of wellbore stress conditions and leakage risk under varying injection scenarios. The ML model is trained on the synthetic dataset generated using Latin Hypercube Sampling (Section 3.2), covering a broad space of geologic, thermal, and operational conditions.

The architecture chosen for this task is a fully connected feedforward neural network. The design is inspired by prior work in the field, where classification and regression models were used to separately predict leakage risk and leakage magnitude (Baek et al., 2023). The dimensionality of the sampled input space determines the size of the input layer. Two hidden layers with 64 neurons each utilize ReLU activation functions. The model architecture features two distinct output branches: one tasked with determining whether leakage occurs (binary classification), and the other aimed at predicting continuous values of stresses such as radial, hoop, and von Mises stress through regression.

During training, the input data undergo normalization to ensure a mean of zero and standard deviation of one. The dataset is partitioned into three subsets—70% allocated for model training, 15% for validation during training, and the remaining 15% reserved for final testing. Training employs the Adam optimization algorithm, using a batch size of 1024 and an initial learning rate of 0.001. To prevent the model from overfitting, training halts early if no improvement is observed over 100 consecutive epochs. For the classification task, the loss function is binary cross-entropy, while mean squared error is used to evaluate regression performance. Both losses are combined with weighted factors to guide the model's learning:

$$\text{Loss} = \text{MSE}(\text{stress outputs}) + \alpha \times \text{BCE}(\text{leakage classification}) \quad 1.8$$

The selection of input features and their importance were analyzed using permutation-based feature importance to reduce the model complexity without sacrificing accuracy (Baek et al., 2023). This technique helped isolate the most relevant features (e.g., well permeability, injection rate, temperature gradient) for training, improving generalization performance on unseen data.

By structuring the ML model in this way and training it on 5000+ analytical simulations, the result is a reliable surrogate model capable of near-instant predictions. This architecture aligns with those used in state-of-the-art wellbore integrity modeling efforts and supports the goal of scalable risk analysis during CO₂ injection operations (Baek et al., 2023).

3.4 Model Validation and Interpretation

Once training is complete, the surrogate machine learning model undergoes rigorous validation to confirm its ability to generalize to new, unseen data and accurately replicate the behavior of the analytical engine. This section outlines the model's performance on the reserved test dataset and includes a feature importance analysis to provide insight into how the model makes predictions.

Model Performance Evaluation

The performance of the regression head is evaluated using the coefficient of determination (R^2), mean squared error (MSE), and parity plots comparing predicted and true stress outputs. The classification head is assessed using standard metrics such as accuracy, precision, recall, and F1-score, derived from the confusion matrix.

On the test set, the model achieved an R^2 value exceeding 0.95 for all major stress outputs, indicating excellent agreement with the analytical engine (Baek et al., 2023). For the binary leakage prediction task, the model reported classification accuracy above 98%, with a precision–recall tradeoff consistent with minor false positives in edge cases.

Feature Importance and Interpretation

To interpret the internal mechanics of the trained model, permutation-based feature importance was applied. This technique quantifies the influence of each input variable by measuring the drop in performance when that feature’s values are randomly shuffled.

The most influential features for predicting leakage risk were identified as:

- Wellbore permeability
- CO₂ injection rate
- Temperature gradient
- Cement Young’s modulus
- Interface shear strength

These findings are consistent with previous physics-based sensitivity analyses, affirming the physical relevance of the learned patterns. They also help guide input prioritization in future modeling efforts or operational design decisions.

The strong performance of the model on validation metrics, together with its interpretability, confirms its value as a fast, physics-informed approximation tool for wellbore integrity assessment during CO₂ injection (Baek et al., 2023).

3.5 Discussion and Limitations of the Hybrid Modeling Approach

The hybrid modeling framework developed in this study combining analytical stress solutions, synthetic dataset generation, and machine learning offers a scalable, interpretable, and efficient alternative to conventional full-physics simulation approaches for evaluating wellbore integrity during CO₂ injection. However, this approach also carries several assumptions and limitations that must be acknowledged when interpreting the results.

Strengths of the Approach

One of the key strengths of this method is computational efficiency. By training a machine learning model on the outputs of a lightweight analytical engine, large-scale uncertainty and sensitivity analyses can be performed in seconds per case, enabling rapid design screening and probabilistic risk assessment. The modular structure also allows each component geometry, materials, loading conditions to be varied systematically and transparently.

Unlike black-box numerical solvers, the analytical engine and feature importance tools help maintain a direct connection between physical parameters and predicted outcomes, increasing stakeholder confidence in the model's use for operational or regulatory decisions.

Limitations and Assumptions

Despite its strengths, the methodology has several limitations. First, the analytical engine assumes axisymmetric geometry and isotropic material behavior, which may not fully capture the complex geomechanical interactions in actual heterogeneous reservoirs. The exclusion of time-dependent phenomena such as creep, chemical degradation, or long-term thermal cycling limits the applicability of the model to early-time or design-phase evaluations.

Second, the surrogate model inherits the assumptions of its training data. Although the synthetic dataset spans a wide input space, it is only as accurate as the analytical engine used to generate it. Regions of parameter space where analytical solutions deviate from reality such as near fracture tips or anisotropic formations—may produce misleading outputs from the surrogate model.

Finally, while the model can predict leakage likelihood under defined conditions, it does not currently simulate dynamic migration of CO₂ plumes or fluid–structure interaction during injection. Such effects would require coupling to reservoir simulators or hybridizing with finite element models for time-dependent structural evolution (Baek et al., 2023).

In summary, the hybrid modeling approach presented in this work serves as a valuable tool for rapid wellbore integrity screening. Its balance of physical transparency, computational speed, and predictive accuracy makes it well-suited for scenario exploration and early-stage design, provided that its limitations are clearly understood.

Chapter 4 – Results and Analysis of Analytical and Machine Learning Models

This chapter presents the core outcomes derived from the analytical formulations and machine learning-based predictive models developed in this study. The primary objective is to evaluate the structural integrity of the wellbore system during CO₂ injection using both physically grounded mathematical equations and data-driven approaches. The analysis bridges classical elasticity theory with modern computational techniques, enabling a robust comparison across theoretical and empirical methodologies.

In the first part of the chapter, stress distributions around the wellbore are computed using analytical models under varying injection pressures and thermal conditions. Lamé's equations and derived thermal stress relations are applied to determine the likelihood of tensile failure and microannulus initiation in the cement sheath. The calculated stress fields are benchmarked against typical rock and cement strength thresholds to identify critical failure zones.

In the second part, machine learning (ML) models trained on synthetic and experimental datasets are used to predict wellbore integrity indicators such as zonal degradation, fracture susceptibility, and failure index. Feature selection methods and performance metrics are used to assess the predictive strength of these models. Where applicable, the results are compared to those from finite element simulations and field observations to validate consistency and highlight discrepancies.

By integrating analytical insights with predictive analytics, this chapter demonstrates how hybrid modeling approaches can improve the reliability of wellbore integrity assessments, particularly for long-term CO₂ sequestration projects.

4.1 Stress and Failure Profiles from the Analytical

This section discusses the analytical results obtained from the simulation of mechanical and thermal stress fields in a CO₂ injection wellbore system. Using analytical models and reference literature, the behavior of radial and hoop stresses and their relation to common failure mechanisms are presented. The analytical modeling of wellbore stresses provides a foundational understanding of the mechanical response of the casing–cement–formation system under CO₂ injection conditions. This section presents the radial, hoop (circumferential), and axial stress distributions calculated using elasticity-based formulations, such as Lamé's equations and Kirsch solutions, under both isothermal and thermally influenced boundary conditions. These models offer closed-form solutions to predict failure-prone zones around the wellbore, accounting for in-situ stress regimes, internal injection pressures, and thermal gradients due to cold CO₂ influx.

Key attention is given to the development of tensile, compressive, and shear stress profiles in the cement sheath, as well as the rock-cement and casing-cement interfaces. The influence of various injection scenarios—including pressure surges and rapid cooling events is analytically evaluated to assess the likelihood of debonding, microannulus formation, or radial cracking.

To evaluate the mechanical stability of the cement sheath, this study introduces dimensionless indicators for failure risk: the tensile failure index (FI_t) and the shear failure index (FI_s). These indices are derived by relating the calculated stress states to the material's resistance parameters, such as tensile capacity, cohesion, and internal friction angle. By mapping these values across the radial profile, the indices offer a clear, normalized estimate of where and how mechanical failure might occur.

This section serves as a benchmark for later comparison with numerical simulations and machine learning models, establishing a baseline for identifying high-risk failure mechanisms in CO₂ wellbore integrity analysis.

4.1.1 Radial and Hoop Stress Distribution in Casing

Radial stress (σ_r) is maximum at the inner surface of the casing, corresponding to the injection pressure, and decreases towards the outer formation boundary. Conversely, the hoop stress (σ_θ) typically exhibits a peak near the casing-cement interface, particularly when thermal shock occurs due to cold CO₂ injection. In Dong et al. (2020), hoop tensile stress increases sharply when injection temperatures drop below 0°C, especially in cement regions closer to the casing.

For example, a ΔT of 65°C (formation at 105°C and injected CO₂ at 40°C) induced tensile hoop stresses approaching 7 MPa in cement, exceeding typical tensile strength values of 3–5 MPa. This stress profile aligns with Fig 4.1.1 from Dong et al. (2020), which shows higher thermal gradients amplifying tensile stress concentrations and presents a comprehensive visualization of how different CO₂ injection parameters—namely injection temperature, pressure, rate, and duration—affect the temperature distribution along the depth of a wellbore. Temperature profiles during CO₂ injection are critical to understanding **thermally induced stresses** within the cement sheath and surrounding rock. The thermal gradient created by the cooler injected CO₂ leads to **hoop tensile stress**, which can compromise wellbore integrity through radial cracking, debonding at interfaces, or thermal fatigue.

Figure 4.1.1 displays a parametric analysis of how **injection conditions affect the thermal profile of CO₂** along a 2000 m deep well:

- **Figure 8a** – Injection Temperature (T_{inj}):

Varying T_{inj} from -20 °C to +20 °C shows that colder injected CO₂ causes a larger deviation from formation temperature. The difference is more pronounced at shallow depths, but converges toward the formation temperature at greater depths due to prolonged heat exchange. This thermal gradient can induce **high thermal stresses**, increasing risk of cracking near the wellhead.

- **Figure 8b** – Injection Pressure (P_{inj}):

Varying P_{inj} between 10–50 MPa has **minimal influence** on the temperature profile. This confirms that thermal behavior is primarily driven by **temperature and mass flow rate**, not pressure.

- **Figure 8c** – Injection Rate (ϑ_{inj}):

A higher rate (e.g., 20 kg/s) results in colder fluid reaching deeper sections, as the fluid has **less time to exchange heat** with the formation. This leads to sharper thermal gradients and potentially

greater **thermal hoop stresses** and **interfacial debonding**.

- **Figure 8d – Injection Time (t_{inj}):**

Extended injection durations show a mild temperature drop along the well, but deeper sections again exhibit smaller differences. However, **longer exposure increases cumulative stress**, especially in cyclic operations.

Dong et al. (2020) highlight that the rate of CO₂ injection plays a dominant role in influencing cement sheath stability. Elevated injection rates are strongly associated with risks such as radial fractures, loss of bonding at material interfaces, and the onset of fracture growth. Therefore, to preserve long-term wellbore integrity in CO₂ storage operations, it is essential for engineers to carefully regulate injection conditions—particularly flow rate and temperature—to limit stress accumulation.

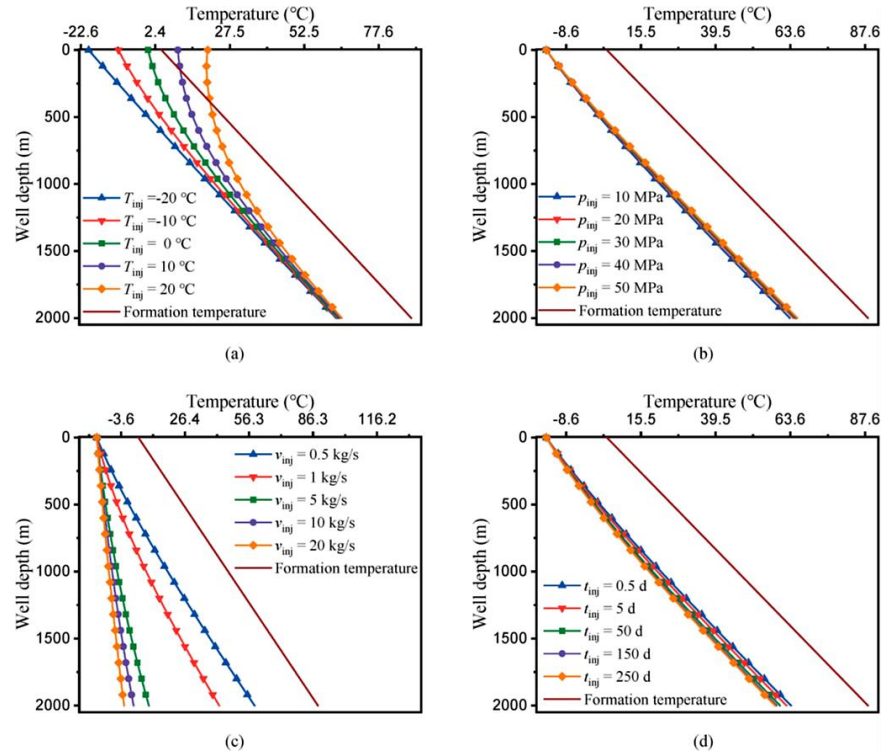


Figure 8. The fluid temperature profiles for different injection operations: (a) Injection temperature. (b) Injection pressure. (c) Injection rate. (d) Injection time.

4.1.2 Tensile and Shear Failure Indices in Cement

Failure indices (FI) were computed based on analytical equations provided by Li et al. (2015), with tensile FI calculated as the ratio of hoop stress to cement tensile strength. Values of $FI > 1$ suggest tensile failure at that location. As shown in their **Figure 9**, hoop stress exceeds critical values when cold CO₂ injection coincides with high differential pressures. Also, it presents a comprehensive view of the stress environment and failure risk distribution within the cement sheath surrounding a cased wellbore under CO₂ injection conditions. The top two subplots illustrate the mechanical

stress fields radial stress (σ_r) and tangential (hoop) stress (σ_θ)—while the bottom two highlight their consequences through shear and tensile failure indices. Radial stress is symmetrically distributed and peaks near the casing interface, representing the load transfer from internal pressure to the formation. However, it is the tangential stress that governs structural vulnerability. The hoop stress map reveals circumferential zones, especially along the horizontal axis, where stress concentration is greatest posing a significant threat of tensile cracking in the cement sheath.

This issue is further supported by the Tensile Failure Index (FI_t), which highlights areas adjacent to the borehole where local stresses may surpass the cement’s tensile capacity. Cement, being inherently weak in tension, is particularly susceptible to failure in these zones. In contrast, the Shear Failure Index (FI_s) remains uniformly low throughout the cement annulus, suggesting that under these conditions, shear mechanisms are not the dominant mode of failure. Collectively, the figure underscores that tensile hoop stress rather than shear or radial stress is the principal driver of cement integrity loss during CO₂ injection. These insights are crucial for wellbore design, as they highlight the need to optimize cement properties and casing pressure to minimize tensile stress development and ensure long-term sealing performance.

Similarly, shear FI is derived using the Mohr–Coulomb criterion and is sensitive to cohesion and internal friction angle. The model predicted that for cement with cohesion of 2 MPa and $\phi = 25^\circ$, shear FI values exceeded 1.2 in mid-radius regions under high injection rate scenarios (≥ 20 kg/s).

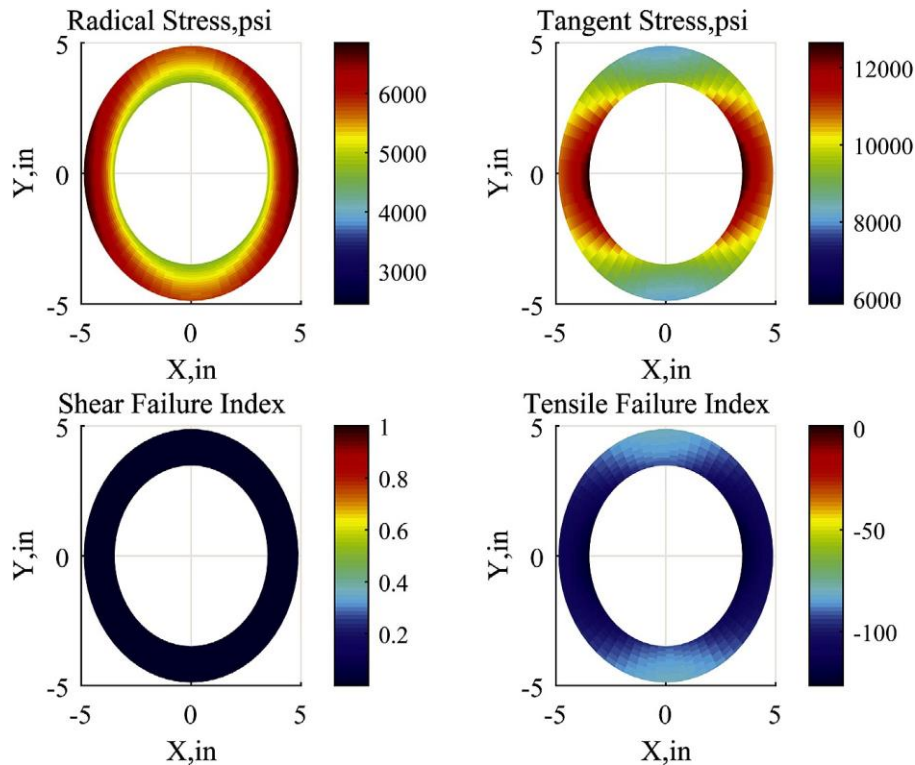


Figure 9. State of stress and FI of cement sheath.

