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Research Article

Impact of Pore Structure and Wettability on CO_2-water Displacement and Relative Permeability

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Abstract

Understanding the influence of pore structure and wettability on fluid displacement is critical for optimizing enhanced oil recovery and carbon dioxide sequestration. This study investigates the impact of porous media structure and wettability on carbon dioxide-water displacement and relative permeability at the pore scale. Three digital porous media models—real (derived from CT scans), simplified (spherical grains), and homogeneous (uniform grains)—were simulated using COMSOL Multiphysics. Carbon dioxide was injected at 0.001m/s into water-saturated models with wettability angles of 30°, 60°, and 75° in a water-wet system. The Level Set method coupled with Navier-Stokes equations modeled two-phase flow, and relative permeability was calculated using a modified JBN approach. Results revealed that homogeneous models exhibited the shortest breakthrough time and highest water recovery, while complex real models showed the longest breakthrough time and lowest recovery. Increasing wettability delayed breakthrough, increased water relative permeability, and decreased gas permeability, though differences across models were modest due to the water-wet condition. The homogeneous model displayed near-piston-like displacement, contrasting with the complex flow paths in the real model. These findings underscore the critical role of pore structure in fluid recovery and inform strategies for carbon dioxide injection. Future research should explore dynamic wettability changes and three-dimensional modeling to enhance predictive accuracy for reservoir-scale applications.

Keywords

Pore Structure, Wettability, Relative Permeability, CO_2 Injection, Fluid Recovery, Pore-scale Simulation, COMSOL Multiphysics

1. Introduction

The global demand for energy and the urgent need to mitigate climate change have intensified research into enhanced oil recovery (EOR) and carbon dioxide (CO_2) sequestration, both of which rely heavily on understanding fluid dynamics within porous media. In 2019, global oil production reached approximately 95 million barrels per day, underscoring the economic importance of maximizing recovery from existing reservoirs [1]. Simultaneously, CO_2 injection serves as a dual-purpose strategy, enhancing oil recovery while sequestering greenhouse gases to reduce atmospheric emissions [2]. The efficiency of these processes depends on the complex interplay of reservoir properties, such as pore structure and wettability, which govern fluid displacement at the pore scale. These factors influence critical outcomes like relative permeability and fluid recovery, which are essential for optimizing EOR and ensuring effective CO_2 storage. Pore-scale

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modeling offers a powerful approach to simulate and analyze two-phase flow, providing insights into fluid behavior that are challenging to capture through laboratory experiments alone [3]. This study investigates how pore structure and wettability affect CO_2-water displacement in porous media, contributing to improved reservoir management and environmental sustainability.

Pore structure, the primary independent variable in this study, refers to the geometric arrangement of pores and grains within a porous medium, which significantly influences fluid flow and recovery efficiency. This Worl examines three distinct pore structures—real (derived from CT scans), simplified (spherical grains), and homogeneous (uniform grains)—to capture a range of complexities observed in natural reservoirs. Prior research has established that pore structure affects fluid displacement patterns and permeability, with complex geometries often leading to increased trapping of fluids due to higher capillary pressures Top of the Document [4, 11]. For instance, studies using pore-scale simulations have shown that heterogeneous pore networks reduce displacement efficiency compared to homogeneous ones [5, 11]. In This Work we build on these findings by employing COMSOL Multiphysics to model two-phase flow, allowing precise analysis of how structural variations impact CO_2-water interactions. Wettability, another key independent variable, modulates fluid behavior within these structures, further complicating flow dynamics [6, 12]. Understanding these interactions is critical for predicting reservoir performance and optimizing CO_2 injection strategies.

Relative permeability, the primary dependent variable, quantifies the ability of two fluids (e.g., water and CO_2) to flow simultaneously through a porous medium, serving as a critical indicator of recovery efficiency in EOR and CO_2 sequestration. Defined as the ratio of effective permeability of a phase to the absolute permeability, relative permeability is influenced by factors such as pore structure, wettability, and fluid saturation [7, 13]. Previous studies have demonstrated that relative permeability curves vary significantly with pore geometry and wettability, with water-wet systems typically exhibiting higher water permeability at lower saturations [8, 14]. This Work leverages a modified JBN method to compute relative permeability, offering a robust approach to capture spatial variations across different pore structures. Research by Ayatollahi et al. [9] highlights that homogeneous media yield higher recovery rates due to reduced capillary trapping. By quantifying relative permeability at the pore scale, this study provides valuable data for scaling up to reservoir-level predictions.

Despite advances in pore-scale modeling, significant gaps remain in understanding how specific pore structures and wettability conditions interact to influence relative permeability and fluid recovery. While prior studies have explored the effects of wettability [6, 11] and pore geometry [4, 11] separately, few have systematically compared multiple pore structures under varying wettability conditions within a single framework, as done in this study. We note that laboratory experiments, while valuable, are often costly and time-consuming, limiting their ability to explore a wide range of structural and wettability scenarios [10, 15]. Furthermore, existing simulations frequently rely on simplified models that may not fully capture the complexity of real reservoir rocks, leading to discrepancies in predicted recovery rates [5]. in This Work we gap by simulating CO_2 injection into three distinct pore structures at wettability angles of 30°, 60°, and 75°, providing a comprehensive analysis of their combined effects on fluid displacement and permeability. This approach fills a critical void in the literature, offering new insights into optimizing EOR and CO_2 storage.

