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 CO_2 emissions from industrial sources. The effectiveness of CCS relies heavily on understanding the multiphase behavior and fluid flow in geological formations where CO_2 is injected for long-term storage. This paper investigates the multiphase behavior and fluid flow dynamics during CO_2 sequestration, focusing on the interaction between supercritical CO_2 ($scCO_2$), 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 CO_2, offering insights into optimizing injection strategies and predicting long-term storage behavior.

Keywords: CO_2 Sequestration, Supercritical CO_2, Multiphase Flow, Geological Storage

1. Introduction

Carbon dioxide (CO_2) sequestration is an integral part of global efforts to combat climate change by reducing greenhouse gas emissions. CCS involves capturing CO_2 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 CO_2 in subsurface environments [2, 3]. When CO_2 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 CO_2 (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 CO_2, which are critical for ensuring the safety and efficacy of storage.

Understanding the multiphase behavior of $scCO_2$ and brine within the porous media of geological formations is crucial for predicting the fate of injected CO_2 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 CO_2 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 CO_2 storage dynamics and inform the development of more effective CCS strategies.

2. Literature Review

CO_2 Sequestration Mechanisms

The primary mechanisms for CO_2 sequestration in geological formations include structural trapping, residual trapping, solubility trapping, and mineral trapping. Structural trapping involves the physical containment of CO_2 beneath impermeable caprocks. Residual trapping occurs when CO_2 becomes immobilized in pore spaces due to capillary forces. Solubility trapping involves the dissolution of CO_2 into formation brine, reducing the volume of free-phase CO_2 [6-9]. Mineral trapping results from the chemical reactions between dissolved CO_2 and formation minerals, leading to the precipitation of stable carbonate minerals.

Supercritical CO_2 Properties

When CO_2 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 CO_2 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 CO_2 with geological formations, making it essential to consider $scCO_2$ in CCS applications.

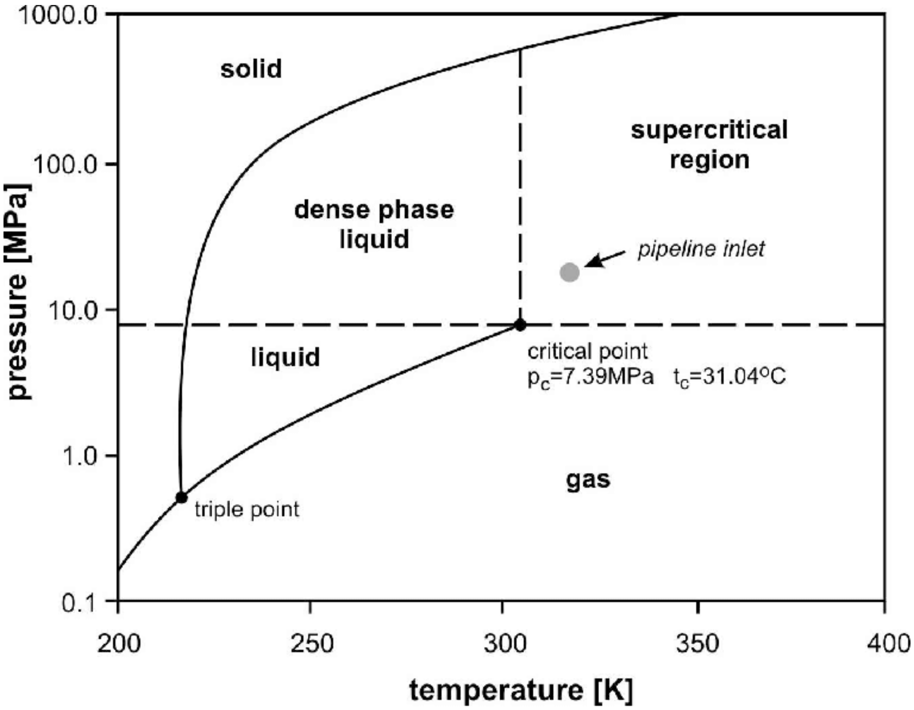

Fig. 1 CO_2 phase diagram.