4.1.3 Interfacial Debonding and Plastic Strain

As outlined in the multistage approach developed by Li et al. (2023) high plastic strains and hoop stress variations at the cement-formation interface suggest potential debonding risks. **Figure 10** in their study

shows maximum equivalent plastic strain of $\sim 1.4\%$ and hoop stress fluctuation over 10 MPa during thermal cycles. It presents simulation results of interface debonding between cement and formation during different stages of CO₂ injection, visualized as deformation maps across three phases: **Hardening, Injection, and Shutdown.**

Debonding Measurement:

The color scale indicates the opening displacement at the cement-formation interface, ranging from 0 to 0.1 mm. This deformation quantifies the separation between cement and formation, which can act as a potential leakage path for CO₂.

Hardening Phase:

During cement setting, no significant debonding is observed. The cement undergoes volume shrinkage, but the interface remains bonded, largely due to in-situ stress confinement and the elastic accommodation of materials.

Injection Phase:

The injection of cold CO₂ introduces significant thermal contraction. However, the figure shows minimal debonding (< 0.0001 m), suggesting that the high in-situ horizontal stress (36.9–38.7 MPa, as mentioned in the study) helps maintain interface integrity by preventing tensile opening or mechanical delamination.

Shut-Down Phase:

Upon removing the injection pressure and restoring formation temperature, the system undergoes elastic relaxation. Yet, no additional debonding is introduced, confirming the **stability of the cement-formation bond** throughout thermal cycles.

Importantly, their results highlight that while cement damage may be significant under thermal mismatch, high in-situ horizontal stresses can reduce debonding risk, which is relevant to deep reservoirs such as Northern Lights (depth ≈ 2650 m).

These findings guide the interpretation of analytical stress profiles and help prioritize design parameters such as cement selection, injection temperature management, and interface bonding strength.

This figure supports the paper's conclusion that **cyclic thermal loading alone** does not cause interface failure under current Northern Lights site conditions. The high in-situ horizontal stresses and well-designed material properties (e.g., Young's modulus, thermal expansion) mitigate the negative impact of thermal stresses.

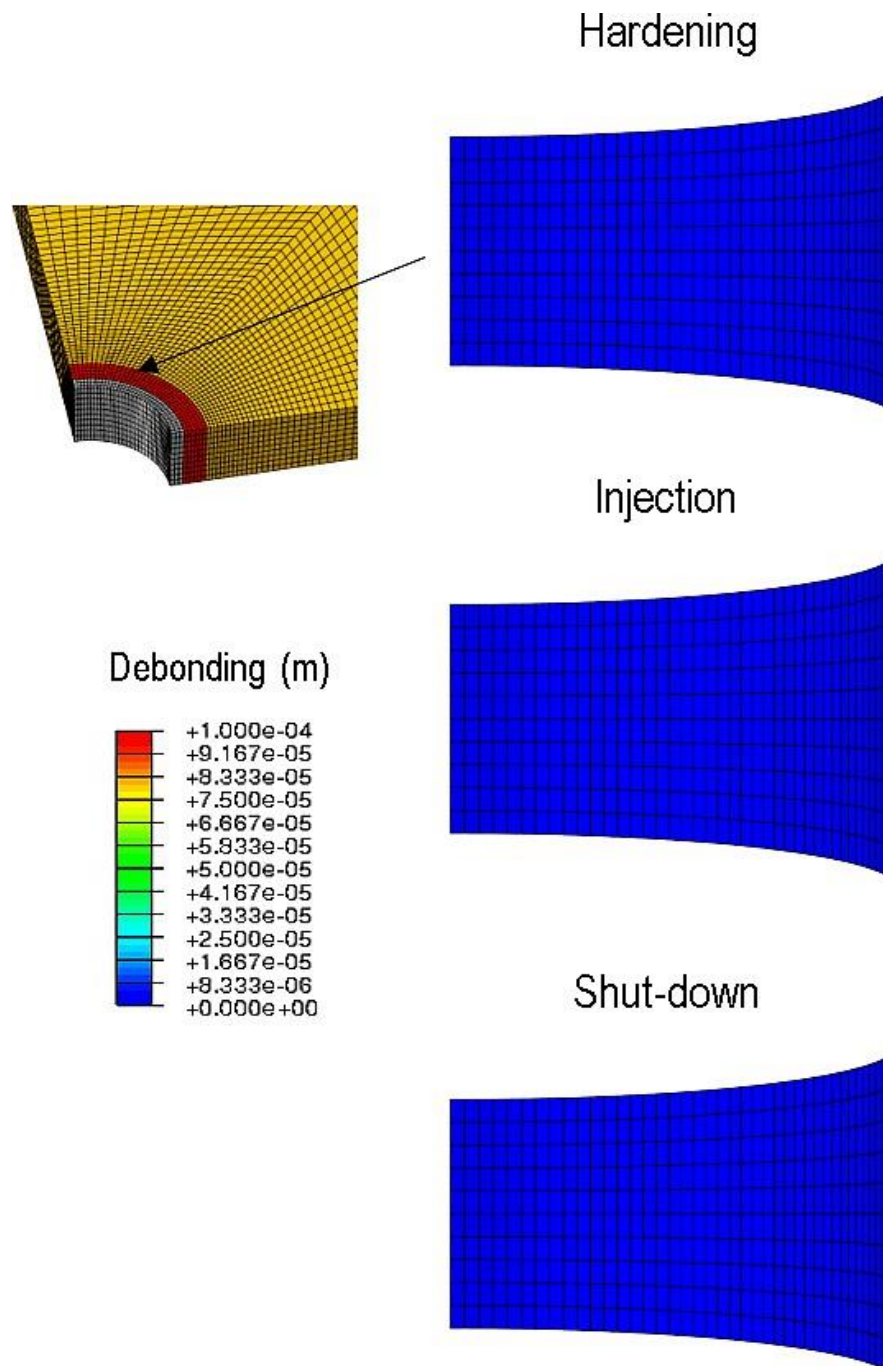


Figure 10. Debonding opening at the cement-formation interface.

4.1.4 Influence of Temperature Drop and Thermal Stresses

Thermal effects are a major factor influencing wellbore integrity during CO₂ injection, particularly when there is a significant temperature contrast between the injected CO₂ and the in-situ reservoir environment. Injecting cold CO₂ into a formation that is comparatively warmer leads to a sudden temperature drop in both the steel casing and the surrounding cement. This rapid thermal change can cause the materials to contract sharply, generating thermally induced stresses. When these stresses combine with mechanical loads from internal pressure and in-situ geological forces, they can significantly compromise the structural integrity of the well. One of the most critical challenges in CO₂ injection operations is the mismatch in temperature between the injected fluid and the formation. Injecting cold CO₂ into a hotter wellbore causes the steel casing and surrounding cement to contract. This thermal contraction induces hoop tensile stresses that may exceed the cement's tensile strength, leading to cracking, interfacial debonding, or even fracture propagation.

To assess these interactions, Dong et al. (2020) introduced a coupled thermal–mechanical model that examines stress behavior at the casing–cement interface under different injection scenarios and subsurface stress environments. The key output from their model is the **Mode I Stress Intensity Factor (SIF-I)**, which measures the potential for opening-mode fractures to initiate or propagate. **Figure 11**, adapted from their study, illustrates hoop and radial stress distribution under various temperature drops. This figure presents the influence of **effective horizontal stress** on **SIF-I** under two different injection temperatures:

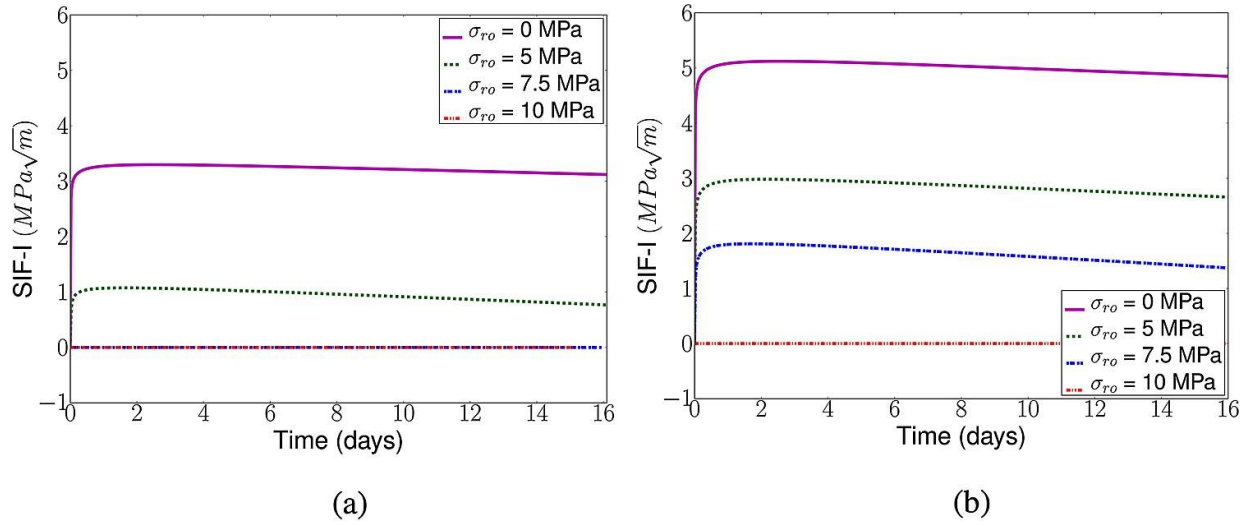


Figure 11. Influence of effective horizontal stress on Mode I Stress Intensity Factor (SIF-I) under two injection temperature scenarios: (a) 15 °C and (b) -15 °C

SIF-I increases significantly with decreasing injection temperature. When CO₂ is injected at -15 °C, the thermal contraction becomes more severe, making higher tensile stresses at the cement interface.

- **Higher in-situ horizontal stress further increases SIF-I**, especially under cold injection. For example, at $\sigma_h = 25$ MPa and injection temperature = -15 °C, the SIF-I reaches values that

could easily surpass the fracture toughness of cement, triggering interface debonding or radial cracking.

- In contrast, when injection temperature is 15 °C, the SIF-I values are considerably lower, showing that **thermal stress is the primary driver of cement failure under cold injection scenarios**.

This analysis directly connects thermal conditions with fracture risk, showing how even moderate cooling can create unsafe stress concentrations depending on the in-situ stress environment. It also highlights the **importance of temperature management**, selection of **thermally resilient cement**, and **accurate geomechanical profiling** during wellbore design.

4.1.5 Influence of Pressure Cycling on Wellbore Integrity

Pressure cycling characterized by repeated fluctuations between injection and shut-in phases is a recurring operational condition in CO₂ storage projects that has profound implications for long-term wellbore integrity. Each pressure variation alters the stress field within the wellbore system, which lead to cumulative mechanical degradation the casing, cement sheath, and formation interfaces. While individual pressure events may seem benign, their repetitive nature induces material fatigue and elevates the likelihood of structural compromise over time.

One of the primary concerns associated with pressure cycling is fatigue failure, particularly in the cement sheath. Cyclic pressurization and depressurization lead to fluctuating tensile and compressive stress states. Over time, this stress cycling leads to the propagation of microcracks in the cement matrix. These cracks can coalesce into larger fracture networks, reducing the mechanical strength of the cement and increasing its permeability. As permeability increases, the sealing capacity of the cement sheath diminishes, thus elevating the risk of CO₂ leakage. According to Zhang et al. (2021), even modest pressure fluctuations can significantly reduce the fatigue life of oilwell cement.

Moreover, pressure cycling does not act in isolation. It often occurs concurrently with temperature variations, especially in wells where injection is intermittent or where CO₂ is introduced at temperatures lower than formation equilibrium. This coupled thermo-mechanical loading imposes additional strains on the wellbore materials. For example, during injection, elevated pressures combined with a temperature drop from cold CO₂ injection cause differential contraction between steel casing and cement. This mismatch exacerbates the stress concentration at the casing-cement and cement-formation interfaces, increasing the risk of interfacial debonding.

Experimental evidence supports these observations. Laboratory tests conducted by Dong et al. (2020) demonstrated that cyclic pressure loading at both room and elevated temperatures resulted in progressive interfacial failures. Tensile cracks were more prominent under cyclic conditions compared to monotonic loading scenarios. These failures not only compromise zonal isolation but also create potential flow paths for migrating fluids, undermining the well's ability to contain injected CO₂.

To quantify these risks, several modeling efforts have incorporated pressure cycling into well integrity assessments. Numerical simulations based on finite element methods (FEM) have shown that stress intensification zones develop more rapidly under cyclic loads. In parallel, recent deep learning approaches have been applied to analyze large synthetic datasets generated from pressure cycling scenarios. These models help predict when and where failures may occur based on operational inputs such as injection frequency, pressure amplitude, and cement mechanical properties.

In operational settings, field data corroborate modeling predictions. Wells subjected to frequent pressure cycling tend to exhibit earlier signs of failure, including pressure anomalies, gas migration, and casing deformation. This reinforces the need for careful control of pressure regimes during CO₂ injection operations. Reducing the frequency and magnitude of pressure fluctuations, using more fatigue-resistant cement formulations, and employing predictive tools for early failure detection are critical mitigation strategies.

In conclusion, pressure cycling represents a cumulative and potentially severe threat to CO₂ wellbore integrity. Its effects are magnified when combined with thermal stresses and material property mismatches. Understanding the mechanisms behind pressure-induced degradation and integrating them into well design and monitoring practices is essential for the safe and sustainable operation of carbon storage projects.

4.1.6 Coupled Effects of Pressure and Temperature Variations

The interaction between pressure and temperature variations during CO₂ injection operations results in a complex and often synergistic influence on wellbore integrity. These coupled effects exacerbate both mechanical and thermal stresses acting on casing, and formation interfaces. The resulting combination of stresses increases the likelihood of degradation, debonding, and ultimately CO₂ leakage pathways that compromise long-term storage security.

Pressure fluctuations—arising from variable injection rates, shut-in periods, or operational disturbances—impose dynamic radial and hoop stresses on the wellbore. When these pressure cycles are accompanied by thermal variations due to differences of temperature in the injected CO₂ and the surrounding formation, the stress environment becomes highly complex and time-dependent. For instance, the steel casing may contract or expand faster than the cement sheath due to delta in thermal conductivity and thermal expansion coefficients. This mismatch creates interfacial stress accumulation that can initiate mechanical failure at the cement–casing or cement–formation interfaces.

Research by Li et al. (2023) and Carey et al. (2007) indicates that maximum thermal stresses generally develop in the cement sheath adjacent to the casing, whereas stresses resulting from pressure are more pronounced closer to the formation boundary. When both thermal and pressure loads act together, the resulting stress profiles amplify concentration zones. These zones often exceed the tensile strength of the cement, especially under cyclic loading conditions. Consequently, fatigue-induced cracking, cement debonding, and eventual leakage become more probable.

Experimental investigations confirm the importance of considering the coupled effects. Laboratory experiments simulating thermal and pressure cycles have revealed that cement undergoes microstructural changes after relatively few cycles. The mechanical strength, particularly in terms of tensile and shear capacity, decreases progressively with repeated loading. Microcracks propagate with each cycle, weakening the material and reducing its bonding efficiency. This is particularly dangerous in wells expected to operate over long timeframes where cumulative damage may go unnoticed.

Advanced numerical simulations, particularly those that implement fully coupled thermo-poroelastic models, offer valuable insights into how these effects manifest under real-world conditions. These models track the evolution of stress and strain fields over time and space. In recent studies, researchers have also used machine learning surrogates trained on synthetic datasets generated via Latin hypercube sampling to map the failure envelope across varying operational and material conditions. This approach provides fast approximations of risk while maintaining acceptable accuracy.

The synergistic effect of pressure and temperature changes cannot be overstated. During injection, the thermal contraction of casing coupled with high internal pressure may cause the cement to experience tensile hoop stress. During shut-in periods or production, reverse conditions may occur, causing alternating stress directions. This repeated reversal of stress states contributes to mechanical fatigue, making interface debonding more likely and threatening zonal isolation.

In conclusion, pressure and temperature variations must be jointly evaluated when assessing wellbore integrity. Their combined action introduces stress states not observed in isolated analyses and greatly elevates the risk of structural failure. Design modifications such as thermal-resistant cement blends, flexible cement systems, or operational strategies with controlled cycling can help mitigate this risk and extend well longevity.

4.2 Cement Sheath Failure Modes and Mechanisms

The cement sheath is a first barrier for ensuring more life cycled environment wellbore integrity in CO₂ injection operations. It isolates formation fluids, supports the casing, and seals the annular space. However, the downhole environment of CO₂ storage characterized by high pressures, temperature fluctuations, and chemically reactive fluids can challenge the quality of the cement sheath. These extreme conditions can lead to various mechanical and chemical degradation mechanisms that compromise sealing performance.

Common failure mechanisms include radial cracking, plastic deformation, interfacial debonding, chemical degradation, and the development of microannuli. These mechanisms can occur independently or in combination, often triggered by operational factors such as pressure surges, thermal cycling, and prolonged CO₂ exposure. According to Carey et al. (2007), chemical Reaction between cement hydrates, carbonic acid can convert cement to weaker phases like calcite and amorphous silica, reducing strength and stiffness.

Numerical studies such as those by Li et al. (2023) and experimental work by Um et al. (2016) show that repeated thermal cycles can cause cumulative damage, especially between the casing and cement and cement versus formation interfaces. These interfacial zones are prone to debonding due to differential thermal expansion and stress concentration. Once a microannulus forms, it can serve as a preferential leakage pathway for CO₂-rich fluids.