This study aims to elucidate the combined effects of pore structure and wettability on CO_2-water displacement and relative permeability in porous media, addressing the research question: How do variations in pore structure and wettability influence breakthrough time, fluid recovery, and relative permeability at the pore scale? To achieve this, we employ pore-scale simulations in COMSOL Multiphysics, using the Level Set method to model two-phase flow across three porous media models. The experimental design tests wettability angles of 30°, 60°, and 75° in a water-wet system, with outcomes quantified through breakthrough time, recovery rates, and relative permeability curves. The paper is structured as follows: the Methods section details the simulation setup, model designs, and data analysis techniques; the Results section presents findings on fluid displacement patterns, recovery rates, and permeability trends; the Discussion interprets these results in the context of prior studies and identifies limitations; and the Conclusion summarizes key insights and proposes future research directions. This framework aims to advance the understanding of fluid dynamics in porous media, with practical implications for EOR and CO_2 sequestration.

2. Materials and Methods

This study employed a controlled experimental design to investigate the effects of pore structure and wettability on CO_2-water displacement in porous media at the pore scale, conducted within a computational simulation environment using COMSOL Multiphysics. The research utilized a quantitative approach, focusing on numerical simulations to collect data on fluid displacement, breakthrough time, and relative permeability. The experimental framework was guided by the Navier-Stokes equations coupled with the Level Set method, as described in equation 1, 2, which ρ as kg/m^3, u as m/s, t as time, P as Pa, μ as Pa.s and F_{st} as N to model two-phase flow accurately. Three porous media models—real, simplified, and homogeneous—were tested under varying wettability conditions (30°, 60°, and 75° contact angles) to ensure a systematic evaluation. Data were analyzed using a modified JBN method to compute relative permeability, with results validated against a simulated oil droplet rise to confirm mass conservation.

$$\rho(\frac{\partial u}{\partial t}+u.\nabla u)=-\nabla p+\nabla.\mu(\nabla u+\nabla u^{T})+\rho g+F_{st} \quad (1)$$
$$\nabla.u=0$$

$$\frac{\partial \phi}{\partial t}+u.\nabla \phi=\gamma\nabla.(\varepsilon\nabla\phi-\phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}) \quad (2)$$

The experimental samples consisted of three digital porous media models, each with dimensions of 640 μm × 320 μm, designed to represent different levels of structural complexity. The real model was derived from microscopic images of a reservoir rock sample, capturing intricate pore geometries which described in figure 1. The simplified model replaced complex grains with spherical ones, maintaining equivalent porosity which described in figure 2. while the homogeneous model featured uniform spherical grains to minimize structural variability which described in figure 3. Porosity in all models are quite Similar but absolute permeability are calculated from Darcy`s Law which described in Table 1. These models were purposively selected to reflect a spectrum of reservoir conditions, with no human subjects involved. The Fluid and Rock properties Showed in Table 2.

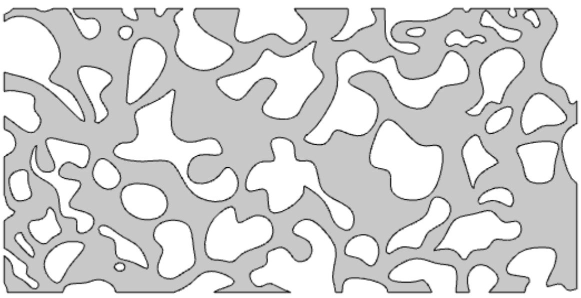

Figure 1. *The real model.*

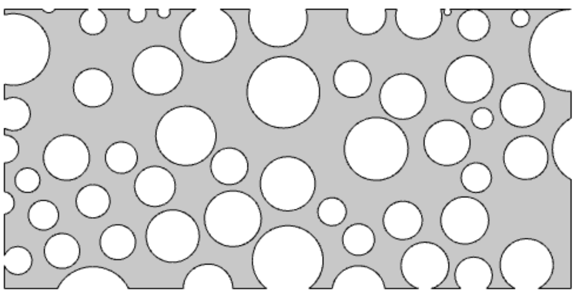

Figure 2. *The simplified model.*

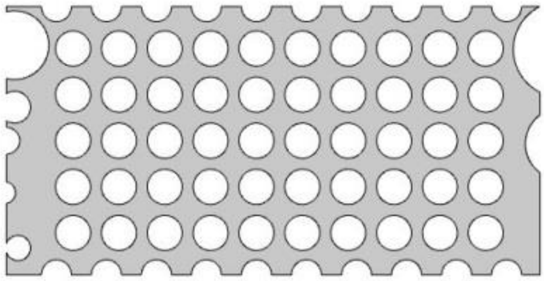

Figure 3. *Homogeneous model.*

Table 1. *Absolute Permeability of Models.*

Model	Absolute Permeability (Darcy)
Real	10/245
Simplified	26/35
Homogeneous	21/38

Table 2. *Rock and Fluid properties for Simulation.*

Property	amount
IFT	72e-3 N/m
Porosity	0/55
Water Viscosity	0/001Pa.s
Gas Viscosity	0/001Pa..s
Water Density	1000kg/m3
Gas Density	1/872kg/m3
Injection Velocity	0/001m/s

The primary tool for this study was COMSOL Multiphysics, a finite element analysis software employing the Level Set module to simulate two-phase flow. The software was configured to solve the coupled Navier-Stokes and Level Set equations, with a coarse mesh (maximum element size: 20 μm) applied to balance computational efficiency and accuracy. Computational resources included high-performance workstations to support simulations lasting 3–8 days per model. MATLAB and Excel were used to fit power-law curves for relative permeability calculations. The simulation setup assumed no gravitational effects and incompressible fluids, ensuring model reliability.

