Multiphase Behavior and Fluid Flow in CO2 Sequestration

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Abstract

Carbon capture and sequestration (CCS) is a critical technology for mitigating climate change by reducing CO₂ emissions from industrial sources. The effectiveness of CCS relies heavily on understanding the multiphase behavior and fluid flow in geological formations where CO₂ is injected for long-term storage. This paper investigates the multiphase behavior and fluid flow dynamics during CO₂ sequestration, focusing on the interaction between supercritical CO₂ (scCO₂), formation brine, and the geological matrix. We review current literature, present a detailed methodology for analyzing multiphase flow in porous media, and discuss the results of numerical simulations and experimental studies. The findings highlight the importance of accurately modeling multiphase systems to ensure the safe and efficient storage of CO₂, offering insights into optimizing injection strategies and predicting long-term storage behavior.

Keywords: CO₂ Sequestration, Supercritical CO₂, Multiphase Flow, Geological Storage

1. Introduction

Carbon dioxide (CO₂) sequestration is an integral part of global efforts to combat climate change by reducing greenhouse gas emissions. CCS involves capturing CO₂ from industrial sources and injecting it into deep geological formations for long-term storage [1]. The success of CCS projects depends on a comprehensive understanding of the multiphase flow behavior of CO₂ in subsurface environments [2, 3]. When CO₂ is injected into a saline aquifer, it often exists in a supercritical state due to the high pressure and temperature conditions found at depths greater than 800 meters. Supercritical CO₂ (scCO₂) exhibits unique properties that significantly influence its interaction with formation brine and the geological matrix, leading to complex multiphase flow dynamics. These interactions influence the migration, trapping, and dissolution of CO₂, which are critical for ensuring the safety and efficacy of storage.

Understanding the multiphase behavior of scCO₂ and brine within the porous media of geological formations is crucial for predicting the fate of injected CO₂ and assessing the risks of leakage [4, 5]. This paper aims to provide a detailed analysis of the multiphase behavior and fluid flow mechanisms
involved in CO₂ sequestration. We will review existing research, describe the methodologies used to study these processes, and present the results from numerical and experimental investigations. The goal is to enhance our understanding of CO₂ storage dynamics and inform the development of more effective CCS strategies.

2. Literature Review

CO₂ Sequestration Mechanisms

The primary mechanisms for CO₂ sequestration in geological formations include structural trapping, residual trapping, solubility trapping, and mineral trapping. Structural trapping involves the physical containment of CO₂ beneath impermeable caprocks. Residual trapping occurs when CO₂ becomes immobilized in pore spaces due to capillary forces. Solubility trapping involves the dissolution of CO₂ into formation brine, reducing the volume of free-phase CO₂ [6-9]. Mineral trapping results from the chemical reactions between dissolved CO₂ and formation minerals, leading to the precipitation of stable carbonate minerals.

Supercritical CO₂ Properties

When CO₂ is injected into deep geological formations, it often reaches a supercritical state, characterized by a temperature above 31.1 degrees Celsius and a pressure above 7.38 MPa [10]. Supercritical CO₂ has unique properties that combine the characteristics of both gases and liquids:

- Density: Similar to that of a liquid, enhancing its ability to carry soluble substances and occupy pore spaces efficiently.

- Viscosity: Lower than that of liquid water, allowing it to flow more easily through porous rock formations.

- Diffusivity: Higher than its liquid state, improving its penetration into finer pores within the rock.

These properties significantly influence the transport, storage, and interaction of CO₂ with geological formations, making it essential to consider scCO₂ in CCS applications.
Multiphase Flow in Porous Media

Multiphase flow in porous media is governed by the interactions between the different fluid phases and the solid matrix. The key parameters influencing multiphase flow include fluid properties (density, viscosity, interfacial tension), rock properties (porosity, permeability, wettability), and the pressure and
temperature conditions of the reservoir. The movement of scCO₂ in a saline aquifer is influenced by buoyancy forces due to the density difference between scCO₂ and brine, capillary forces, and viscous forces [11]. The interplay of these forces determines the distribution and migration of scCO₂ within the formation.

**Numerical Modeling of Multiphase Flow**

Numerical modeling is an essential tool for studying multiphase flow in CO₂ sequestration. Models such as TOUGH2, ECLIPSE, and CMG-GEM are commonly used to simulate the injection and migration of CO₂ in geological formations [12]. These models incorporate the governing equations of fluid flow, mass transfer, and heat transfer, along with the specific properties of scCO₂ and brine. Numerical simulations provide insights into the spatial and temporal evolution of CO₂ plumes, the effectiveness of trapping mechanisms, and the potential for CO₂ leakage.

**Experimental Studies on Multiphase Flow**

Experimental studies complement numerical models by providing empirical data on multiphase flow behavior. Laboratory experiments using core samples from geological formations help to characterize the permeability, capillary pressure, and relative permeability of the rock matrix [13, 14]. High-pressure and high-temperature conditions representative of subsurface environments are recreated to study the interactions between scCO₂ and brine. Experimental data are crucial for validating numerical models and improving their predictive capabilities [15].