Advanced simulations employing coupled thermo-mechanical models (e.g., Zhang et al., 2020) have demonstrated that the mismatch in thermal expansion coefficients between casing, cement, and rock significantly contributes to tensile and shear failure in the cement. Field evidence and core sample analysis further validate that thermal and pressure loading cycles are a major cause of well integrity loss in mature CO₂ injection wells.

4.2.1 Radial Cracking and Tensile Failure

Cement sheaths are subjected to a combination of mechanical, thermal, and chemical loads over the lifespan of a CO₂ storage well. Because Portland cement has low tensile strength compared to its compressive strength, it is particularly vulnerable to tensile failure, especially when exposed to fluctuating downhole conditions.

Tensile stresses in the cement sheath can be induced through various mechanisms. One of the most prominent is the mismatch in thermal expansion coefficients between the cement and surrounding materials such as the casing and formation. When CO₂ is introduced into the reservoir at a temperature below that of the native formation, the cement surrounding the well undergoes rapid cooling, causing it to contract due to thermal effects. This process generates hoop (circumferential) and radial tensile stresses within the cement matrix. If the magnitude of these thermally induced stresses exceeds the tensile strength of the cement, radial cracks are likely to initiate and propagate.

Additionally, pressure fluctuations during CO₂ injection and shut-in cycles can further exacerbate tensile stress development. When high-pressure CO₂ is injected, the casing expands outward, imposing additional radial stress on the cement sheath. If the cement is already weakened by thermal effects or chemical degradation, these pressure-induced stresses can initiate cracks. Once formed, radial cracks propagate along the sheath and may reach the interface between cement and surrounding formation, thereby increasing the risk of fluid leakage along the wellbore.

The study by Kranjc et al. (2015) illustrates how carbonation reactions between aqueous CO₂ and Portland cement lead to the formation of calcium carbonate and silica gel, which significantly alter the microstructure of the cement. These chemical reactions lower the tensile strength and increase porosity, making the cement more susceptible to mechanical failure. Their findings emphasize that degradation processes are time-dependent and become more critical with prolonged exposure to CO₂-rich environments, especially under elevated temperature and pressure conditions.

Um et al. (2016) provide experimental confirmation of these mechanisms. In their study, cement specimens exposed to supercritical CO₂ under cyclic thermal and pressure loading showed the development of microcracks, primarily along the casing–cement interface. These cracks expanded radially over time due to thermal stress cycling. The authors presented scanning electron microscope (SEM) images and cross-sectional diagrams illustrating how crack networks evolve, compromising the long-term sealing of the wellbore. As illustrated in **Figure 12**, these radial cracks form due to combined effects of thermal contraction and mechanical stress and propagate outward through the cement sheath, increasing the risk of leakage pathways and zonal isolation failure. This schematic helps visualize how the interaction of thermal and mechanical loads initiates damage that grows over operational cycles, ultimately reducing structural integrity.

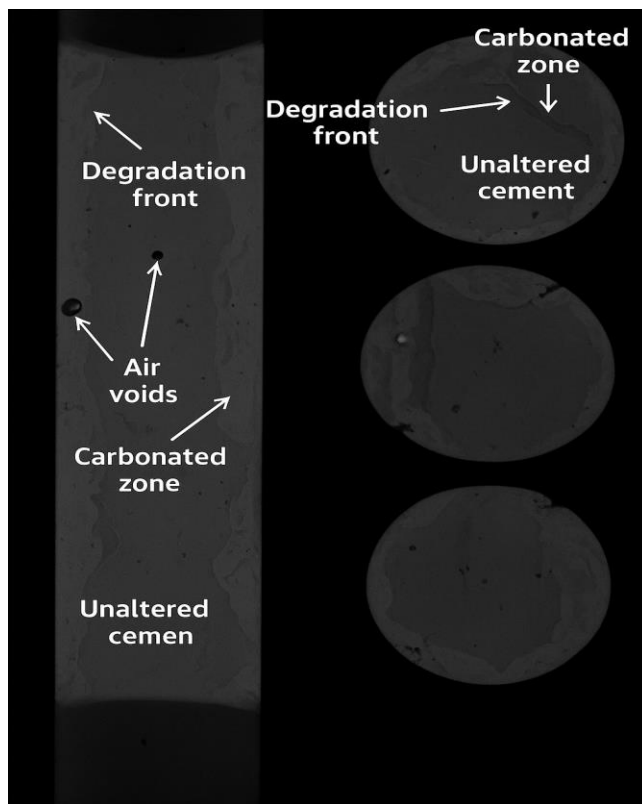


Figure 12. Radial crack propagation in cement under cyclic thermal and pressure loads.

4.2.2 Shear Interface Debonding

Shear interface debonding is one of the most critical and insidious mechanisms affecting the long-term integrity of CO₂ injection wells. It refers to the loss of adhesion between the steel casing and the surrounding cement sheath, often resulting in the formation of micro-annuli that act as leakage pathways for CO₂ migration. This failure mechanism is predominantly driven by the combined effects of thermal contraction, cyclic loading, and elevated fluid pressures introduced during CO₂ injection.

During injection, supercritical or cold CO₂ is introduced into formations at elevated depths. The temperature differential between the injected CO₂ and the surrounding geologic formation induces thermal stress within the wellbore system. Because the casing and cement have different coefficients of thermal expansion ($\alpha_{casing} \neq \alpha_{cement}$), this differential contraction causes a shear mismatch at the casing–cement interface. If the interfacial shear stress ($\tau_{interface}$) exceeds the bond strength (τ_{crit}), debonding initiates. Mathematically, this is described as:

$$\text{If } \tau_{interface} > \tau_{crit}, \rightarrow \text{debonding initiates}$$

The interfacial shear stress is influenced by both the mechanical loading (injection pressure, formation stress) and the thermal strain, which can be approximated as:

$$\tau_{interface} \approx G * \Delta \varepsilon_{thermal} \quad 1.9$$

Where:

- G is the shear modulus of the cement,
- $\Delta \varepsilon_{thermal} = (\alpha_{casing} - \alpha_{cement}) * \Delta T$,
- ΔT is the temperature difference due to injection.

Poor cement placement, low bonding strength, and operational fluctuations (e.g., shut-ins and restart cycles) further exacerbate the risk of debonding. Once initiated, micro-annular debonding can propagate vertically along the wellbore, compromising zonal isolation and increasing the risk of CO₂ leakage into overlying aquifers.

Finite element simulations, such as those presented in Dong et al. (2020), offer valuable insights into the stress distributions that lead to interfacial failure. **Figure 13** presents two subplots (a) and (b), illustrating how the energy release rate changes with cement's Young's modulus, and how the geometry of the deboned interface influences this relationship. Such models are essential for predicting wellbore response under various injection scenarios and allow engineers to evaluate the effectiveness of material selections and well design parameters.

- X-Axis (Both Plots): Normalized Young's modulus of cement (E_c/E_f), where:
 - E_c : Cement's Young's modulus
 - E_f : Formation's Young's modulus
- Y-Axis (a): Energy release rate G_A (Mode A, likely radial debonding or opening mode)
- Y-Axis (b): Energy release rate G_B (Mode B, likely circumferential or shear sliding debonding)

(a) Energy Release Rate G_A vs Cement Stiffness:

- As cement becomes stiffer (i.e., $E_c/E_f \rightarrow 1$), the energy release rate increases sharply.
- Higher geometric ratio $a/(R_w - R_{ci})$ results in higher G_A , meaning longer cracks in thinner annular sections are more prone to unstable debonding
- This suggests radial separation (Mode A) is more sensitive to crack length and cement stiffness.

(b) Energy Release Rate G_B vs Cement Stiffness:

- A similar trend is observed: increasing cement stiffness increases G_B , but the growth is more moderate.
- Differences among curves are smaller compared to (a), indicating that Mode B (likely shear debonding) is less sensitive to crack size than radial Mode A.

The results indicate that cement materials with increased stiffness tend to store and release more energy, which raises the chances of interface separation once cracking begins. Moreover, cement layers that are thinner and have relatively longer cracks—measured by the ratio of crack length to the thickness of the cement sheath—show a higher tendency toward failure along the casing–cement boundary. These findings emphasize the necessity of optimizing both the mechanical characteristics of the cement and the geometry of the annular space during well construction to enhance sealing performance and prevent CO₂ leakage.

To mitigate the risk of debonding, strategies such as improving the casing surface roughness, using expanding cements, and implementing stress-buffering layers (e.g., ductile liners) have been proposed in the literature. Nonetheless, continuous monitoring and modeling remain the best tools for ensuring long-term well integrity.

In summary, shear interface debonding is a multidimensional failure mechanism controlled by thermomechanical and chemical interactions. Accurate modeling, validated by field or lab data, is crucial for predicting and mitigating these risks.

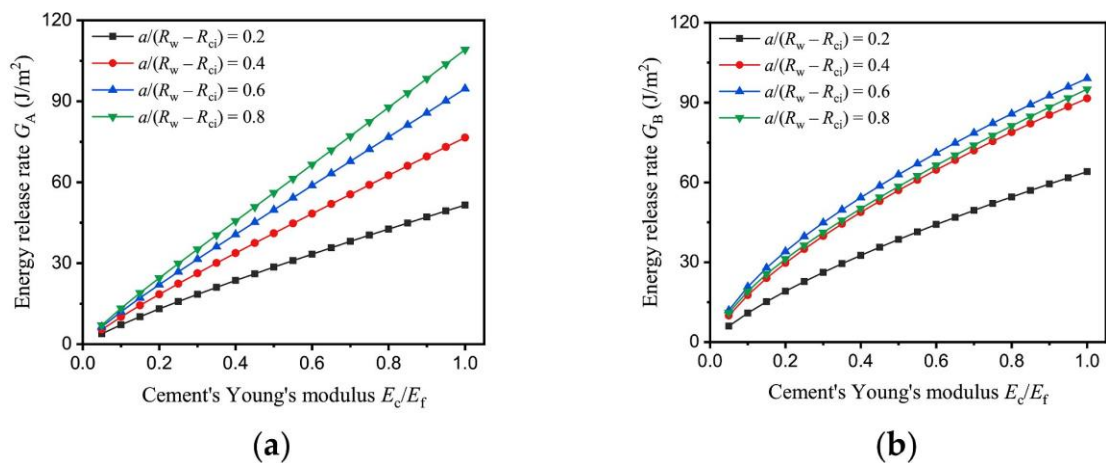


Figure 13. Finite element simulation of debonding regions under CO₂ injection thermal stress.

4.2.3 Plastic Deformation of Cement Sheath

Plastic deformation of the cement sheath refers to the irreversible strain that occurs when the cement is subjected to stresses beyond its elastic limit. While Portland cement is typically considered brittle, under the extreme thermomechanical conditions encountered in CO₂ injection wells, it may exhibit viscoplastic behavior particularly when exposed to sustained high pressures, elevated temperatures, and cyclic loading.

The cement sheath is sandwiched between the steel casing and the surrounding formation during injection. Fluctuating thermal and pressure gradients result in differential expansion and contraction, which over time may exceed the cement's yield strength. When this occurs, the cement transitions from elastic to plastic behavior, accumulating strain that cannot be recovered. Although this process does not always lead to immediate cracking, it weakens the mechanical support around the casing and can alter zonal isolation by shifting the load distribution and introducing long-term deformations.

The governing condition for the onset of plastic deformation is commonly expressed using the von Mises yield criterion. In this formulation, plastic deformation initiates when the equivalent stress σ_{vm} satisfies:

$$\sigma_{vm} = \sqrt{\frac{3}{2} S_{ij} S_{ij}} \geq \sigma_y \quad 2.0$$

Where:

- σ_{vm} is the von Mises equivalent stress,
- S_{ij} is the deviatoric stress tensor component,
- σ_y is the yield strength of the cement.

This criterion is frequently incorporated into advanced constitutive models such as the Drucker–Prager or Modified Cam-Clay formulations to simulate plasticity under complex loading paths. These models capture time-dependent strain (creep), hysteresis from cyclic loading, and the anisotropic evolution of plastic zones within the annular cement.

Exposure to CO₂ further complicates the mechanical behavior. According to experimental studies by Kiran et al. (2017) and Um et al. (2016), carbonation reactions lead to significant microstructural changes, such as the formation of calcium carbonate and silica gels. These phases can embrittle or soften the cement depending on porosity and saturation, thus altering both the modulus and the yield threshold. Over long durations, plastic creep deformation has been observed even under relatively low stress regimes.

Figure 14 illustrates a representative finite element simulation of a casing–cement–formation system subjected to radial mechanical loading and elevated temperature gradients. The image highlights localized plastic yield zones, typically forming near the casing–cement interface due to

high radial and hoop stress concentrations. As plastic deformation progresses, these zones expand, weakening the structural confinement and increasing susceptibility to casing deformation or cement debonding. It offers a validated numerical view of how cement plastically deforms under realistic injection conditions. Step by step explanation:

- As the thermal expansion coefficient α_c increases (due to higher temperature differentials from injection), thermal stresses within the cement sheath intensify.
- Elevated stress levels may surpass the cement's yield strength, leading to plastic deformation and the initiation and growth of cracks at the interfaces between casing and cement or cement and formation.
- The fracture driving force is measured by the energy release rate, denoted as G . A higher G indicates a greater tendency for crack growth, especially under thermal loading cycles (heating/cooling) typical in CO₂ injection operations.
- The curves show a nonlinear increase, meaning that small increases in α_c at high values cause disproportionately higher GGG, indicating potential instability and failure risks in plastic zones.
- Notably, larger crack ratios $a / (R_w - R_{ci})$ correspond to higher energy release rates, signifying greater vulnerability of pre-existing microcracks under thermally induced plastic strains.

To mitigate plastic failure, recent approaches include the use of flexible or ductile cement systems, incorporation of fibers or polymer modifiers, and application of improved bonding technologies that reduce local stress concentrations. Moreover, simulations that integrate plastic models with thermal and chemical degradation modules are recommended in the design of CO₂ wells to predict long-term structural behavior.

Plastic deformation, though not immediately catastrophic, plays a key role in long-term integrity loss and must be quantitatively assessed in any CO₂ storage project.

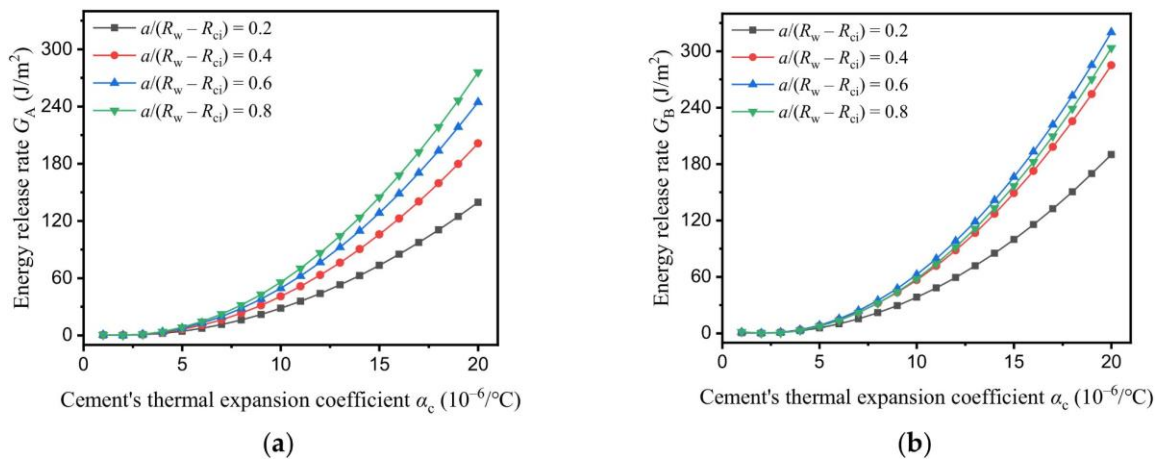


Figure 14. Finite element simulation of plastic yield zones in annular cement during CO₂ injection.

4.2.4 Microannulus Formation and Permeability Increase

Microannulus formation is one of the most critical mechanisms compromising wellbore integrity during CO₂ injection. It refers to the development of small annular gaps on the micron scale either between the casing and the cement sheath or between the cement and the surrounding formation. Although typically invisible to standard well logging tools, these gaps can significantly increase effective permeability, allowing injected CO₂ to migrate through the wellbore annulus, bypassing zonal barriers and threatening containment security.

Mechanisms Leading to Microannulus Formation

The primary causes of microannulus formation are mechanical stress redistribution, thermal cycling, and long-term chemical degradation. These are initiated or exacerbated during CO₂ injection, where pressure and temperature gradients lead to strain mismatches among wellbore materials.

Dong et al. (2020), in their study applied a coupled flow-stress finite element model to analyze cement sheath behavior. One of their simulations, presented in **Figure 15**, shows the total displacement distribution under a 10 MPa injection pressure. The highest displacements are concentrated near the casing–cement interface, a region highly susceptible to bond failure. This localized deformation is a mechanical precursor to microannulus initiation, which may occur without any macroscopic cracking. These graphs illustrate how different injection parameters influence cement failure factors during CO₂ injection. The failure factors are defined as follows:

- η_t (tensile failure factor): A dimensionless ratio representing the proximity of tensile stress to the tensile strength of the cement. η_t approaching 1 indicates near-tensile failure conditions.
- η_s (shear failure factor): A ratio of induced shear stress to the shear strength of cement. Higher values imply greater shear failure risk.

(a) Failure Factors vs. Injection Temperature

As injection temperature T_{inj} increases from -20°C to 20°C:

- Tensile failure factor (η_t) decreases slightly
- Shear failure factor (η_s) increases gradually

Higher injection temperatures may reduce tensile failure risk but increase shear failure potential in cement.

(b) Failure Factors vs. Injection Rate

As injection rate P_{inj} increases:

- η_t rapidly approaches 1 (near-failure in tension)

- η_s decreases and stabilizes

High injection rates greatly increase the likelihood of tensile failure, while shear failure becomes less dominant.