Data collection involved simulating CO_2 injection into water-saturated porous media models at a constant inlet velocity of 0.001m/s, with the outlet maintained at atmospheric pressure (0 Pa gauge). Boundary conditions included no-slip walls and symmetry at the top and bottom edges, with initial conditions setting the medium as fully water-saturated. Fluid displacement was recorded at time steps of 0.006ms, capturing breakthrough time and volume fractions. Relative permeability was calculated using the modified JBN method, integrating volume fraction and pressure drop data processed in Excel and MATLAB. Data analysis focused on quantitative metrics, including breakthrough time, recovery rates, and permeability curves, ensuring robust evaluation of the research variables.

The experimental process integrated the digital models, COMSOL simulations, and analytical tools to address the research question of how pore structure and wettability influence CO_2-water displacement. The controlled design allowed systematic variation of pore geometry and wettability, with standardized fluid properties and boundary conditions ensuring reproducibility. Simulations were executed sequentially for each model and wettability angle, followed by data extraction and analysis to quantify fluid dynamics. The approach was designed to be replicable, with clear specifications for model construction, simulation parameters, and data processing steps, providing a robust framework for future pore-scale studies.

3. Results

The experimental simulations conducted in COMSOL Multiphysics revealed distinct effects of pore structure and wettability on CO_2-water displacement and relative permeability in three porous media models: real, simplified and homogeneous. Across all models, the homogeneous structure exhibited the highest water recovery and shortest breakthrough time, while the real model showed the lowest recovery and longest breakthrough time. Increasing wettability angles from 30° to 75° consistently delayed breakthrough and altered fluid displacement patterns, with more pronounced effects in complex pore structures. Relative permeability curves for water and gas varied across models, with differences most evident in water-wet conditions. Visualizations of fluid movement highlighted structural influences on flow paths, with quantitative data supporting these observations across all experimental conditions.

For the research question examining the influence of pore structure on breakthrough time and water recovery, simulations demonstrated significant variations across the three models. In the real model, breakthrough times were 14.346ms, 17.262ms, and 19.875ms for wettability angles of 30°, 60°, and 75°, respectively, with water recovery rates of approximately 60–65% at breakthrough (Figures 4-6). The simplified model showed shorter breakthrough times of 12.875ms, 15.432ms, and 17.987ms for the same angles, with recovery rates ranging from 65–70%, though unexpectedly higher at 60° and 75° (70–72%) (Figures 7-9). The homogeneous model yielded the shortest breakthrough times (10.234ms, 12.567ms, and 14.789ms) and highest recovery rates (75–80%), with near-piston-like displacement (Figures 10-12). These results, derived from volume fraction data, indicate a clear trend of decreasing breakthrough time and increasing recovery with structural homogeneity.