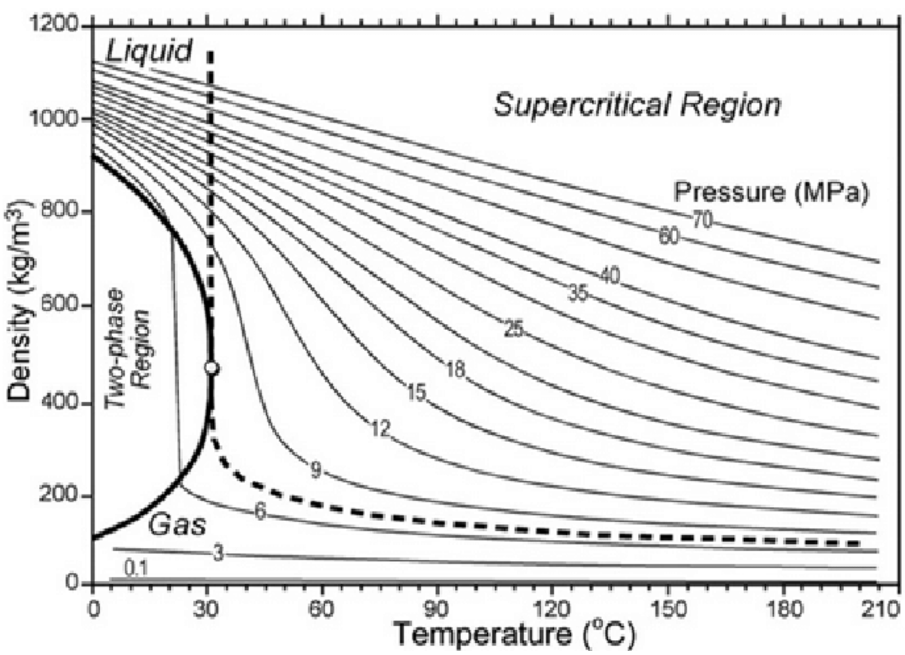

Fig. 2 CO_2 density diagram.

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 $scCO_2$ in a saline aquifer is influenced by buoyancy forces due to the density difference between $scCO_2$ and brine, capillary forces, and viscous forces [11]. The interplay of these forces determines the distribution and migration of $scCO_2$ within the formation.

Numerical Modeling of Multiphase Flow

Numerical modeling is an essential tool for studying multiphase flow in CO_2 sequestration. Models such as TOUGH2, ECLIPSE, and CMG-GEM are commonly used to simulate the injection and migration of CO_2 in geological formations [12]. These models incorporate the governing equations of fluid flow, mass transfer, and heat transfer, along with the specific properties of $scCO_2$ and brine. Numerical simulations provide insights into the spatial and temporal evolution of CO_2 plumes, the effectiveness of trapping mechanisms, and the potential for CO_2 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 $scCO_2$ 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 CO_2 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**:

$$q_\alpha = -\frac{k k_{r\alpha}}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha g \nabla z) \tag{1}$$

where q_α is the flow rate of phase α (gas or liquid), k is the absolute permeability of the porous medium, and $k_{r\alpha}$ is the relative permeability to phase α, and μ_α is the viscosity of phase α. p_α is the phase pressure, ρ_α is the density of phase α, g is the acceleration due to gravity, and z is the depth.

2. **Mass Conservation for Each Phase**:

$$\frac{\partial(\emptyset \rho_\alpha S_\alpha)}{\partial t} + \nabla \cdot (\rho_\alpha q_\alpha) = q_{\alpha,s} \tag{2}$$

where $\emptyset$ is the porosity, S_α is the saturation of phase α, and $q_{\alpha,s}$ is a source or sink term for phase α.

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**:

$$P_c = P_{nw} - P_w = \sigma \cos(\theta) \left(\frac{1}{r}\right) \tag{3}$$

where P_{nw} and P_w are the non-wetting and wetting phase pressures, respectively, σ is the interfacial tension, θ 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 $scCO_2$ in the saline aquifer are significantly influenced by the heterogeneity of the geological formation. High-permeability zones facilitated the rapid migration of $scCO_2$, while low-permeability zones acted as barriers, promoting the accumulation of $scCO_2$ and enhancing residual and solubility trapping. The simulations showed that higher injection rates resulted in larger $scCO_2$ plumes, increasing the risk of $scCO_2$ reaching the caprock and potentially leaking. However, optimized injection strategies, such as pulsed injection, were found to improve the efficiency of CO_2 trapping by promoting better mixing with formation brine.

1. **Relative Permeability Models**:

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

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 CO_2 distribution and migration paths, emphasizing the role of formation heterogeneity. The results indicated how variations in permeability and fluid properties influence the effectiveness of CO_2 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 $scCO_2$-brine system exhibited strong capillary forces, which contributed to the effective immobilization of CO_2 in the pore spaces. The relative permeability curves showed that $scCO_2$ 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 $scCO_2$ within the core samples, confirming the preferential flow paths and the regions of CO_2 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 CO_2sequestration. The heterogeneity of the formation plays a crucial role in determining the migration and trapping of $scCO_2$. High-permeability zones can facilitate CO_2 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 CO_2 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 $scCO_2$ 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 CO_2 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 CO_2 sequestration. Future models should integrate more complex physical phenomena such as non-Newtonian fluid behaviors, geochemical interactions between CO_2 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 CO_2 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 CO2 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 CO_2 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 $scCO_2$, 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 CO_2 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 CO_2 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

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