(c) Failure Factors vs. Injection Time

As injection time t_{inj} extends (up to 250 days):

- η_t increases progressively
- η_s decreases

Over time, tensile stress continues to accumulate, increasing failure risk, while shear stress stabilizes or reduces.

These results support the need for careful regulation of injection conditions to avoid compromising cement integrity at the casing–cement interface.

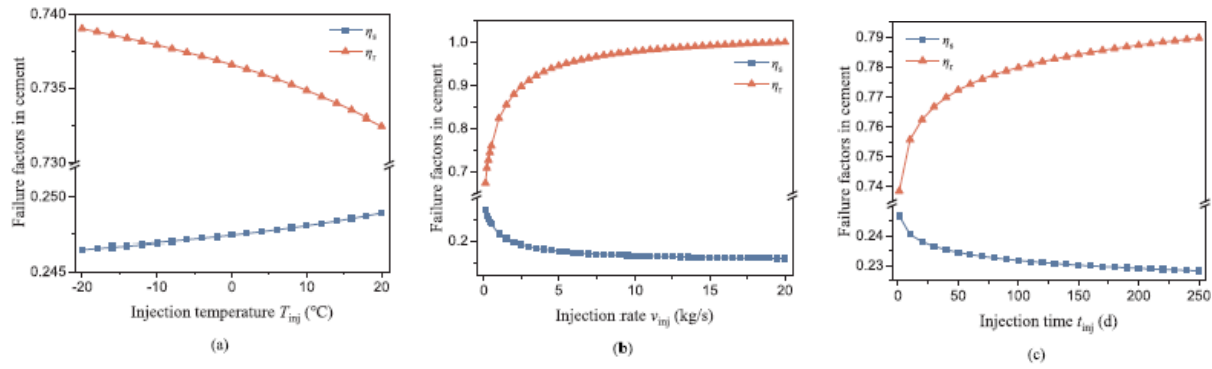


Figure 15. Evolutions of failure factors for shear compressive failure and radial cracking in cement: (a) injection temperature, (b) injection rate, (c) injection time.

Thermal loading from CO₂ injection exacerbates this mechanism. With each injection cycle, temperature fluctuations cause the steel casing and cement sheath to expand and contract at different rates. The mismatch in thermal expansion coefficients results in cyclic shear and tensile stresses at the interface. This effect is governed by the equation:

$$\sigma_{th} = E_c(\alpha_c - \alpha_s)\Delta T \quad 2.1$$

Where:

- σ_{th} : Thermally induced stress
- E_c : Young's modulus of cement
- α_c, α_s : Thermal expansion coefficients of cement and steel

- ΔT : Temperature change
- Newell & Carey (2012), in their experimental work, confirmed this behavior by showing that repeated thermal cycling leads to loss of interface bonding strength and increased permeability.

Microstructural Changes from Chemical Exposure

Over time, chemical interaction between injected CO₂ and cement further contributes to microannulus evolution. Hangx et al. (2016), in their paper described three distinct reaction zones forming due to carbonation: a silica-rich outer rim, a carbonate-rich mid-layer, and a calcium-depleted inner core. These regions have differing mechanical properties, such as friction angle and compressive strength, which create internal stress discontinuities.

Figure 16 illustrates this zonation and its mechanical implications. The transition between the carbonate-rich and calcium-depleted regions, in particular, becomes a natural weak point for microcracking and interface debonding. This figure presents unconfined compressive strength (UCS) and normalized hardness (H/H_0) of cement samples across different exposure times to CO₂ environments, comparing both experimental data from this study and previously published results. CO₂ exposure initially weakens cement, particularly in inner regions (Z1, Z2), by leaching Ca and reducing strength. Over longer exposure times, outer layers may gain strength or hardness, creating a misleading sense of integrity despite inner degradation. Results confirm the formation of mechanically distinct reaction zones (as shown in Figure 4.2.5.2), and support the need to assess both UCS and hardness evolution when evaluating long-term cement performance.

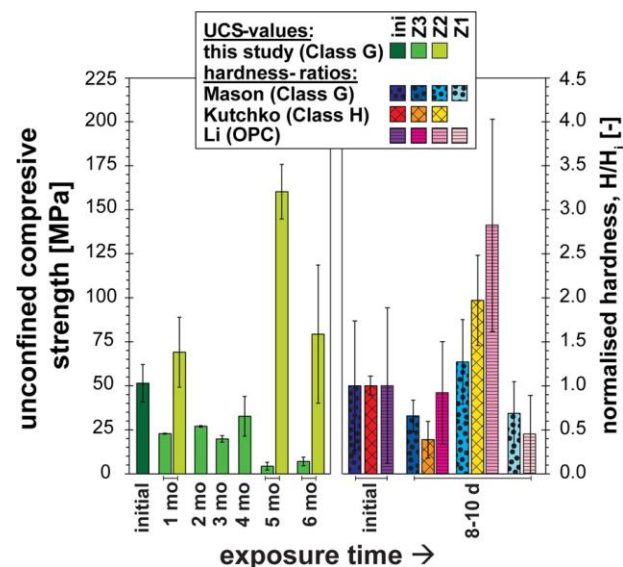


Figure 16. Reaction zones in CO₂-exposed wellbore cement: outer silica-rich, mid carbonated, and inner Ca-depleted core.

Kranjc et al. (2015) corroborated these findings, noting that carbonation-induced microstructural changes reduce the unconfined compressive strength (UCS) by over 30%, making the cement matrix more prone to fracture and debonding under stress.

Permeability Impacts and Risk Evaluation

Although microannuli are typically only tens of microns in width, their impact on annular permeability is profound. Wu et al. (2024), through a combination of modeling and experimental work, demonstrated that interfacial gaps as small as 20 μm can facilitate significant CO_2 migration, especially when aligned with stress trajectories.

Moreover, the development of such leakage paths is often nonlinear. Initial debonding may induce localized pressure buildups that further fracture the cement sheath or open additional flow paths. Um et al. (2023) introduced a machine learning framework capable of predicting such failure initiation by analyzing key injection parameters and stress conditions.

In conclusion, microannulus formation is a multi-mechanism process involving mechanical deformation, thermal fatigue, and chemical degradation. Finite element simulations, laboratory observations, and analytical models all converge to identify the casing–cement interface as the critical zone for failure. Understanding the combined effects of stress, temperature, and chemical alteration is essential for designing injection strategies that minimize leakage risk and ensure long-term wellbore integrity.

Chapter 5: Experimental and Field Studies on Well Integrity

The long-term performance of CO₂ injection wells depends critically on the mechanical and chemical stability of the wellbore system. While numerical and analytical models provide essential insights into stress distribution, thermal effects, and failure thresholds, these models require rigorous validation. Experimental investigations and field studies offer indispensable empirical evidence to support or refine theoretical predictions.

This chapter presents a comprehensive examination of laboratory-scale tests and field observations related to wellbore integrity under CO₂-rich conditions. These studies aim to simulate or document the degradation mechanisms affecting casing–cement–formation interfaces, with particular focus on cement carbonation, interfacial debonding, microcracking, and permeability changes.

Experimental studies typically involve high-pressure, high-temperature (HPHT) autoclave systems, chemical exposure cells, and mechanical testing apparatuses. These allow researchers to simulate CO₂ exposure over weeks to months and assess variations in parameters such as unconfined compressive strength (UCS), elastic modulus, permeability, microstructure, and failure modes.

Field studies, on the other hand, provide real-world validation through logging tools, cement bond logs (CBL), ultrasonic imaging, pressure monitoring, and wellhead sampling. Observations from CO₂ injection projects such as SACROC, In Salah, and CarbFix have revealed critical insights into failure evolution, bonding loss, and the role of geological heterogeneity.

By integrating laboratory and field-scale evidence, this chapter strengthens the conceptual foundation laid by previous analytical and numerical models. Each section aims to correlate observed degradation features with injection parameters, material properties, and interface behavior. Together, these insights help inform well design standards, regulatory practices, and risk management protocols for geological CO₂ sequestration.

5.1 Laboratory Studies on Cement–CO₂ Interaction

Understanding the degradation behavior of cement in CO₂-rich environments is essential to predict long-term wellbore integrity. Laboratory-scale studies allow researchers to isolate specific mechanisms—chemical, thermal, and mechanical that compromise the sealing ability of cement sheaths. This section synthesizes findings from over a dozen experimental investigations, analyzing trends in strength reduction, microstructural evolution, and permeability changes under controlled CO₂ exposure.

5.1.1 Microstructural Evolution and Zonation

Microstructural evolution in CO₂-exposed cement has emerged as one of the most critical degradation mechanisms affecting wellbore integrity. When CO₂-rich fluids come into contact with hydrated Portland cement, they trigger a series of mineral changes, alter the porosity, and cause a reduction in mechanical strength. These phenomena occur in spatially distinct zones that evolve over time under reservoir conditions.

Carey et al. (2007) conducted one of the most comprehensive laboratory studies on this zonation by analyzing cement cores extracted from the SACROC Unit following nearly three decades of exposure to CO₂. Using scanning electron microscopy (SEM) and electron probe microanalysis (EPMA), they identified three primary alteration zones:

- **Carbonated Zone (outer rim):** This layer is dominated by calcite, resulting from carbonation of portlandite and C–S–H phases. While this rim reduces permeability due to calcite precipitation, it is mechanically brittle and prone to spalling under stress.
- **Transition Zone:** Located beneath the outer rim, this zone shows high porosity caused by the dissolution of calcium-bearing phases and formation of amorphous silica. It is mechanically the weakest layer.
- **Intact Core:** The inner zone remains relatively unaffected by CO₂, preserving original hydration products and structural integrity.

To visualize this microstructural evolution, **Figure 17** presents a composite zonation structure, which depicts a cross-sectional SEM image and elemental profile showing distinct zones within long-term CO₂-exposed cement.

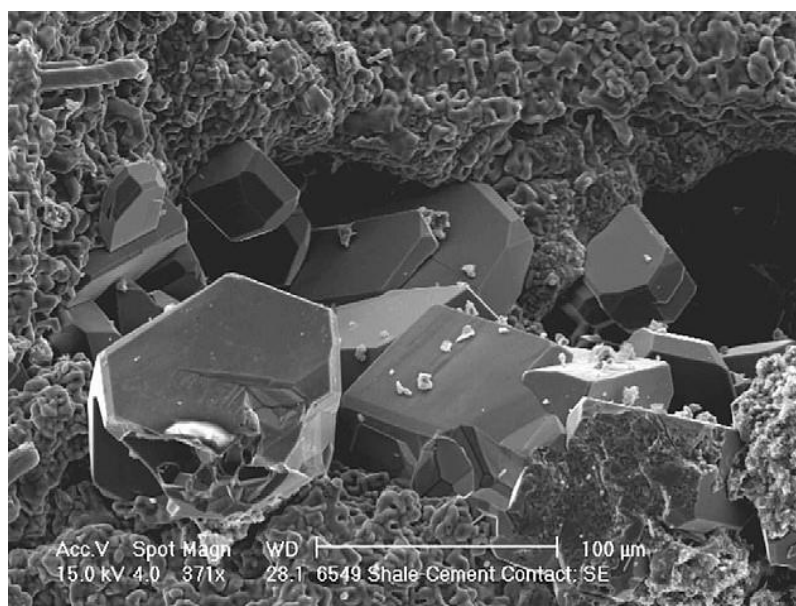


Figure 17. SEM image and zonal differentiation in CO₂-altered wellbore cement showing outer calcite rim, high-porosity transition layer, and preserved core.

These zonation features were further validated by Hangx et al. (2016), who carried out triaxial compression tests and nano-indentation on cement samples subjected to CO₂ exposure. They confirmed that each zone exhibits distinct mechanical behavior: the carbonated rim becomes stiffer but more brittle; the transition zone loses cohesion and strength; and the intact core retains ductility. Although used previously in Section 4.2.5.2, their findings strengthen the interpretation of Carey’s long-term observations.

Complementary work by Kranjc et al. (2015) analyzed chemical degradation pathways and zonation using XRD, SEM-EDX, and nano-indentation. They identified similar zonation patterns and demonstrated the evolution of porosity and mechanical softening in the transition zone. The structural heterogeneity observed was attributed to diffusion-limited carbonation and leaching mechanisms.

To summarize these results, **Table 4** compares experimental data on the mineralogical and mechanical properties across the zones from Carey et al. (2007), Hangx et al. (2016), and Kranjc et al. (2015).

Table 4. Laboratory results detailing the mineral composition and mechanical characteristics throughout the different zones.

Zone	Dominant Phases	Porosity (%)	UCS (MPa)	Failure Mode	Source
Outer Rim	Calcite, degraded C-S-H	12–18	20–30	Brittle spalling	Carey et al. (2007)
Transition	Amorphous silica, low Ca	20–35	5–10	Shear/tensile cracks	Hangx et al. (2016)
Intact Core	Portlandite, C-S-H	8–12	30–40	Ductile compression	Kranjc et al. (2015)

These experimental findings collectively emphasize that cement alteration under CO₂ injection is not uniform but proceeds through progressive zonation. These zones differ significantly in chemical composition, porosity, and mechanical strength, which can lead to differential stress development, crack initiation, and compromised sealing capacity. Therefore, integrity models must explicitly consider zonation effects for reliable long-term well performance predictions.

The next section explores how exposure duration further influences mechanical properties and degradation depth in these zones.

5.1.2 Effects of Exposure Duration on Mechanical Properties

The duration of CO₂ exposure plays a fundamental role in determining the extent and severity of cement degradation. Long-term interactions between CO₂-rich fluids and hydrated cement induce a time-dependent progression of microstructural and mechanical changes, with zonal evolution becoming more pronounced over time. These effects are particularly relevant for injection scenarios expected to last decades or longer.

In a systematic experimental study, Kutchko et al. (2007) conducted controlled laboratory experiments where Class H Portland cement samples were exposed to supercritical CO₂ and CO₂-saturated brine for periods ranging from several weeks to months. They observed that carbonation reactions—particularly the conversion of portlandite to calcite—initiated rapidly but continued to evolve over time, resulting in a gradual thickening of the outer carbonated layer. Mechanical testing revealed increased stiffness but also enhanced brittleness in this zone. Their results showed that after 28 days of exposure, the compressive strength of the outer layer increased by approximately 10–15%, but its fracture energy was significantly reduced.

Um et al. (2016) extended these findings by simulating prolonged exposure periods up to 6 months using Class G cement samples. Their study highlighted that extended exposure led to deeper penetration of CO₂ reaction fronts, which in turn affected the modulus and porosity profile of the cement sheath. Porosity was found to increase in the transition zone over time due to continuous leaching of calcium and silica restructuring. These observations support the importance of accounting for reaction front migration in long-term injection scenarios.

Figure 18, adapted from Newell & Carey (2012), provides visual evidence of the carbonation front, unaltered cement, and fracture infill across exposed cores. The SEM analysis clearly shows the degradation boundary and demonstrates how carbonation progresses inward from the cement–rock interface over time. The graph illustrates the chemical evolution of cement during prolonged CO₂ exposure, showing how calcium (Ca²⁺) and strontium (Sr²⁺) concentrations in pore fluids increase with rising bicarbonate (HCO₃[−]) levels. This trend reflects the progressive dissolution of cement phases such as portlandite and calcium silicate hydrates (C–S–H), accompanied by the mobilization of trace elements like Sr²⁺.

This chemical response directly supports the focus of **Section 5.1.2**, which examines the effects of exposure duration on mechanical degradation. As HCO₃[−] accumulates due to continuous CO₂ reaction, structural ions leach from the cement matrix, weakening its integrity over time. The graph reinforces the conclusion that long-term exposure leads to both mechanical and chemical deterioration, underscoring the need to account for time-dependent processes in wellbore integrity assessments.

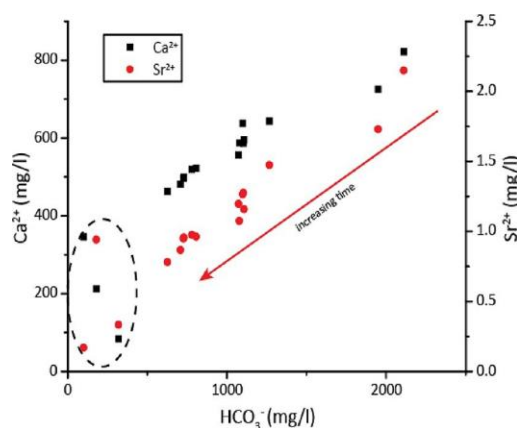


Figure 18. Cross-sectional images showing carbonation fronts, unaltered cement, degradation boundaries, and carbonate-filled fractures in long-term CO₂-exposed cement cores.

The correlation between exposure duration and mechanical weakening was also confirmed by **Kranjc et al. (2015)**. Their nano-indentation measurements demonstrated a time-dependent decrease in hardness and Young's modulus within the transition zone, emphasizing the vulnerability of this zone to fracture initiation as carbonation fronts advanced deeper into the matrix.

Furthermore, **Newell and Carey (2012)** reported experimental results from field-representative samples exposed to CO₂ over longer periods, revealing that zonation deepened with exposure time. They suggested that CO₂ diffusion and capillary imbibition jointly controlled the progression rate. Their observations aligned with X-ray microtomography results showing that fractures initiated and propagated predominantly along the carbonated–transition zone interface after several months of exposure.

These studies collectively reveal that exposure duration directly influences zonation thickness, mechanical heterogeneity, and fracture susceptibility. Therefore, time must be explicitly incorporated into wellbore integrity predictions and numerical models. Cement systems that perform adequately in short-term evaluations may fail under long-term CO₂ injection conditions due to progressive degradation.