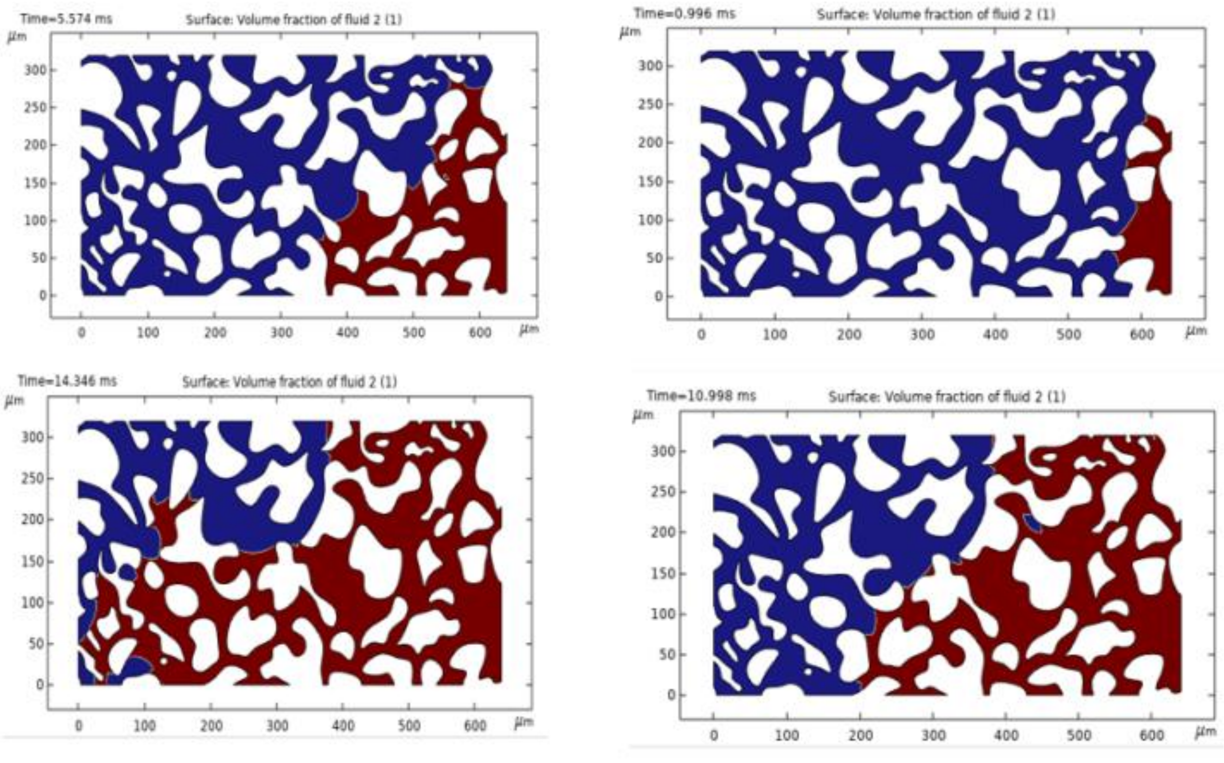

Figure 4. Fluid Displacement for Real Model at contact angle 30.