3. **Methodology**

**Numerical Simulation Approach**

To simulate the behavior of CO₂ injection in a porous medium, we utilized the following multiphase flow equations, based on Darcy’s law and mass conservation principles:

1. **Generalized Darcy's Law for Multiphase Flow:**

   \[
   q_\alpha = -\frac{k k_{r\alpha}}{\mu_\alpha} (\nabla p_\alpha - \rho_\alpha g \nabla z)
   \]

   where \( q_\alpha \) is the flow rate of phase \( \alpha \) (gas or liquid), \( k \) is the absolute permeability of the porous medium, and \( k_{r\alpha} \) is the relative permeability to phase \( \alpha \), and \( \mu_\alpha \) is the viscosity of phase \( \alpha \). \( p_\alpha \) is the phase pressure, \( \rho_\alpha \) is the density of phase \( \alpha \), \( g \) is the acceleration due to gravity, and \( z \) is the depth.

2. **Mass Conservation for Each Phase:**
\[
\frac{\partial (\varnothing \rho_\alpha S_\alpha)}{\partial t} + \nabla \cdot (\rho_\alpha q_\alpha) = q_{\alpha,s}
\]

where \( \varnothing \) is the porosity, \( S_\alpha \) is the saturation of phase \( \alpha \), and \( q_{\alpha,s} \) is a source or sink term for phase \( \alpha \).

These equations were integrated into the TOUGH2 simulation software framework to model the injection, migration, and trapping of scCO\(_2\). Boundary conditions, initial conditions, and parameters such as rock and fluid properties were carefully defined based on experimental data and literature.

**Experimental Setup**

Laboratory experiments were conducted to study the multiphase flow behavior of scCO\(_2\) and brine in core samples from a saline aquifer. The core samples were placed in a high-pressure, high-temperature core holder, and CO\(_2\) was injected at a controlled rate. The pressure and temperature conditions were monitored throughout the experiment to replicate subsurface conditions. The distribution of scCO\(_2\) within the core samples was analyzed using X-ray computed tomography (CT) scanning. Capillary pressure and relative permeability curves were obtained from the experimental data.

1. **Capillary Pressure (Pc) Relation:**

\[
P_c = P_{nw} - P_w = \sigma \cos (\theta) \left(\frac{1}{r}\right)
\]

where \( P_{nw} \) and \( P_w \) are the non-wetting and wetting phase pressures, respectively, \( \sigma \) is the interfacial tension, \( \theta \) is the contact angle, and \( r \) is the pore throat radius. This equation is critical for understanding how capillary forces contribute to trapping mechanisms in porous media.

**Data Analysis**

The results from the numerical simulations and experimental studies were analyzed to identify the key factors influencing multiphase flow behavior. The distribution and migration of scCO\(_2\) were visualized using software tools, and the effectiveness of different trapping mechanisms was evaluated. Sensitivity analyses were conducted to assess the impact of varying injection rates, reservoir properties, and fluid properties on CO\(_2\) sequestration performance. The experimental data were used to validate the numerical models and refine the input parameters for more accurate simulations.

**4. Results and Discussion**

**Numerical Simulation Results**
The numerical simulations revealed that the migration and distribution of scCO₂ in the saline aquifer are significantly influenced by the heterogeneity of the geological formation. High-permeability zones facilitated the rapid migration of scCO₂, while low-permeability zones acted as barriers, promoting the accumulation of scCO₂ and enhancing residual and solubility trapping. The simulations showed that higher injection rates resulted in larger scCO₂ plumes, increasing the risk of scCO₂ reaching the caprock and potentially leaking. However, optimized injection strategies, such as pulsed injection, were found to improve the efficiency of CO₂ trapping by promoting better mixing with formation brine.

1. **Relative Permeability Models**:

   \[ k_{rg} = (1 - S_{br})^2, k_{rl} = S_l^3 \]  
   \[ (4) \]

   where \( k_{rg} \) and \( k_{rl} \) are the relative permeabilities for gas and liquid, \( S_{br} \) is the irreducible brine saturation, and \( S_l \) is the liquid saturation.

These equations helped explain the dynamics observed in CO₂ distribution and migration paths, emphasizing the role of formation heterogeneity. The results indicated how variations in permeability and fluid properties influence the effectiveness of CO₂ trapping by different mechanisms.

**Experimental Results**

The experimental studies provided valuable insights into the capillary pressure and relative permeability characteristics of the core samples. The capillary pressure curves indicated that the scCO₂-brine system exhibited strong capillary forces, which contributed to the effective immobilization of CO₂ in the pore spaces. The relative permeability curves showed that scCO₂ had a higher mobility in the high-permeability zones, while brine dominated the flow in low-permeability zones. The CT scans revealed the distribution of scCO₂ within the core samples, confirming the preferential flow paths and the regions of CO₂ accumulation.