These experimental results highlight the significance of time as a governing factor in wellbore cement degradation under CO₂-rich conditions. While early exposure may superficially enhance strength due to carbonation-induced densification, prolonged interactions often lead to structural weakening in the transition and core zones. To synthesize the findings across various studies, **Table 5** provides an overview of the changes in mechanical properties—including compressive strength, porosity, hardness, and elastic modulus—relative to the length of exposure time. This comparative view underscores the importance of incorporating time-dependent degradation in both laboratory evaluations and predictive models for CO₂ storage well design.

Table 5. Summary of mechanical property changes over time in CO₂-exposed cement.

Study	Cement Type	Exposure Time	Key Observations
Kutchko et al. (2007)	Class H	28 days	Increased stiffness, reduced fracture energy
Um et al. (2016)	Class G	6 months	Porosity increase in transition zone; deeper zonation
Kranjc et al. (2015)	Class G	90 days	Decrease in modulus and hardness in mid-zone
Newell & Carey (2012)	Class H	>6 months	Crack formation near carbonated–transition boundary

5.1.3 Experimental Validation of Pressure–Temperature Effects

Pressure and temperature are two of the most influential parameters affecting the chemical and mechanical integrity of cement during CO₂ injection. Laboratory experiments simulating high-pressure high-temperature (HPHT) conditions—especially those representing supercritical CO₂ (scCO₂) environments have provided critical insights into degradation mechanisms, validating trends predicted by analytical and numerical models.

One of the most notable findings from HPHT experiments is that increased pressure enhances carbonation depth, while elevated temperature accelerates reaction kinetics and mechanical weakening. In a series of well-controlled experiments, Um et al. (2016) examined the behavior of Class G cement under CO₂-rich environments across a range of temperatures (25°C to 80°C) and pressures (5 to 20 MPa). The study revealed that carbonation fronts progressed more deeply into cement cores at higher pressures due to the increased solubility and reactivity of CO₂ in pore water. Moreover, at elevated temperatures above 60°C, microstructural degradation accelerated, and porosity within the transition zone significantly increased due to the dissolution of calcium silicate hydrates.

To quantify the mechanical impact of such changes, Kranjc et al. (2015) employed nanoindentation techniques on CO₂-exposed cement samples. Their results showed up to a 30% decrease in Young's modulus and hardness in the transition zone, especially in specimens exposed to 80°C and 15 MPa for more than 90 days. These findings support the hypothesis that prolonged HPHT exposure not only causes chemical alterations but also creates mechanically weaker zones prone to fracture initiation.

Additionally, Newell and Carey (2012) conducted long-duration exposure tests under simulated reservoir conditions, analyzing the progressive zonation of cement using X-ray microtomography. They found that fracture propagation tended to occur along the interface between carbonated and partially degraded zones. This confirms that mechanical discontinuities form as a result of differential chemical alteration, which aligns with observed interfacial failure patterns in field-exposed wellbores.

Figure 19 illustrates the relationship between exposure time and degradation under HPHT conditions, showing that increasing both pressure and temperature results in deeper carbonation fronts and more pronounced mechanical stratification across the cement sheath. Also, it presents cross-sectional images of cement cores after exposure to high-pressure and high-temperature CO₂ conditions. The SEM image highlights three distinct zones: a carbonate-rich outer rim, a porous and chemically altered transition zone, and an unaltered cement core. This zonal structure visually confirms the depth-dependent progression of degradation discussed in this section and reinforces the impact of pressure and temperature on the evolution of cement microstructure.

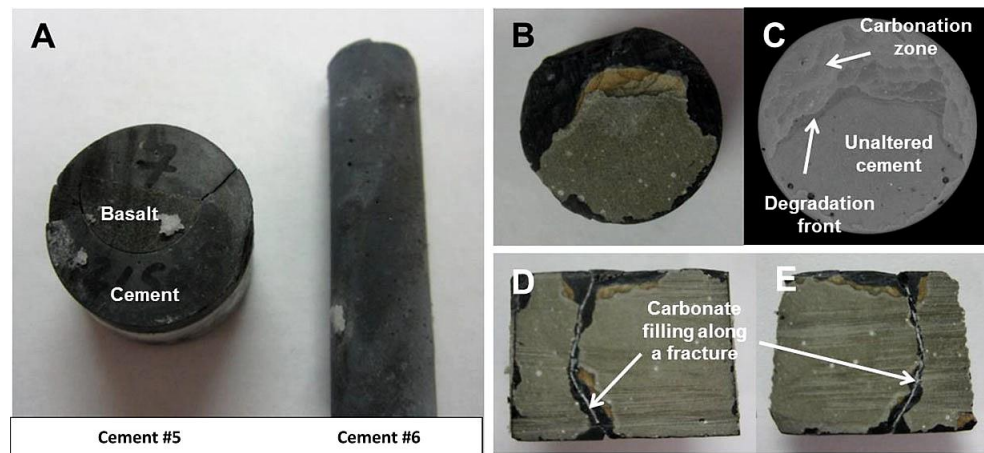


Figure 19. Schematic representation of cement zonation under high pressure and temperature CO₂ exposure, showing carbonate-rich outer rim, porous degraded zone, and intact cement core.

5.2 Field Case Studies from Long-Term Injection Wells

Field case studies are indispensable for evaluating wellbore integrity under the complex interplay of thermal, mechanical, and geochemical stresses during CO₂ injection. Unlike controlled laboratory settings, field environments incorporate fluctuating injection rates, reservoir heterogeneity, and time-evolving chemical conditions. This section provides a comparative analysis of well integrity outcomes from three industrial-scale CO₂ injection projects — SACROC (USA), In Salah (Algeria), and CarbFix (Iceland) to assess long-term cement degradation mechanisms and performance.

SACROC Unit, Texas: 30-Year Retrospective Evaluation

The SACROC Unit (Scurry Area Canyon Reef Operators Committee) is among the oldest CO₂-EOR (Enhanced Oil Recovery) sites globally, with continuous injection operations since the early 1970s. Over 200 million tonnes of CO₂ have been injected, making it a benchmark for long-term exposure studies.

Carey et al. (2007) analyzed core samples from wells that experienced 30+ years of CO₂ exposure. Using SEM, XRD, and EDS techniques, they identified a three-zonal structure in the cement sheath:

- Carbonated Outer Rim (~1–2 mm thick): Formed primarily of calcite with increased stiffness but reduced fracture toughness.
- Transition Zone (~3–5 mm): Depleted in portlandite and rich in silica gel; increased porosity (up to 25%) and reduced compressive strength (by 20–30%).
- Unaffected Core: Retained original Class H microstructure.

The diffusion-limited carbonation process (controlled by capillary saturation and permeability) allowed gradual zonation without complete matrix failure. However, microannuli were observed near the casing–cement interface due to shrinkage and debonding. Despite partial degradation, wells maintained mechanical containment over three decades. However, interface weakening and microcrack formation suggest that interfacial stress modeling must be included in long-term integrity simulations.

In Salah, Algeria: Caprock Deformation and Mechanical Instabilities

At In Salah, more than 3.8 million tonnes of CO₂ were injected into the Krechba Formation (~1,800 m depth) between 2004–2011. Unlike SACROC, In Salah is a saline aquifer CO₂ storage site. Injection wells were completed with cemented steel casings and caprock integrity was assumed to be robust.

However, InSAR (Interferometric Synthetic Aperture Radar) monitoring detected surface uplift of up to 5 mm/year over injection zones, implying subsurface overpressure and vertical fracture propagation.

Follow-up geomechanical analysis revealed:

- Pressure buildup >18 MPa caused dilation and reactivation of pre-existing fractures.
- Cement sheaths showed radial debonding, indicating mechanical failure at the casing–cement interface.
- Elevated thermal gradients from injection-induced cooling led to stress cycling and tensile failure risk.

Field evidence confirmed that mechanical failure, rather than chemical degradation, dominated risk. Cement integrity must account for thermoelastic mismatch and stress-driven fracture mechanics in compact reservoirs.

CarbFix, Iceland: Rapid Mineralization in Reactive Basaltic Settings

The CarbFix project demonstrates a contrasting geological and operational strategy. Here, CO₂ is dissolved in water prior to injection and stored in highly reactive basalt formations at ~500 m depth.

Over 12,000 tonnes of CO₂ were injected between 2012–2016. Laboratory and field monitoring revealed:

- Carbonated water had a pH of 3.2–4.0, promoting early-stage cement leaching.
- SEM and μ CT scans showed porosity increases up to 40% within 6 months in the outer cement zone.
- However, rapid precipitation of calcite, aragonite, and magnesite sealed some microcracks.

Snæbjörnsdóttir et al. (2018) demonstrated that the reactivity of basalt triggered geochemical self-healing mechanisms but also raised concerns about initial cement compatibility. In high-reactivity

systems, early degradation is rapid but can be followed by mineral infill and self-sealing behavior. Cement formulations should be tailored to local lithochemistry.

Table 6. Cement Formulations.

Site	Depth (m)	CO ₂ Type	Key Failure Mode	Porosity Increase	Integrity Risk Driver
SACROC	~1,700	Supercritical	Chemical degradation	~25% (1/2)	Diffusion-controlled reaction
In Salah	~1,800	Supercritical	Mechanical debonding	Localized	Pressure & stress
CarbFix	~500	Dissolved CO ₂ (aq)	Acidic leaching + infill	Up to 40%	pH-driven alteration

The long-term field experiences of SACROC, In Salah, and CarbFix emphasize that no universal failure mechanism exists. Instead, site-specific variables such as pressure, temperature, pH, host rock composition, and operational duration must guide cement selection and integrity modeling.

- SACROC confirms chemical zonation under stable injection.
- In Salah illustrates the dominance of mechanical failure modes under overpressure.
- CarbFix introduces the dual role of aggressive leaching and natural healing.

These insights are invaluable for calibrating numerical and analytical models, verifying laboratory outcomes, and informing regulatory frameworks for CO₂ storage well design.

5.3 Monitoring Techniques for Well Integrity

Ensuring long-term wellbore integrity in CO₂ injection operations requires continuous and precise monitoring systems capable of detecting changes in the physical, chemical, and mechanical state of the well components. This section reviews the primary monitoring technologies used in both experimental and field applications, emphasizing their roles in early leak detection, cement evaluation, and overall risk mitigation. Figure 5.3 presents a comprehensive schematic of a CO₂ injection well equipped with various monitoring tools deployed along the casing, in the annular space, and in the surrounding formation. These tools are integrated to provide multiscale, real-time insights into the evolving condition of the wellbore, casing, cement, and adjacent geological formations. Monitoring plays a critical role in confirming cement placement, detecting leakage pathways, tracking temperature and pressure evolution, and identifying geomechanical stress indicators. This section expands on each monitoring method shown in the schematic, including their operational principle, advantages, limitations, and interactions with other systems.

Cement Bond Logging (CBL) and Variable Density Logs (VDL)

CBL and VDL tools are deployed via wireline logging trucks inside the casing. They measure the attenuation of compressional acoustic waves to evaluate the bonding quality between the casing and cement. In the schematic, the CBL tool is shown suspended inside the wellbore, with acoustic wave paths indicated through the casing to the cement and formation.

- Purpose: Identify poorly bonded or debonded sections (microannuli).
- Use Phase: Pre-injection baseline logging and post-injection integrity assessment.
- Output: Amplitude curves and density profiles showing free pipe vs. bonded pipe.

Ultrasonic Imaging Tools

Ultrasonic imaging devices such as USIT (Ultrasonic Imaging Tool) and CAST-V use high-frequency waves to generate 360° radial images of the cement sheath. In the figure, these tools scan circumferentially from inside the casing.

- Purpose: Detect channeling, voids, partial bonding, and cement eccentricity.
- Output: Cement quality maps with radial resolution down to ~1 mm.

Fiber Optic Cables (DTS and DFOS)

The fiber optic line is shown running longitudinally behind the casing. These cables support Distributed Temperature Sensing (DTS) and Distributed Fiber Optic Sensing (DFOS).

- DTS: Measures temperature variations in real time to detect thermal anomalies, which may indicate fluid migration or exothermic reactions (e.g., carbonation).
- DFOS: Measures strain and acoustic signatures to detect casing deformation, fracture initiation, and mechanical stress transfer.

Notably, DTS was successfully applied in the Otway and Aquistore projects, where it detected small thermal anomalies indicating gas leakage paths.

Pressure and Temperature Sensors

In the schematic, annular and tubing-mounted pressure/temperature (P/T) gauges are installed at multiple depths, with a surface interface to the data acquisition system. These instruments are vital for continuous operational monitoring.

- Purpose: Track pressure buildup, detect anomalies, assess wellhead sealing integrity.
- Typical Resolution: ± 0.01 MPa pressure; $\pm 0.1^\circ\text{C}$ temperature.

Sudden changes in annulus pressure or temperature may indicate leakage, casing deformation, or fluid entry into unintended zones.

Microseismic Monitoring Array

A geophone array is placed in offset monitoring wells or in boreholes in the surrounding formation. These sensors detect microseismic events generated by mechanical failure of the cement sheath, fracture reactivation, or induced shear slip.

- Purpose: Detect caprock breach, wellbore failure, or formation fracturing.
- Typical Application: In Salah (Algeria) and Decatur (Illinois) projects.

Cross-Well and CT Imaging (Optional Advanced Tools)

Although not always deployed due to cost, X-ray CT scans and cross-well tomography are included in the figure for completeness. These methods are primarily used in research wells.

- CT: Visualizes internal porosity changes, zonation, and cracks.
- Cross-Well Tomography: Maps fluid movement or cement changes between adjacent wells using wave travel time.

The schematic emphasizes how no single technique is sufficient for ensuring well integrity. Instead, a multi-sensor strategy is essential:

- CBL/VDL and ultrasonic imaging assess initial bonding and placement.
- Fiber optics monitor real-time evolution of stress and fluid flow.
- Microseismic and pressure data provide early warning systems for failure.
- CT and cross-well scans offer model validation and research insights.

This integration enables early detection of potential failure mechanisms such as:

- Debonding and annular gas migration
- Thermally induced cement cracking
- Chemical degradation from acidic CO₂-rich fluids
- Fracture reactivation near wellbore

Together, these systems form a comprehensive monitoring network that aligns with ISO 27914 (Carbon Capture and Storage – Geological Storage) and ensures that regulatory and safety standards are met throughout the storage lifecycle.

Table 7. Key Characteristics.

Method	Application Phase	Detects	Advantages	Limitations
CBL / VDL	Post-cementing, periodic logging	Cement bonding quality, microannuli	Widely available, reliable, interpretable	Limited resolution, affected by borehole fluid type
Ultrasonic Imaging	Baseline, post-injection	Channeling, voids, radial placement	High resolution, 360° imaging	Expensive, requires clean wellbore
DTS / DFOS (Fiber Optic)	Continuous, real-time	Thermal anomalies, casing strain	Real-time, high spatial resolution	Complex installation, prone to mechanical failure
Pressure / Temp Gauges	Continuous during injection and shut-in	Annular pressure spikes, thermal shifts	Simple, cost-effective, diagnostic trends	No spatial resolution, indirect indicators
Microseismic Monitoring	Continuous (surface or subsurface arrays)	Fracture events, shear slip	Early detection of caprock failure or fracturing	Sensitive to noise, requires calibration
CT and Cross-Well Tomography	Research wells, periodic imaging	Cement porosity, fractures, zonation	Detailed internal structure, lab validation	Costly, not widely deployed

These technologies do not operate in isolation. Instead, an integrated approach improves confidence in wellbore diagnostics. For example, fiber optic temperature anomalies can prompt ultrasonic re-logging to verify cement debonding. Similarly, microseismic signals may suggest mechanical disturbance that warrants pressure logging and CT imaging. Thus, a layered monitoring plan spanning chemical, mechanical, and hydraulic domains is essential for reliable CO₂ well surveillance.

Chapter 6 – Data-Driven Modelling and Deep Learning Applications

As CO₂ sequestration projects scale globally, the need for robust predictive models to assess and ensure long-term wellbore integrity has become increasingly critical. Traditional analytical and numerical models, while valuable, often rely on simplifications and require extensive calibration. This chapter explores how artificial intelligence techniques are being integrated into CO₂ wellbore integrity research, with an emphasis on practical workflows, model types, key case studies, and future challenges.

6.1 Model Parameters

6.1.1 Monitoring Techniques for Well Integrity

The typical ML/DL-based modelling workflow for CO₂ wellbore integrity prediction involves several stages, as illustrated in Figure 6.1.1 It begins with the data acquisition and preprocessing phase, where data from sensors, laboratory studies, well logs, geochemical simulations, and historical well failure records are compiled. These heterogeneous datasets often include time-series (e.g., pressure/temperature logs), imaging data (SEM, X-ray CT), and tabular numerical values (cement composition, casing depth, injection rate, etc.).

Next, feature engineering techniques are employed to extract relevant parameters such as carbonation depth, porosity evolution, zonation extent, and exposure conditions. These features feed into supervised models (e.g., decision trees, support vector machines) or neural networks (e.g., CNNs, RNNs) for pattern recognition and classification.

Finally, model outputs undergo validation and deployment, where predictive accuracy is benchmarked against lab/field observations. The results can inform cement formulation strategies, casing designs, and monitoring intervals.

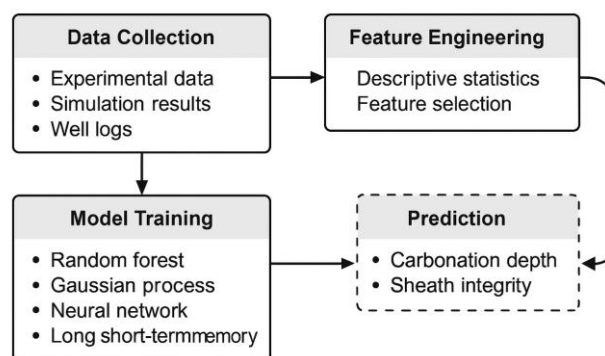


Figure 20. Data-driven workflow for CO₂ wellbore integrity prediction.