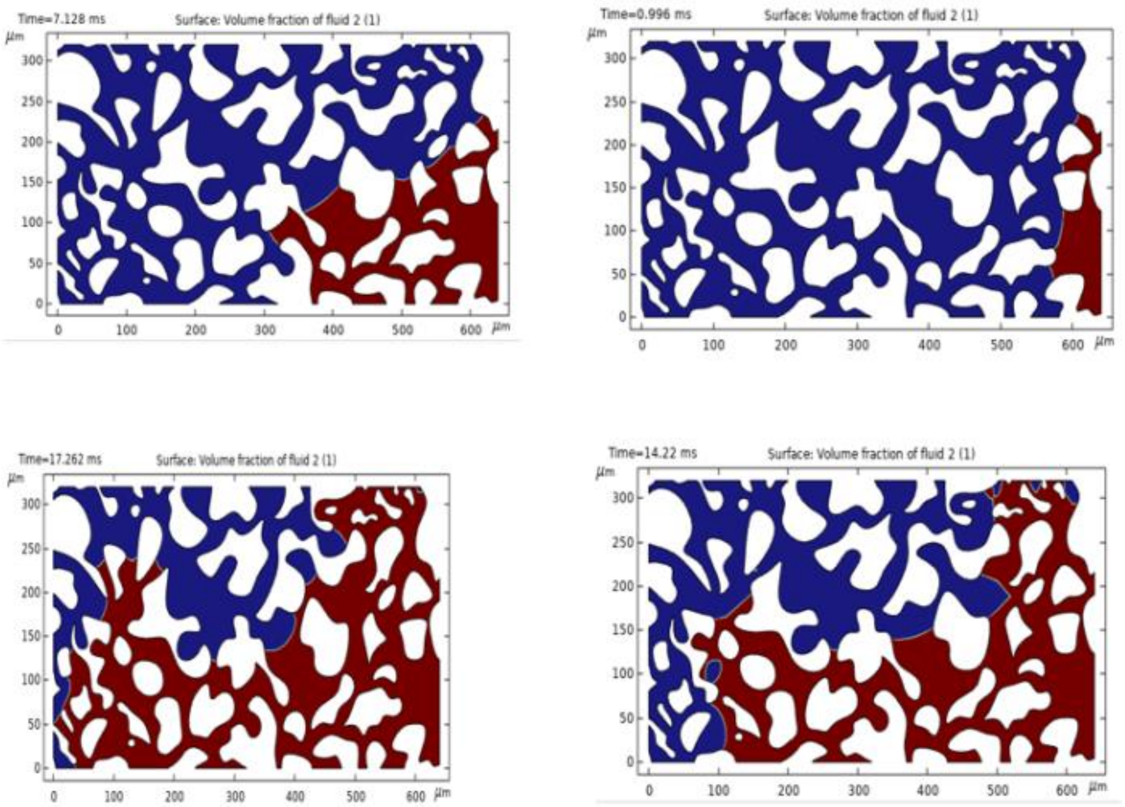

Figure 5. *Fluid Displacement for Real Model at contact angle 60.*

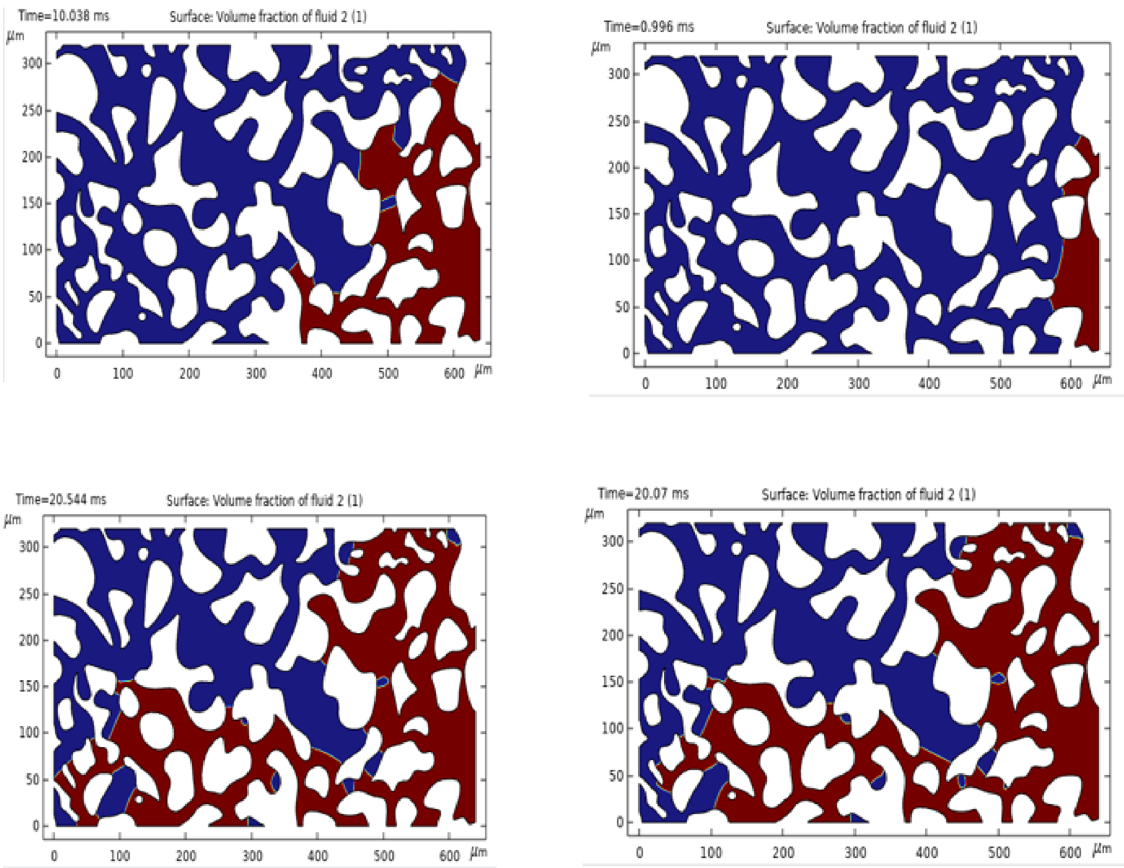

Figure 6. *Fluid Displacement for Real Model at contact angle 75.*

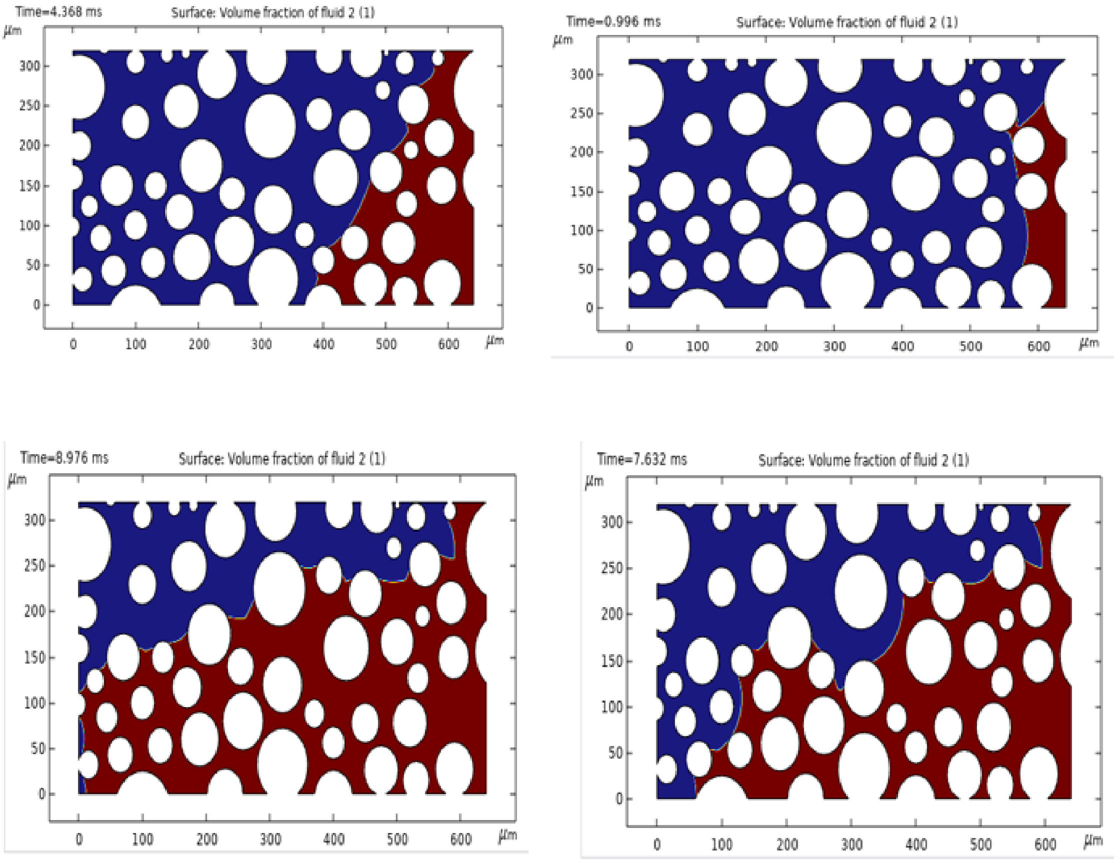