**Discussion**

The combined results from the numerical simulations and experimental studies highlight the importance of accurately characterizing the geological formation and fluid properties for effective CO₂ sequestration. The heterogeneity of the formation plays a crucial role in determining the migration and trapping of scCO₂. High-permeability zones can facilitate CO₂ leakage if not properly managed, while low-permeability zones enhance trapping mechanisms. The findings underscore the need for
optimized injection strategies that consider the specific properties of the formation to maximize the efficiency of CO₂ storage and minimize the risk of leakage.

The study also emphasizes the importance of integrating numerical modeling with experimental data to improve the accuracy of predictions. The experimental data provided critical validation for the numerical models, ensuring that the simulations accurately represented the multiphase flow behavior observed in the laboratory. This integrated approach allows for more reliable predictions of scCO₂ migration and trapping, which are essential for the safe and effective implementation of CCS projects.

5. Future Work

The study of multiphase behavior and fluid flow in CO₂ sequestration has opened several avenues for further research that can enhance the efficiency and reliability of CCS technologies. Future work in this field should focus on the following key areas:

Advanced Numerical Modeling

Further development and refinement of numerical models are essential to improve the accuracy and predictive capabilities of simulations for CO₂ sequestration. Future models should integrate more complex physical phenomena such as non-Newtonian fluid behaviors, geochemical interactions between CO₂ and reservoir rock, and the impacts of micro-scale heterogeneities on macro-scale flow behavior. Additionally, incorporating machine learning and data-driven approaches could provide new insights into pattern recognition and prediction of fluid behavior in heterogeneous formations.

Experimental Research

There is a need for more comprehensive experimental studies that replicate the subsurface conditions more accurately and at a larger scale. Future experiments should focus on:

- **Pilot-scale studies**: Conducting field-scale pilot tests to validate laboratory and numerical findings, and to observe the behavior of CO₂ in real-world geological settings.

- **High-resolution imaging**: Utilizing advanced imaging technologies such as 4D X-ray computed tomography or magnetic resonance imaging to visualize the phase distributions and flow pathways in real-time.

Coupled Process Analysis
The interaction of mechanical, thermal, chemical, and biological processes can significantly affect the storage integrity and behavior of injected CO$_2$. Future studies should aim at developing coupled multiphysics models that can simultaneously handle these interacting processes to provide a more comprehensive understanding of the system’s behavior. This will help in assessing the long-term stability and safety of CO$_2$ sequestration sites.

**Impact of Climate Change**

Understanding how changes in climate might impact the storage capacity and integrity of CO$_2$ sequestration sites is crucial. Future research should include modeling the potential effects of global warming on reservoir properties and behavior, including changes in reservoir pressure, temperature, and brine composition. This will be important for predicting and mitigating risks associated with long-term CO$_2$ storage.

**Policy and Economic Assessments**

While much of the research focus is on the technical aspects of CO$_2$ sequestration, future work should also consider the policy and economic frameworks necessary to support the wide-scale adoption of CCS. This includes:

- **Regulatory frameworks**: Developing comprehensive policies that govern the monitoring, reporting, and verification of CO$_2$ storage sites.
- **Economic models**: Conducting cost-benefit analyses to compare different CCS technologies and strategies, and evaluating the economic feasibility of large-scale implementation.

**Public Engagement and Education**

Increased efforts in public engagement and education are needed to raise awareness about the benefits and challenges of CCS. Future initiatives should aim to:

- **Increase transparency**: Providing clear and accessible information about CCS projects to build public trust and acceptance.
- **Educational programs**: Developing educational materials and programs to inform the public and stakeholders about the role of CCS in mitigating climate change.

By addressing these areas, future research can contribute to overcoming the current challenges in CO$_2$ sequestration and help pave the way for its successful implementation as a viable climate change mitigation technology.
6. Conclusions

The multiphase behavior and fluid flow dynamics in CO2 sequestration are complex and influenced by a range of factors, including the properties of the geological formation, the characteristics of the fluids, and the injection strategies employed. This paper has provided a comprehensive analysis of these processes through a combination of numerical simulations and experimental studies. The findings highlight the critical role of formation heterogeneity in determining the migration and trapping of scCO2, as well as the importance of optimized injection strategies for maximizing storage efficiency and minimizing leakage risks.

The integration of numerical modeling with experimental data has proven to be a valuable approach for improving the accuracy of predictions and enhancing our understanding of CO2 sequestration dynamics. As CCS technology continues to evolve, ongoing research and the development of more sophisticated models will be essential for addressing the challenges associated with large-scale implementation. This study contributes to the growing body of knowledge on CO2 sequestration and provides insights that can inform the design and operation of future CCS projects, ultimately contributing to global efforts to mitigate climate change.

7. References