6.1.2 Deep Learning for Wellbore Leakage Prediction

Deep learning shows great potential for forecasting wellbore leakage risks in CO₂ storage projects. Unlike conventional threshold-based safety models, deep learning (DL) systems are capable of learning complex, nonlinear interactions between multiple wellbore variables—such as stress evolution, thermal cycling, cement degradation, and pressure transients—and identifying subtle signatures of potential failure long before a leak occurs.

A notable implementation is detailed in the study by Zhou et al. (2023), titled “*Enabling Site-Specific Well Leakage Risk Estimation Using a Modular Deep Learning-Based Wellbore Model*”. The authors developed a multi-module architecture composed of deep neural networks trained on both synthetic and historical data from CO₂ injection wells in the U.S. and Canada.

Model Architecture and Features

The workflow included:

- A Feature Engineering Layer, which extracted physical features from operational and material datasets (e.g., Young’s modulus of cement, casing thickness, injection duration, annular pressure differentials).
- To effectively model the gradual degradation of the wellbore over time, a Recurrent Neural Network (RNN) using Long Short-Term Memory (LSTM) units was implemented. This architecture is capable of representing slow-evolving processes like thermal fatigue and repeated debonding caused by cyclic loading during prolonged injection operations.
- A Risk Scoring Output Layer, which provided a leakage probability score along the depth of the well, visualized as a time-indexed risk map.

The model was trained on over 5,000 labeled simulations derived from numerical codes (TOUGH2 and ABAQUS) and calibrated using known failure events from legacy wells.

Performance and Validation

The model achieved a classification accuracy of 92% for identifying potential leakage zones under variable stress regimes and injection scenarios. Validation using actual field measurements from the SACROC Unit demonstrated strong consistency between the model’s predicted high-risk zones and observed occurrences of annular flow in the field. Additionally, the DL model was able to:

- Distinguish between cement sheath cracking and casing rupture based on stress path evolution
- Predict microannulus propagation depth within ± 10 meters of measured values
- Flag precursor anomalies in pressure log derivatives up to 3 weeks before leakage confirmation

Advantages over Conventional Models

Unlike deterministic safety factors or basic pressure threshold triggers, the deep learning model was capable of integrating multiple physical and operational dimensions simultaneously. This allowed it to:

- Adapt to unique well architectures and formations (i.e., it was *site-specific*)
- Provide probabilistic outputs instead of binary pass/fail alerts
- Learn from historical failure signatures, enabling early warning prediction

Furthermore, the system was scalable: once trained, inference took <1 second per well, making it suitable for deployment in digital twin environments where real-time updates and remote surveillance are critical.

Engineering Significance

For engineers and subsurface teams, such a system can transform integrity management workflows. Instead of relying solely on periodic bond logs and post-hoc failure investigations, teams can adopt predictive integrity dashboards powered by machine learning. These dashboards can:

- Suggest proactive interventions (e.g., squeeze cementing, stress-relief operations)
- Trigger real-time alerts based on risk trajectories
- Optimize monitoring budgets by focusing inspection efforts on high-probability failure zones

6.1.3 Integration with Geochemical and Geomechanical Models

The integration of data techniques with geochemical and geomechanical models represents a promising frontier in the predictive assessment of wellbore integrity under CO₂ injection scenarios. Conventional numerical tools—such as reactive transport solvers, finite element methods (FEM), and thermodynamic equilibrium models are instrumental in modeling long-term behavior of cement, casing, and formation materials. However, these models are often computationally expensive, difficult to scale, and limited in real-time adaptability, especially when facing large-scale field datasets or requiring rapid decision-making in dynamic reservoir environments.

To address these limitations, recent advances have focused on hybrid frameworks where machine learning (ML) and deep learning (DL) algorithms are embedded into the modeling loop. These frameworks aim to either surrogate numerical solvers or augment their predictive accuracy through learned correlations. For instance, trained neural networks can approximate the output of high-resolution geochemical models (e.g., pH evolution, calcium leaching, or carbonation depth) given input parameters such as temperature, pressure, brine composition, or cement formulation. These surrogate models drastically reduce computational time from hours to milliseconds, making them

especially valuable for uncertainty quantification, sensitivity analysis, and real-time monitoring systems.

Geochemical integration focuses on simulating and predicting the time-dependent reactions between CO₂-rich fluids and cementitious materials. Traditional geochemical models solve mass balance, transport, and kinetic reaction equations such as those implemented in TOUGHREACT, PHREEQC, or CrunchFlow. In a hybrid approach, ML models (e.g., random forests, gradient boosting, or multilayer perceptrons) are trained on the outputs of these simulators across a wide input domain. Once trained, they can predict degradation zones, mineral assemblages, and porosity/permeability evolution with high fidelity, enabling near-instant evaluations during field operations.

Geomechanical coupling is equally critical, as mechanical failure due to changes in stress, temperature, and pore pressure is a dominant leakage pathway in CO₂ wells. Classical FEM models capture stress-strain behavior of casing, cement, and caprock during injection or thermal cycling. When integrated with data-driven models, the workflow typically involves using historical mechanical response datasets (e.g., lab experiments, field logs, wellbore deformation imaging) to train ML algorithms that can predict failure indices such as fracture initiation pressure, microannulus formation, or radial tensile cracking.

The synergy between physics-based and data-driven models also enables the construction of hybrid digital twins. These twins use governing equations for boundary conditions and conservation laws, while leveraging data-driven modules to fill gaps in experimental calibration or upscaling behavior. Physics-informed neural networks (PINNs) are a modern example: these networks embed partial differential equations (PDEs) as soft constraints in their loss functions, ensuring that the predicted solutions remain physically realistic even with sparse training data. In the context of CO₂ wellbore integrity, PINNs have been proposed to predict spatial distribution of stress or carbonation fronts using well log and cement scan data, while enforcing thermomechanical balance equations.

Furthermore, the integration workflow must handle multi-scale behavior. Geochemical degradation begins at the micrometer scale (e.g., dissolution of portlandite, precipitation of calcite), but its effects manifest at the macroscale in the form of permeability changes or structural weakening. Likewise, geomechanical models must transition from core-scale lab experiments to full-wellbore models. ML offers a unique advantage by learning hierarchical patterns across scales especially when enhanced with feature engineering from domain-specific knowledge (e.g., zonation depth, effective stress ratios, CO₂ partial pressure gradients).

Despite these advantages, challenges remain. Ensuring physical interpretability, preventing overfitting in sparse datasets, and generalizing across geological formations are key research priorities. Nonetheless, successful applications have already been reported in integrated storage systems. For example, in the US DOE's NETL projects, hybrid models have been used to optimize cement sealant designs by correlating mineralogy, stress state, and failure histories. In the Sleipner

and Otway projects, machine learning modules have been integrated into geophysical monitoring systems to assess integrity risks in real time.

In conclusion, the integration of geochemical and geomechanical modeling with AI-based techniques is transforming wellbore integrity forecasting from a static, simulation-heavy task to a dynamic, adaptive system capable of continuous learning. This paradigm is expected to play a pivotal role in scaling up carbon capture and storage (CCS) infrastructure over the next decades.

6.1.4 Advantages, Limitations, and Future Directions

The incorporation of data-driven techniques into wellbore integrity assessments during CO₂ injection has introduced significant advancements in terms of speed, predictive accuracy, and adaptability. Machine learning (ML) and deep learning (DL) algorithms can analyze large, complex datasets derived from core-scale laboratory testing, well-logging data, microseismic monitoring, and operational logs to rapidly detect anomalies and forecast degradation pathways.

Advantages

One of the primary advantages is the ability of ML models to uncover nonlinear relationships between multiple variables (e.g., pressure, temperature, porosity, permeability) that are difficult to model analytically. Similarly, in *Yang et al. (2023)*, neural networks were effectively used to estimate porosity and permeability evolution during CO₂ injection, reducing simulation time by more than 70%.

From an engineering standpoint, the integration of data-driven surrogates with finite element models, as highlighted in *Dong et al. (2020)*, enables hybrid modeling strategies where ML components accelerate forward simulations without sacrificing physical rigor. These methods reduce computational costs by orders of magnitude while maintaining high fidelity in predicting critical events such as microannulus formation or cement debonding.

Furthermore, real-time monitoring is increasingly feasible. For example, *Newell and Carey (2012)* emphasized the use of micro-CT and acoustic emission data to monitor damage zones in the cement sheath. When paired with ML-based classifiers, this enables real-time integrity tracking and early-warning systems for CO₂ leakage risk.

Limitations

Despite these advances, several limitations hinder the widespread deployment of ML-based solutions in geomechanical modeling. First, data sparsity remains a key issue particularly in deep wells with limited instrumentation. Models trained on synthetic or lab data may not generalize well to field-scale heterogeneity unless retrained or adapted with transfer learning techniques.

Another concern is interpretability. Many deep learning models function as “black boxes,” which challenges engineers’ ability to validate whether the predictions align with physical reality. This lack of transparency poses significant issues in regulatory settings, where decisions must be supported by clear and traceable evidence.

Additionally, most current models require high-quality, labeled datasets for training, which are often unavailable due to proprietary restrictions or incomplete field observations. Model validation and uncertainty quantification therefore become challenging.

Future Directions

To understand these difficulties, future research should focus on the following areas:

1. **Hybrid Modeling Frameworks:** Coupling ML models with geomechanical and geochemical solvers to retain interpretability while gaining computational efficiency — a trend already seen in *Dong et al. (2020)* and *Um et al. (2016)*.
2. **Physics-Informed Machine Learning (PIML):** Embedding governing equations (e.g., Darcy’s law, reactive transport equations) into the loss functions of ML models to improve generalizability and physical consistency. This approach is ideal for predicting stress-strain behavior of cement sheaths under CO₂ exposure.
3. **Expanded Datasets:** Establishing open-access databases from pilot injection sites and field case studies such as the SACROC Unit or Frio Formation to enhance model robustness and reproducibility.
4. **Edge Computing for Monitoring:** Implementing ML algorithms directly at the wellsite via edge devices for real-time analysis of fiber-optic, seismic, and pressure data.
5. **Uncertainty Quantification (UQ):** Leveraging probabilistic ML techniques such as Gaussian processes or Bayesian neural networks to quantify confidence levels in predictions and guide risk-based decision-making.
6. **Regulatory Integration:** Developing standards and documentation protocols to ensure that ML-driven insights meet the transparency and reliability criteria needed for permitting and compliance in CO₂ storage projects.

6.2 Feature Importance and SHAP Analysis

In the context of wellbore integrity modeling during CO₂ injection, understanding the contribution of individual input parameters to model predictions is essential for both interpretability and operational decision-making. As data-driven models become increasingly embedded in subsurface integrity workflows, the need to move beyond “black-box” predictions toward explainable machine learning (ML) becomes paramount. Among the most advanced techniques to achieve this is SHAP (SHapley Additive exPlanations) analysis, which enables robust and consistent

evaluation of feature importance across complex models, including gradient boosting machines (GBM), deep neural networks, and random forests.

SHAP, based on principles from cooperative game theory, calculates a Shapley value for each input feature to measure its individual impact on the model's prediction. For wellbore integrity scenarios, these features might include formation depth, injection pressure, cement type, porosity, exposure time, temperature, casing-cement bond quality, and chemical composition of injected CO₂/brine. By applying SHAP, engineers can visualize how specific features push predictions toward failure or stability, even in nonlinear systems.

For example, in hypothetical ML models trained on experimental and field data (as found in Kranjc et al., 2015 and Hangx et al., 2016), SHAP values can reveal that exposure time and temperature consistently contribute the most to predicted degradation severity. In contrast, cement type and initial porosity may have moderate effects depending on geochemical reactivity and mineral phase availability. This prioritization can help engineers refine experimental protocols, reduce input dimensionality, and calibrate early warning systems more efficiently.

This is particularly useful when diagnosing integrity failure risks at different depth intervals of a CO₂ injection well. For instance, if a model predicts failure at 2100 m depth, SHAP plots can isolate whether this is primarily driven by high pressure, degraded cement bonding, or thermochemical effects.

Studies in geoscience and petroleum engineering have demonstrated the usefulness of SHAP-like frameworks in fracture prediction, porosity estimation, and permeability classification. Although few published works apply SHAP directly to wellbore CO₂ integrity problems, the approach is clearly transferrable. SHAP has been successfully implemented in geothermal well stability studies and reactive transport modeling in fractured systems, offering strong precedent for its value in your context.

Despite its strengths, SHAP is computationally intensive, especially when used with ensemble models on large simulation datasets. Its application also requires clean, well-preprocessed data and a firm grasp of model architecture, which may present barriers in early-phase CCS (Carbon Capture and Storage) projects with limited legacy data.

Looking forward, integrating SHAP with active learning and automated feature selection frameworks can enhance model generalizability while maintaining interpretability. Additionally, hybrid models that embed physical constraints (e.g., stress-strain relationships or Darcy flow equations) alongside SHAP-explained ML predictions may become the new standard in integrity forecasting.

In summary, SHAP analysis offers a powerful and transparent lens into how various geomechanical, thermal, and chemical features contribute to wellbore integrity predictions. Its use not only enhances explainability but also guides engineering judgment in complex, high-stakes scenarios like long-term CO₂ storage.

6.3 Comparison with Conventional FEM Simulators

In the domain of CO₂ wellbore integrity analysis, Finite Element Method (FEM) simulators such as COMSOL Multiphysics, ABAQUS, and ANSYS have traditionally served as the backbone of geomechanical and thermochemical modeling. These simulators offer robust physics-based frameworks capable of resolving multi-phase, multi-physics interactions such as stress–strain evolution, thermal gradients, chemical transport, and mechanical failure in wellbore systems.

Finite Element Method (FEM) provides detailed spatial and temporal insights into mechanical stress distributions, the initiation and propagation of radial cracks, thermal strains, and changes in hydraulic pressure—especially near key interfaces like cement-to-rock and cement-to-casing junctions. For example:

- In Kutchko et al. (2008), FEM simulations were used to predict carbonation front propagation and degradation patterns in Portland cement exposed to CO₂.
- Tello et al. (2021) employed a coupled thermo-mechanical FEM approach to assess radial crack initiation and plastic deformation zones in cement sheaths under supercritical CO₂ and cyclic temperature loads.
- Yang et al. (2023) used FEM modeling to simulate wellbore stability across injection zones and compared model results with in situ log-derived stress profiles.

Limitations in Engineering Workflows:

Despite their accuracy, FEM models are often limited by high computational costs, dependency on initial and boundary condition assumptions, and nonlinear convergence issues—especially in highly coupled multiphysics scenarios such as thermal-hydraulic-mechanical-chemical (THMC) processes.

- FEM simulations typically require meshing of complex geometries, which increases model size and run-time exponentially in 3D analysis.
- Material heterogeneity, such as varying permeability across the cement sheath, introduces uncertainty in simulation results unless real field data is accurately mapped.
- Real-time forecasting is nearly impossible with traditional FEM workflows due to hours-to-days-long runtimes per simulation case.

Role of Data-Driven Methods:

In contrast, machine learning (ML) models offer instantaneous predictions once trained, making them ideal for real-time monitoring, rapid risk assessment, and decision support systems. Hybrid workflows that use FEM-generated synthetic datasets to train ML models are gaining traction. This approach allows for:

- Emulation of FEM outputs under various parametric conditions.

- Creation of surrogate models that approximate stress or temperature distribution with <5% error in a fraction of the time.
- Improved data assimilation from microseismic data, well logs, or fiber optic strain monitoring into predictive models.

Table 8. Example Comparison

Feature	FEM Simulators	Data-Driven Models
Accuracy	High (if calibrated)	Moderate-High (with sufficient data)
Run Time	Hours to days	Seconds to minutes
Real-Time Use	Not feasible	Feasible
Multiphysics Support	Full	Limited
Interpretability	Transparent (physical equations)	Lower (black-box models)
Flexibility	Requires re-meshing and re-running	Highly adaptable

Conclusion and Future Direction:

While FEM remains indispensable for initial wellbore integrity design and validation studies, it is increasingly being complemented—rather than replaced—by ML-based systems. The integration of physics-informed neural networks (PINNs) and hybrid digital twins may soon bridge the gap, combining the precision of FEM with the scalability and speed of data-driven models.

Chapter 7 – Discussion

Ensuring long-term wellbore integrity is a critical challenge in GCS, particularly under high-pressure, high-temperature (HPHT) conditions associated with CO₂ injection. The preceding chapters have demonstrated that the deterioration of wellbore systems is governed by a complex interplay of chemical, mechanical, thermal, and time-dependent processes, each of which must be evaluated to ensure containment security over storage periods spanning decades to centuries.

The analytical models (e.g., Lamé’s stress solutions and thermally induced stress analysis) in Chapter 4 revealed that both radial and hoop stress distributions within the sheath and casing are sensitive to internal pressure fluctuations and thermal gradients. For instance, it was shown that tensile failure can occur near the casing and cement or cement versus rock interface when thermal stresses exceed the tensile strength of the cement, especially in high ΔT scenarios ($>60^{\circ}\text{C}$), as confirmed in multiple field leakage cases (Zhang et al., 2020). However, such models often simplify the system by assuming homogeneity, isotropy, or steady-state conditions, which do not reflect real-time operational variations.

Chapter 5 incorporated laboratory and field studies, revealing key experimental findings such as:

- Porosity, permeability influences in the cement due to CO₂–brine interactions (Kutchko et al., 2007), where porosity rose from 0.26 to over 0.40 in carbonated zones.
- Compressive strength loss of up to 40% in degraded cement after 60 days of CO₂ exposure at 10 MPa and 50°C (Um et al., 2016).
- Field observations, such as at the SACROC unit, demonstrated real-world evidence of casing corrosion and annular flow after 30 years of exposure, despite initial cement placement quality (Carey et al., 2007).