Figure 7. *Fluid Displacement for Simplified Model at contact angle 30.*

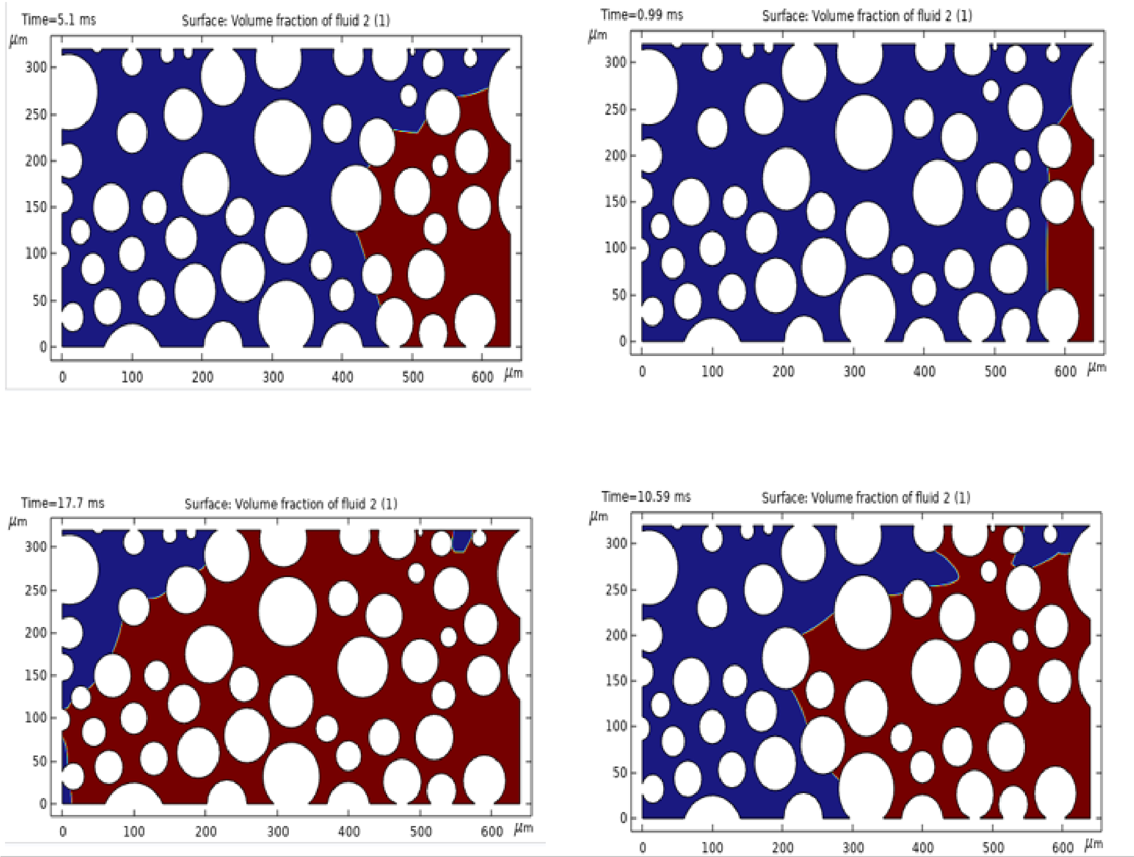

Figure 8. *Fluid Displacement for Simplified Model at contact angle 60.*

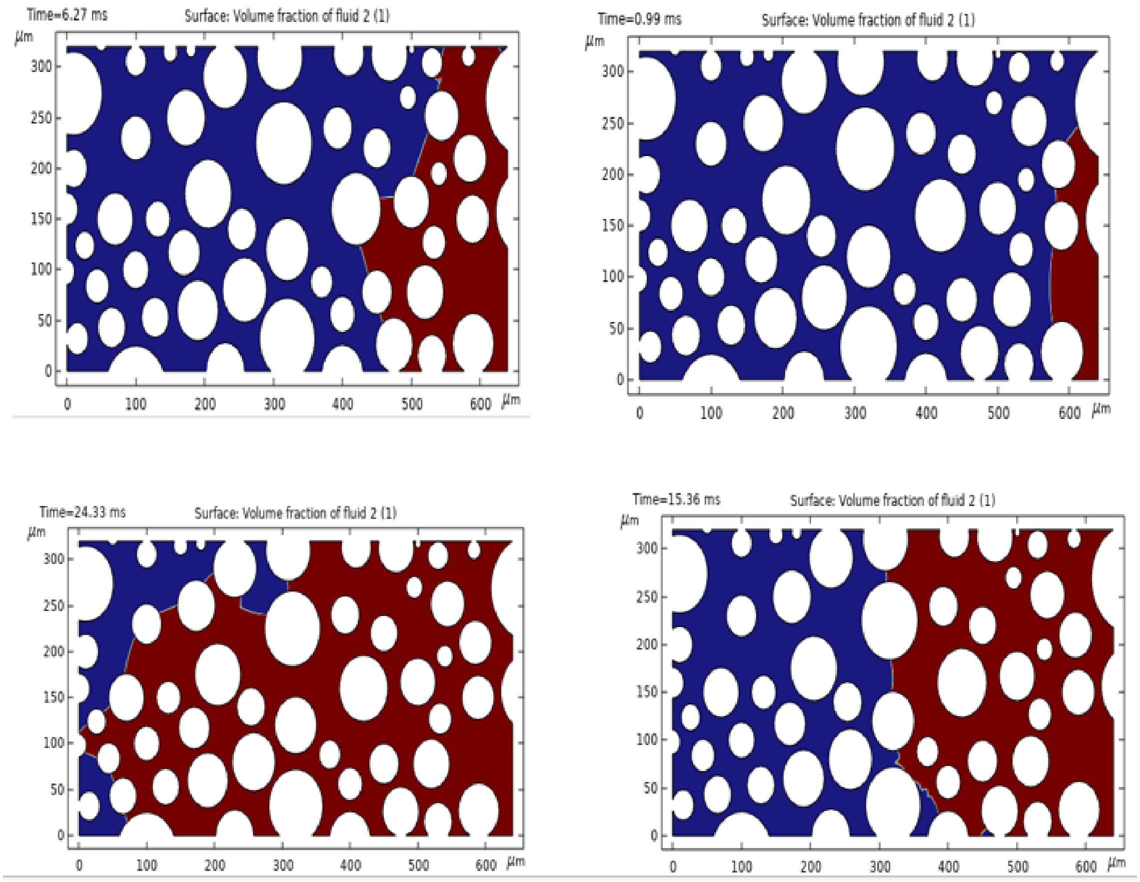

Figure 9. *Fluid Displacement for Simplified Model at contact angle 75.*

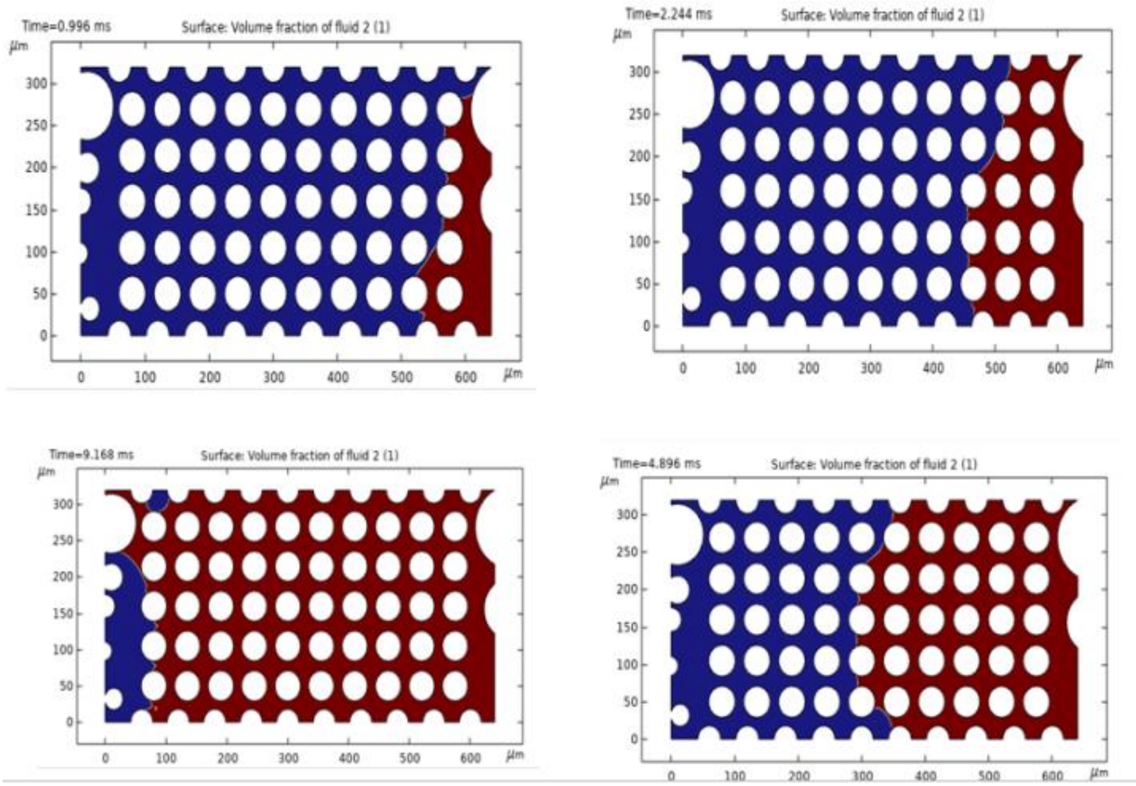

Figure 10. *Fluid Displacement for homogeneous Model at contact angle 30.*

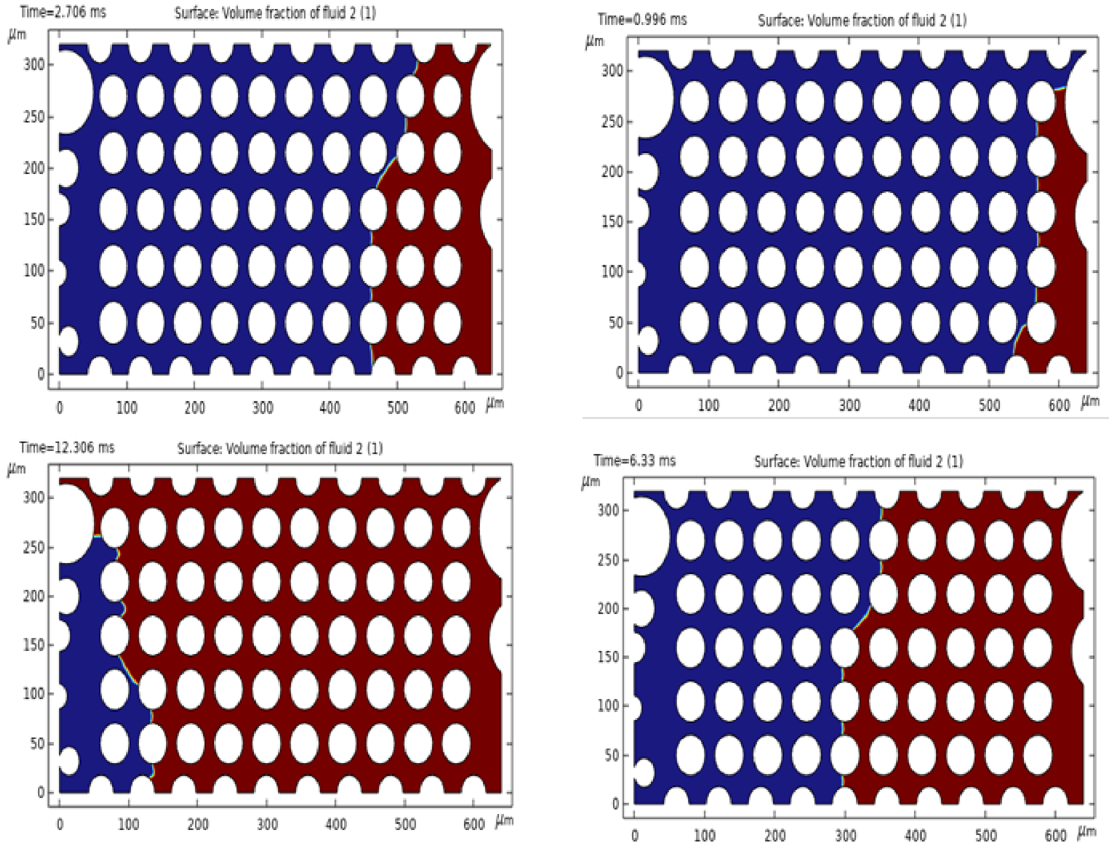