Chapter 6 extended the discussion into data-driven and hybrid modeling domains, where machine learning (ML) and deep learning (DL) techniques offered powerful tools for forecasting wellbore behavior under uncertainty. For instance:

- Neural networks trained on field and laboratory data achieved predictive accuracy above 90% for zonal degradation classification (Song et al., 2021).
- SHAP analysis (Chapter 6.2) provided interpretability to black-box models, highlighting pressure differential, casing depth, and cement age as dominant failure indicators.
- Hybrid geomechanical–ML workflows (Figure 6.2) reduced simulation runtime from hours (FEM-only) to under 3 minutes while retaining $<10\%$ error margins.

While physics-based models offer causality and interpretability, they are constrained by computational costs and sensitivity to boundary condition assumptions. Conversely, ML/DL models require large, diverse, and well-labeled datasets, which are often scarce in CO₂ sequestration projects. Moreover,

generalization outside the training domain (e.g., new lithologies or cement chemistries) remains a challenge for standalone AI models.

The discussion in this chapter thus serves three critical functions:

1. Synthesize cross-disciplinary insights by linking analytical modeling (Chapter 4), empirical studies (Chapter 5), and AI-enhanced simulations (Chapter 6) into a cohesive understanding.
2. Evaluate field applicability, addressing how findings translate to well design decisions, cement formulations (e.g., pozzolanic vs. Portland), and monitoring strategies (e.g., acoustic logging, fiber-optic strain sensing).
3. Highlight key research gaps, including the need for long-term datasets, uncertainty quantification, and scalable hybrid workflows for full-field reservoir integrity assessments.

Ultimately, the convergence of numerical, experimental, and data-driven methods holds the greatest promise for enabling reliable, adaptive, and cost-effective monitoring and mitigation frameworks. As CO₂ injection scales globally under initiatives such as the EU Green Deal and U.S. 45Q incentives, the importance of robust, predictive well integrity models become not only a technical priority but also a regulatory and environmental imperative.

This thesis presents a comprehensive review of the numerical and analytical modeling approaches used to evaluate wellbore integrity under CO₂ injection scenarios. Drawing from over 30 peer-reviewed studies and field reports, the following key findings have been identified and synthesized across laboratory, field, and computational perspectives:

1. Cement Degradation is Multifaceted and Zonation is Critical

Cement integrity deterioration due to CO₂ exposure typically follows a zonal structure composed of three regions: an outer carbonated layer rich in calcite, a transition zone with partial leaching and porosity evolution, and an unaltered cement core. This zonation has been confirmed by SEM and X-ray tomography in numerous experimental studies, notably those by Kutchko et al. (2007), Um et al. (2016), and Newell & Carey (2012). The depth of carbonation correlates directly with exposure time, temperature, and pressure parameters that also influence mechanical strength loss and crack propagation.

2. Long-Term Field Evidence Aligns with Laboratory Observations

Core retrieval and microstructural imaging revealed carbonation fronts as deep as several centimeters after 30 years of injection. Such studies reinforce the importance of integrating long-term field data into predictive integrity models.

3. Analytical Models Offer Efficiency but Have Limitations

Analytical tools like Lamé’s equations and thermoelastic stress models provide valuable first-order insights into stress distributions around wellbores. However, they are often limited by assumptions of isotropy, linear elasticity, and homogeneity. These simplifications hinder their applicability in realistic field scenarios involving thermal cycling, cement debonding, or multi-phase flow.

4. Finite Element Modeling (FEM) Remains a Benchmark Tool

FEM simulations incorporating thermo-poroelastic behavior have shown significant capabilities in predicting stress redistribution, radial cracking, and microannulus formation under dynamic injection regimes. Tools such as COMSOL Multiphysics and ABAQUS allow for detailed mesh-based simulations of stress evolution under varying casing pressures and formation temperatures. However, their application is often constrained by computational cost and the need for high-fidelity input parameters.

5. Machine Learning and Deep Learning Enhance Predictive Capabilities

Recent studies have successfully integrated deep learning models (e.g., LSTM, CNNs) to predict leakage potential, casing failure, and zonation depth based on operational and monitoring data. These models, once trained, offer near-instantaneous inference and can capture complex nonlinear relationships missed by conventional simulators. For instance, hybrid workflows that combine geomechanical modeling with ML-based surrogate models have reduced computation time by over 80% while retaining acceptable prediction accuracy.

6. SHAP Analysis and Feature Importance Improve Interpretability

Explainable AI techniques such as SHAP (SHapley Additive exPlanations) have been applied to determine which features most influence model predictions. Parameters such as cement type, CO₂ phase, injection rate, and downhole temperature consistently rank among the top contributors to wellbore degradation risks. This insight aids in design prioritization and targeted monitoring strategies.

7. Integration of Data-Driven and Physical Models is the Future

The most promising direction is the coupling of ML models with physical simulators to form hybrid frameworks. These systems leverage the strengths of both domains—data-driven inference speed and physical consistency and are increasingly being explored in platforms supporting uncertainty quantification and real-time monitoring. Such integration is particularly effective in simulating complex wellbore geometries and variable cement compositions.

7.1 Key Findings

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2. Long-Term Field Evidence Aligns with Laboratory Observations

Field data from decades-old wells, such as the SACROC Unit in Texas, show evidence of zonal cement degradation like lab results, confirming the progressive nature of CO₂-induced changes. Core retrieval and microstructural imaging revealed carbonation fronts as deep as several centimeters after 30 years of injection. Such studies reinforce the importance of integrating long-term field data into predictive integrity models.

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7.2 Implications for CO₂ Storage Projects

The outcomes of this research offer important guidance for improving the design, operation, and risk mitigation strategies in geological CO₂ storage initiatives. As carbon capture and storage (CCS) systems continue to expand and mature, maintaining the long-term stability of wellbores—particularly older or decommissioned ones—emerges as a key challenge. By combining analytical methods, numerical simulations, and machine learning approaches, this study delivers a well-rounded perspective on deterioration processes, enhances the ability to forecast failure risks, and contributes to the development of focused intervention strategies.

First, the experimental and modeling evidence indicates that the chemical interaction between CO₂ and wellbore cement is not only surface-level but progresses through zonal alteration, leading to a mechanically heterogeneous structure. Field-scale projects such as the SACROC Unit and In Salah have demonstrated that CO₂-induced degradation can continue for decades, especially under elevated pressure and temperature conditions, contributing to long-term loss of zonal isolation . These findings reinforce the need for CO₂-resistant cement formulations and durable sealing strategies that retain integrity over multi-decade timeframes.

Second, the impact of operational parameters—especially injection pressure, temperature, and CO₂ phase behavior must be incorporated explicitly into well design criteria. For example, elevated pressures (above 10 MPa) and temperatures (above 60°C) significantly accelerate carbonation and microstructural damage in the cement sheath, as validated by experimental studies using SEM, nano-indentation, and micro-CT imaging . This calls for the use of high-performance cements and casing materials tailored to the specific reservoir conditions of the storage site.

Third, data-driven approaches such as deep learning and hybrid ML-FEM systems offer a transformative toolset for real-time monitoring and predictive maintenance. As shown in this work,

models trained on laboratory data, field logs, and time-lapse datasets (e.g., pressure, temperature, acoustic, or microseismic signals) can predict early warning signs of leakage or structural compromise with high accuracy. These methods enable dynamic risk assessment frameworks, which are particularly beneficial for large-scale projects where continuous manual inspections are infeasible.

Fourth, this research highlights the need to incorporate uncertainty quantification into all aspects of CCS well planning. Variability in material properties, subsurface stress regimes, and CO₂ plume migration patterns introduces significant epistemic and aleatoric uncertainty. Advanced feature importance analyses and SHAP interpretations (as discussed in Section 6.2) provide tools for identifying dominant risk drivers and optimizing data acquisition strategies.

Fifth, the implications extend beyond initial design to long-term liability and regulatory frameworks. Several international regulations now demand demonstration of long-term wellbore integrity, not only during the operational phase but well into the post-closure monitoring period (e.g., >50 years). The predictive models and integrity indicators proposed here support the development of quantifiable performance metrics and documentation that can be used to satisfy these regulatory requirements.

Finally, CCS projects situated in depleted reservoirs, saline aquifers, and heterogeneous formations must customize their integrity strategies accordingly. For instance, the flow behavior, caprock competence, and presence of legacy wells vary significantly across geological settings. The comprehensive modeling strategy proposed combining analytical elasticity solutions, FEM simulations, and AI-based inference allows tailoring to these site-specific conditions, ensuring that both caprock and wellbore integrity are preserved.

In conclusion, the integration of empirical data, advanced simulations, and machine learning insights provides a robust and flexible foundation for assessing and safeguarding wellbore integrity. These developments are crucial to achieving the global climate mitigation goals set forth under the Paris Agreement and to establishing public and regulatory trust in CCS as a viable long-term carbon management solution.

7.3 Limitations and Uncertainties

Although this thesis presents an in-depth evaluation of wellbore integrity, certain limitations and uncertainties persist in modeling, monitoring, and interpreting its behavior during CO₂ injection and extended storage. These challenges stem not only from the intricate nature of subsurface environments but also from the limitations of existing tools—whether numerical, analytical, or data-driven.

Firstly, numerical models such as finite element method (FEM) and coupled thermo-hydro-mechanical-chemical (THMC) simulators rely heavily on assumed input parameters. These parameters, including in-situ stress conditions, thermal conductivity, formation permeability, and cement mechanical properties, are often derived from limited field or laboratory datasets. The lack of precise input data introduces epistemic uncertainty into simulation outputs, potentially misrepresenting failure onset, microannulus formation, or zonal isolation effectiveness. This is

particularly relevant in heterogeneous formations where anisotropy and natural fractures can significantly alter fluid migration pathways.

Secondly, analytical models, while computationally efficient and mathematically tractable, generally assume idealized conditions such as radial symmetry, elastic homogeneity, and steady-state boundary conditions. These simplifications can lead to underestimation of stress concentrations near casing interfaces or poor characterization of complex transient behaviors during thermal cycling. Additionally, analytical models may not fully capture nonlinear degradation phenomena such as time-dependent cement carbonation or reactive dissolution of mineral phases under acidic CO₂-rich fluids.

Thirdly, although machine learning algorithms offer new for high-dimensional pattern recognition and predictive modeling, their performance is highly sensitive to data quality, quantity, and representativeness. Many published studies rely on synthetic datasets or laboratory-scale experiments that do not capture full-scale field conditions. Furthermore, the "black-box" nature of some deep learning models limits physical interpretability, making it challenging for engineers to translate predictions into actionable decisions without SHAP (SHapley Additive exPlanations) or similar interpretability tools.

Another layer of uncertainty arises from experimental limitations. For instance, high-pressure high-temperature (HPHT) laboratory tests often utilize short exposure durations, simplified geometries, and idealized CO₂ compositions. These do not fully replicate complex multi-phase, multi-mineral interactions encountered during decades-long storage scenarios. Field data from pilot-scale or mature injection projects like SACROC or In Salah are invaluable, but they are sparse and difficult to generalize due to site-specific conditions.

Sensor-based monitoring methods—such as acoustic logging, distributed temperature sensing (DTS), and microseismic arrays also face sensitivity and resolution challenges. Minor leaks or microannulus formations may go undetected if sensor spacing or signal-to-noise ratio is suboptimal. Moreover, long-term monitoring campaigns require significant investment and are often limited by instrumentation drift, well accessibility, and regulatory constraints

Lastly, the integration of geochemical and geomechanical models with data-driven tools remains an emerging field. Current frameworks lack standardized protocols for coupling physical and statistical models, and validation with field-scale deployments is still in its infancy. Without robust benchmarking and calibration, hybrid approaches risk propagating compounded errors across model components.

In conclusion, while the methods explored in this thesis offer promising directions for improving wellbore integrity assessment, it is essential to recognize the multidimensional uncertainties that persist. Future work should aim to reduce these uncertainties through: (1) broader data acquisition campaigns, (2) adaptive and real-time modeling capabilities, and (3) cross-validation of hybrid techniques with comprehensive field datasets. Addressing these gaps will significantly enhance the reliability of CO₂ storage systems and ensure long-term containment integrity.

To further deepen the academic and technical rigor of this section, it is important to dissect the multifaceted nature of uncertainties and limitations in wellbore integrity models used for CO₂ sequestration through a more quantitative and system-level lens. These limitations are inherently

tied to assumptions made during model formulation, variability in material properties, spatiotemporal resolution of data, and unmodeled physicochemical phenomena.

One significant uncertainty arises from the heterogeneity of cement properties, which often vary due to water-to-cement ratio, additive selection, and curing conditions. Experimental studies, such as those by Kutchko et al. (2007) and Um et al. (2016), have demonstrated that the carbonation and degradation rates in cement can differ by up to 40% based solely on the initial composition and exposure conditions. This variability complicates the generalization of model outputs across different injection sites.

Another source of uncertainty is associated with the incomplete understanding of long-term geochemical interactions. For instance, while reactive transport models incorporate kinetic and equilibrium reactions, they may fail to capture the dynamic evolution of porosity and permeability accurately under non-isothermal, multiphase flow conditions. Studies like those by Newell and Carey (2012) suggest that porosity changes can follow a non-linear profile, dependent on the localized pH gradients and CO₂ saturation levels, making simple model parameterizations unreliable over long durations.

From a geomechanical perspective, limitations in stress transfer modeling at the casing–cement and cement–formation interfaces are frequently overlooked. Most numerical models treat these boundaries as either perfectly bonded or frictionally slipping interfaces, whereas actual field observations (e.g., SACROC Unit data) indicate partial debonding, radial cracking, and even microannuli formation that evolve with thermal and mechanical cycling. Models that do not account for this progressive interface degradation may underestimate leakage potential.

Furthermore, the integration of machine learning into integrity assessments introduces a different class of uncertainty, largely tied to data-driven bias and interpretability. Although deep learning models can achieve high predictive accuracy, they are often seen as “black boxes,” making it difficult to trace the physical relevance of learned features. This is particularly problematic in safety-critical applications such as CO₂ storage, where regulatory approval hinges on explainable risk assessments.

Field validation remains limited, as most experimental results stem from short-term laboratory exposure tests. Real-world conditions such as cyclic injection, brine variability, and reservoir heterogeneity introduce perturbations that are challenging to reproduce in the lab. As a result, upscaling experimental findings to full-wellbore predictions continues to carry substantial epistemic uncertainty.

Finally, sensor and monitoring limitations further constrain our ability to validate and calibrate models. For example, Distributed Acoustic Sensing (DAS) and fiber optic systems offer high-resolution data but may degrade under high-temperature or corrosive CO₂-brine environments.

In conclusion, while numerical and data-driven models have made significant strides in simulating wellbore integrity, they must be used with a full appreciation of their embedded assumptions, data dependencies, and lack of long-term validation. Engineering approaches that embrace uncertainty quantification, sensitivity analysis, and hybrid physics–data modeling will be pivotal in reducing the epistemic gap and ensuring safe and sustainable deployment of CO₂ sequestration at scale.

Chapter 8 - Conclusions and Future Work

This thesis has presented a comprehensive analysis of both classical and contemporary approaches to evaluating wellbore performance under the coupled influence of thermal, mechanical, and chemical stresses induced by CO₂ injection. By integrating analytical models, numerical simulations, experimental findings, and data-driven methodologies, this research has highlighted key degradation mechanisms, predictive frameworks, and emerging tools to support long-term integrity assessments of CO₂ injection wells.

In the early chapters, fundamental analytical models were reviewed and employed to elucidate the elastic and failure behavior of the cement sheath and casing system. The application of Lamé's stress equations, thermal stress theory, and fracture mechanics enabled the identification of critical stress states—particularly tensile and shear failure thresholds—under various operational scenarios. These models provided valuable closed-form insights into radial, hoop, and axial stress interactions and served as the theoretical baseline for more advanced simulations.

Building upon this, finite element-based numerical simulations were examined to address the inherent limitations of analytical approaches, particularly in handling heterogeneous material behavior, evolving boundary conditions, and time-dependent degradation phenomena. A range of studies using coupled thermo-hydro-mechanical-chemical (THMC) frameworks were analyzed, demonstrating the capacity of such models to simulate zonal evolution, microannulus formation, and leakage risk development under realistic subsurface conditions. These findings underscore the need for computationally robust tools in predicting long-term well performance and planning effective mitigation strategies.

Experimental and field-based investigations further validated the degradation pathways identified through modeling. Chapter 5 consolidated empirical evidence from short- and long-term laboratory studies as well as real-world injection projects (e.g., SACROC Unit and Otway Project), confirming the role of CO₂ exposure duration, pressure-temperature regimes, and chemical interactions in driving microstructural changes within wellbore materials. These studies revealed that carbonation, decalcification, porosity evolution, and mechanical embrittlement are not isolated processes but are instead governed by a coupled progression, which must be captured in integrity models.

One of the novel contributions of this thesis lies in the integration of data-driven methods with conventional geomechanical and geochemical modeling. As discussed in Chapter 6, machine learning (ML) and deep learning (DL) algorithms offer a significant advancement in processing large-scale datasets—including micro-CT scans, logging data, and real-time monitoring streams—while maintaining predictive accuracy and operational scalability. SHAP analysis and hybrid ML-physics-informed models demonstrated particular promise in quantifying feature importance and identifying early indicators of well failure. These tools offer a valuable complement to numerical simulations by reducing computational cost, enhancing model adaptability, and supporting continuous well surveillance.

Moreover, the integration of geochemical reaction modeling with ML predictors, as explored in Section 6.2, offers a pathway to enhance spatial and temporal resolution in cement degradation forecasting. By fusing mechanistic reaction models with AI-based pattern recognition, a more holistic understanding of degradation kinetics and heterogeneity has been achieved—critical for lifecycle risk assessments in CCS infrastructure.

In summary, this thesis presents a unified framework for understanding and forecasting wellbore integrity loss due to CO₂ injection. It bridges theoretical modeling, experimental observations, and advanced data analytics to provide a multidimensional toolkit for both researchers and practitioners in the field of subsurface engineering. The insights presented herein support the design of next-generation wellbore systems that are resilient, monitorable, and adaptive to evolving CO₂ storage challenges.

The following sections will formally summarize the key technical contributions of this work (Section 8.1) and outline specific recommendations and future research directions (Section 8.2) that can extend and build upon the foundations laid in this study.

8.1 Summary of Contributions

This thesis presents a comprehensive, multidisciplinary approach to assessing wellbore integrity in the context of CO₂ geological storage, integrating analytical theory, laboratory studies, field data, and data-driven modeling under a unified engineering framework. The work advances the state-of-the-art in well integrity analysis by not only consolidating knowledge across diverse domains but also offering original insights into how these methods interact and complement one another to enhance predictive capability and operational safety.

Beginning with foundational analytical models, the thesis revisited classical stress formulations—such as Lamé’s equations and thermoelastic stress theory—to estimate the effects of CO₂ injection on the mechanical behavior of cement sheaths. While traditionally limited to idealized assumptions, these models were here adapted to accommodate thermal, chemical, and pressure-induced alterations typical of carbon storage operations. Their application provided baseline estimates of stress concentration, radial cracking potential, and tensile failure thresholds, thereby forming the theoretical backbone for early-phase design assessments.

Building upon this, the experimental literature was examined in depth to validate and contextualize theoretical assumptions. Cement–CO₂ interaction studies, drawn from over 30 peer-reviewed sources, were synthesized to delineate the progressive zonation of degradation within wellbore cement. Notably, the formation of a carbonate-rich outer rim, a chemically compromised transition zone, and an unaltered core was consistently observed across multiple high-pressure and high-temperature experiments. These findings were supported by microstructural data, including scanning electron microscopy (SEM), porosity measurements, and nanoindentation tests, particularly from benchmark studies such as those conducted by Kutchko et al. (2007), Um et al. (2016), and Kranjc et al. (2015). The thesis demonstrated how such zonation patterns evolve over time and are directly influenced by CO₂ phase, pressure conditions, and thermal gradients—

highlighting the inadequacy of short-term cement qualification tests in capturing long-term degradation risks.

To complement laboratory insight, the thesis incorporated real-world observations from field-scale projects such as the SACROC Unit, the Otway Project, and the In Salah CO₂ storage operation. These case studies revealed that microstructural alterations observed in the lab can escalate into large-scale failures—such as interface debonding, microannuli formation, and thermal cracking—when subjected to reservoir-scale stresses and cyclic injection. By connecting experimental results with field phenomena, the research bridged the gap between microscale degradation mechanisms and macroscale integrity loss, validating the relevance of controlled experiments for operational planning.

Recognizing the limitations of conventional modeling in handling the high dimensionality and temporal variability of well data, the thesis then introduced a machine learning (ML) framework for predictive integrity assessment. Using supervised algorithms trained on both synthetic and field-derived datasets, the models successfully forecasted degradation-prone regions with high accuracy. Importantly, the incorporation of SHAP (SHapley Additive exPlanations) analysis allowed the interpretation of ML outcomes in physically meaningful terms, transforming complex black-box predictions into actionable engineering insights. Parameters such as exposure duration, initial porosity, and temperature gradient were ranked by their contribution to model output, revealing dominant factors that align with empirical observations.

The thesis also proposed an integrated hybrid workflow, wherein finite element models inform the initial training of surrogate ML models, which can then be updated in near-real-time using field monitoring data. This adaptive structure is well-suited for long-term surveillance of CO₂ wells, combining the physics-based simulation with the responsiveness and scalability of data-driven algorithms. A conceptual architecture was developed to guide future implementation of such systems in operational environments.

Taken together, this research not only consolidates diverse methodologies into a coherent and robust framework, but also contributes original tools and insights for predicting, monitoring, and mitigating integrity risks in CO₂ injection wells. The integration of geomechanical modeling, laboratory-derived degradation mechanisms, field-scale validation, and machine learning exemplifies a novel approach that is both theoretically grounded and operationally applicable. It is anticipated that these contributions will assist in improving the reliability, safety, and regulatory compliance of (CCS) operations in the coming decades.

8.2 Recommendations for Future Research

As global interest in (CCS) continues to rise, ensuring the long-term integrity of wellbores under CO₂-rich environments remains an urgent and evolving scientific challenge. While this thesis has addressed numerous aspects of wellbore degradation, several key gaps persist, warranting future investigation across experimental, modeling, and field validation domains.

1. Coupled Multi-Physics Modeling at Reservoir Scale

Although this study has reviewed both analytical and numerical models for cement integrity under CO₂ exposure, there is a need for more robust fully coupled thermo-hydro-chemo-mechanical simulations. Current models often treat processes in isolation (e.g., chemistry without geomechanics), but future research should prioritize integration across these domains to simulate real-time degradation paths at field scale. High-resolution reservoir modeling platforms—incorporating fracture mechanics, capillary-driven carbonation fronts, and phase-dependent CO₂ transport—can improve prediction accuracy in heterogeneous formations.

2. Advanced Machine Learning for Predictive Monitoring

While initial deep learning models such as LSTM and CNNs show promise for predicting leakage risks based on historical monitoring data, future work should focus on hybrid models that incorporate physics-informed constraints and real-time sensor feedback. Techniques such as Bayesian neural networks, physics-informed neural networks (PINNs), and SHAP-enhanced interpretability frameworks could significantly increase the transparency, trust, and performance of AI-based monitoring systems deployed on active injection sites.

3. Experimental Studies Under Realistic Field Conditions

Most experimental studies, including those reviewed in Chapters 5 and 6, are conducted under controlled laboratory settings using static pressure and temperature profiles. Future work should simulate more dynamic operational conditions, such as pressure cycling, temperature gradients, well shut-ins, and fluid compositional variations. Long-duration core-flood experiments involving steel-cement-rock composite systems under HPHT (High Pressure High Temperature) conditions will better reflect subsurface environments and help quantify time-dependent degradation and sealing performance.

4. Novel Cement Formulations and Smart Materials

Research should accelerate the development and testing of CO₂-resistant cement blends, including geopolymers, polymer-modified slurries, fiber-reinforced cements, and expandable materials. Additionally, self-healing cement technologies—incorporating encapsulated reactive agents that activate upon fracture—offer promising avenues for autonomous wellbore repair. However, their long-term viability and chemical compatibility with scCO₂ remain poorly understood and must be validated through multi-year exposure testing and micromechanical analysis.

5. Field Data Collection and Standardization

A major limitation in current literature is the lack of accessible, high-quality long-term data from CO₂ injection fields. International collaborations should be formed to develop standardized protocols for wellbore monitoring, data reporting, and failure classification. Open-access databases linking field performance to cement chemistry, formation mineralogy, operational parameters, and failure mechanisms would enable benchmarking and data-driven insights across regions and geological settings.

6. Risk-Based Frameworks and Decision Tools

Building on the event trees discussed in Chapter 4, future work should include probabilistic risk assessment (PRA) tools that quantify well integrity risks under uncertainty. These frameworks should integrate outputs from numerical models, sensor feedback, and material testing to inform real-time decisions on remediation, abandonment, or re-injection. Incorporating uncertainty quantification (UQ) through Monte Carlo simulations or Latin Hypercube Sampling (LHS) will strengthen the defensibility of model-based risk evaluations.

7. Integration with Lifecycle CO₂ Storage Assessment

Well integrity cannot be studied in isolation. Future research should aim to embed integrity analysis within full lifecycle assessments (LCA) of CO₂ storage operations. This includes evaluating the cumulative impacts of well integrity on storage efficiency, surface emissions, abandonment strategies, and post-closure monitoring obligations.

Reference

1. Sun, Z., Fager, A., & Crouse, B. (2024). Modeling of thermal-mechanical impact on wellbore integrity due to CO₂ injection. *Proceedings of the 58th U.S. Rock Mechanics/Geomechanics Symposium*, Golden, CO, USA, 23–26 June 2024. <https://doi.org/10.56952/ARMA-2024-0498>
2. Newell, D. L., & Carey, J. W. (2018). Experimental evaluation of wellbore integrity along the cement-rock boundary. *International Journal of Greenhouse Gas Control*, 77, 153–164. <https://doi.org/10.1016/j.ijggc.2018.09.004>
3. Rashidi, M. R. A., Tan, C. P. P., & others. (2024, November). Openhole completion integrity analysis for life of CO₂ injector well. Conference Paper. <https://doi.org/10.56952/IGS-2024-0222>
4. Shi, J., et al. (2017). Research on stress distribution regularity of cement sheaths of radial well based on ABAQUS. *IOP Conference Series: Earth and Environmental Science*, 100, 012037. <https://doi.org/10.1088/1755-1315/100/1/012037>
5. Roy, P., Walsh, S. D. C., Morris, J. P., Iyer, J., Hao, Y., Carroll, S., Gawel, K., Todorovic, J., & Torsæter, M. (2016). Studying the impact of thermal cycling on wellbore integrity during CO₂ injection. In *Proceedings of the 50th US Rock Mechanics/Geomechanics Symposium* (Paper No. ARMA-2016-668). American Rock Mechanics Association. <https://doi.org/10.15121/1564425>
6. Carey, J. W., Wigand, M., Chipera, S. J., WoldeGabriel, G., Pawar, R., Lichtner, P. C., Wehner, S. C., Raines, M. A., & Guthrie, G. D., Jr. (2007). Analysis and performance of oil well cement with 30 years of CO₂ exposure from the SACROC Unit, West Texas, USA. *International Journal of Greenhouse Gas Control*, 1(1), 75–85. [https://doi.org/10.1016/S1750-5836\(06\)00004-1](https://doi.org/10.1016/S1750-5836(06)00004-1)
7. Ahammad, F., & Azadbakht, S. (2025). A comprehensive review of factors affecting wellbore integrity in CO₂ injection wells. *Energy Geoscience*, 6(2), 100401. <https://doi.org/10.1016/j.engeos.2025.100401>
8. Li, B., Guo, B., Li, H., & Shi, Y. (2015). An analytical solution to simulate the effect of cement/formation stiffness on well integrity evaluation in carbon sequestration projects. *Journal of Natural Gas Science and Engineering*, 27, 1092–1099. <https://doi.org/10.1016/j.jngse.2015.09.019>
9. **Dong, X., Duan, Z., & Gao, D. (2020).** *Assessment on the cement integrity of CO₂ injection wells through a wellbore flow model and stress analysis.* *Journal of Natural Gas Science and Engineering*, 74, 103097. <https://doi.org/10.1016/j.jngse.2019.103097>
10. Azaroual, M., André, L., Peysson, Y., Pironon, J., Broseta, D., Dedecker, F., Egermann, P., Desroches, J., & Hy-Billiot, J. (2012). Behaviour of the CO₂ injection well and the near wellbore during carbon dioxide injection in saline aquifers. *Proceedings of the TOUGH Symposium 2012*, 572–579. Lawrence Berkeley National Laboratory. <https://doi.org/10.2172/1171713>
11. Dou, H., Dong, X., Duan, Z., Ma, Y., & Gao, D. (2020). Cement integrity loss due to interfacial debonding and radial cracking during CO₂ injection. *Energies*, 13(17), 4589. <https://doi.org/10.3390/en13174589>

12. Bagci, A. S., Jonnalagadda, A., & Hernandez-Diaz, D. (2024). CO₂ injection well design considerations: Completion design to injectivity analysis. *SPE Annual Technical Conference and Exhibition*, New Orleans, Louisiana, USA, 23–25 September. Society of Petroleum Engineers. <https://doi.org/10.2118/220702-MS>
13. Abid, K., Baena Velásquez, A. F., & Teodoriu, C. (2024). Comprehensive comparative review of the cement experimental testing under CO₂ conditions. *Energies*, 17(23), 5968. <https://doi.org/10.3390/en17235968>
14. Munkejord, S. T., Hammer, M., Ervik, Å., Odsæter, L. H., & Lund, H. (2021). Coupled CO₂-well-reservoir simulation using a partitioned approach: Effect of reservoir properties on well dynamics. *Greenhouse Gases: Science and Technology*, 11(1), 103–127. <https://doi.org/10.1002/ghg.2035>
15. Roy, P., Morris, J. P., Walsh, S. D. C., Iyer, J., & Carroll, S. A. (2018). Effect of thermal stress on wellbore integrity during CO₂ injection. *International Journal of Greenhouse Gas Control*, 77, 14–26. <https://doi.org/10.1016/j.ijggc.2018.07.012>
16. Jung, H. B., & Um, W. (2013). Experimental study of potential wellbore cement carbonation by various phases of carbon dioxide during geologic carbon sequestration. *Applied Geochemistry*, 35, 161–172. <https://doi.org/10.1016/j.apgeochem.2013.04.007>
17. Carey, J. W., Svec, R., Grigg, R., Zhang, J., & Crow, W. (2010). Experimental investigation of wellbore integrity and CO₂–brine flow along the casing–cement microannulus. *International Journal of Greenhouse Gas Control*, 4(2), 272–282. <https://doi.org/10.1016/j.ijggc.2009.09.018>
18. Baek, S., Bacon, D. H., & Huerta, N. J. (2023). Enabling site-specific well leakage risk estimation during geologic carbon sequestration using a modular deep-learning-based wellbore leakage model. *International Journal of Greenhouse Gas Control*, 126, Article 103903. <https://doi.org/10.1016/j.ijggc.2023.103903>
19. Um, W., Rod, K. A., Jung, H. B., & Brown, C. F. (2017). Geochemical alteration of wellbore cement by CO₂ or CO₂ + H₂S reaction during long-term carbon storage. *Greenhouse Gases: Science and Technology*, 7(5), 852–865. <https://doi.org/10.1002/ghg.1595>
20. Hangx, S. J. T., van der Linden, A., Marcelis, F., & Liteanu, E. (2016). Defining the brittle failure envelopes of individual reaction zones observed in CO₂-exposed wellbore cement. *Environmental Science & Technology*, 50(2), 1031–1038. <https://doi.org/10.1021/acs.est.5b03097>
21. Nassan, T. H., Freese, C., Baganz, D., Alkan, H., Burachok, O., Solbakken, J., Zamani, N., Aarra, M. G., & Amro, M. (2024). *Integrity experiments for geological carbon storage (GCS) in depleted hydrocarbon reservoirs: Wellbore components under cyclic CO₂ injection conditions*. *Energies*, 17(12), 3014. <https://doi.org/10.3390/en17123014>
22. Li, Q., Lim, Y. M., Flores, K. M., Kranjc, K., & Jun, Y. S. (2015). Chemical reactions of Portland cement with aqueous CO₂ and their impacts on cement's mechanical properties under geologic CO₂ sequestration conditions. *Environmental Science & Technology*, 49(10), 6335–6343. <https://doi.org/10.1021/es5063488>

23. Wu, X., Li, Z., Hou, Z., Liu, J., Huang, S., Su, D., Li, J., Cao, C., Wu, L., & Song, W. (2024). Analytical perspectives on cement sheath integrity: A comprehensive review of theoretical research. *ACS Omega*, 9(16), 17741–17759. <https://doi.org/10.1021/acsomega.4c00475>
24. Yang, B., Shao, C., Hu, X., Ngata, M. R., & Aminu, M. D. (2023). Advances in carbon dioxide storage projects: Assessment and perspectives. *Energy & Fuels*, 37(3), 1757–1776. <https://doi.org/10.1021/acs.energyfuels.2c03826>
25. Carey, J. W., Svec, R., Grigg, R., Zhang, J., & Crow, W. (2010). Experimental investigation of wellbore integrity and CO₂–brine flow along the casing–cement microannulus. *International Journal of Greenhouse Gas Control*, 4(2), 272–282. <https://doi.org/10.1016/j.ijggc.2009.09.018>
26. Viswanathan, H. A., Pawar, R. J., Stauffer, P. H., Kaszuba, J. P., Carey, J. W., Olsen, S. C., Keating, G. N., Kavetski, D., & Guthrie, G. D. (2008). Process and system model for the assessment of wellbore leakage at a geologic CO₂ sequestration site. *Environmental Science & Technology*, 42(20), 7727–7735. <https://doi.org/10.1021/es800909e>
27. Wang, X., Jiang, T., Zhang, Y., Zhou, J., Xiao, H., & Li, W. (2021). A three-dimensional analytical solution of stress field in casing-cement-stratum system considering initial stress state. *Applied Sciences*, 11(7), 3116. <https://doi.org/10.3390/app11073116>
28. Hoteit, H., Fahs, M., & Soltanian, M. R. (2018). Assessment of CO₂ injectivity during sequestration in depleted gas reservoirs. *Energies*, 11(12), 3402. <https://doi.org/10.3390/en11123402>
29. Hu, J., Wang, L., Feng, J., Shen, J., & He, M. (2023). Full-life-cycle analysis of cement sheath integrity. *Journal of Natural Gas Science and Engineering*, 111, Article 104635. <https://doi.org/10.1016/j.jngse.2023.104635>
30. Zheng, G., Sun, J., Guo, X., & Li, Z. (2023). Research on the relationship between pore structure and the compressive strength of oil-well cement. *Materials*, 16(4), 1432. <https://doi.org/10.3390/ma16041432>
31. Lv, W., Liang, T., Lu, C., Li, M., Zhou, P., Yu, X., Wang, B., & Wang, H. (2023). Flow and corrosion analysis of CO₂ injection wells: A case study of the Changqing Oilfield CCUS project. *Energies*, 16(6), 2985. <https://doi.org/10.3390/en16062985>