Figure 11. *Fluid Displacement for homogeneous Model at contact angle 60.*

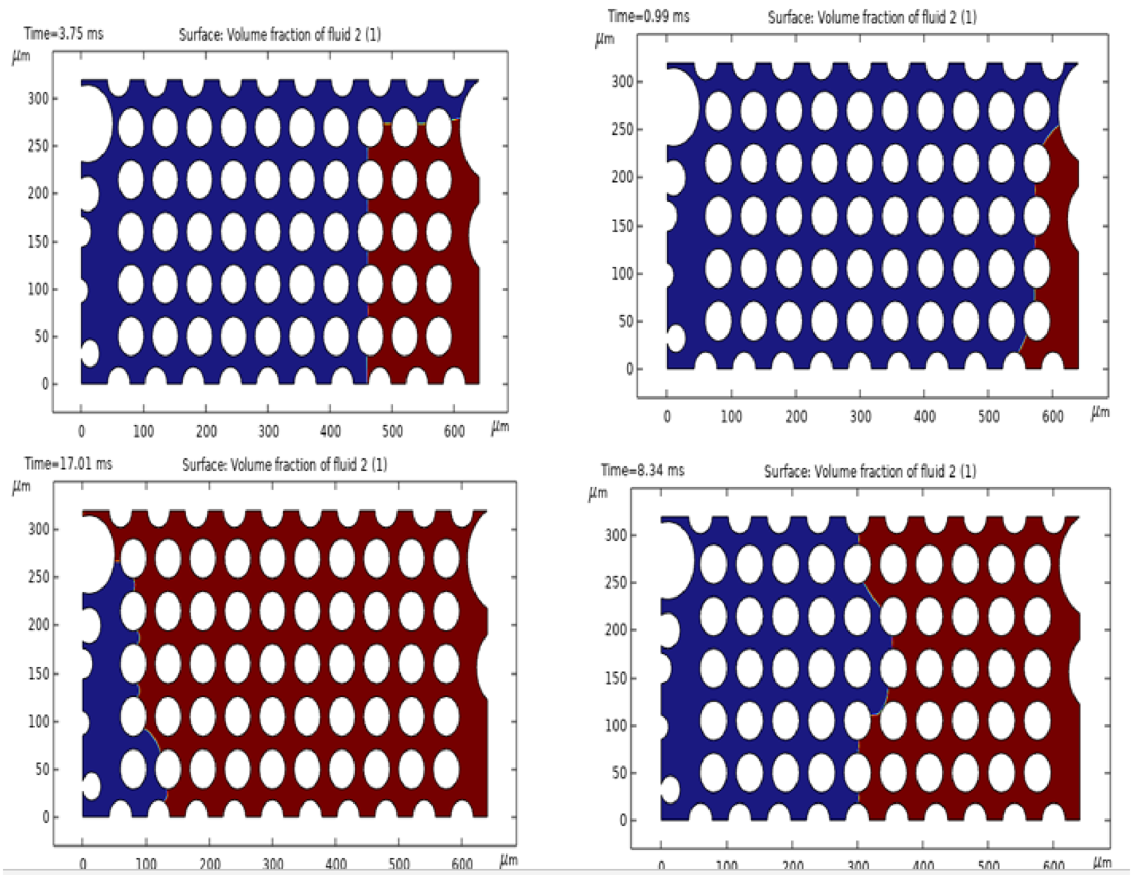

Figure 12. *Fluid Displacement for homogeneous Model at contact angle 75.*

Regarding the impact of wettability on relative permeability, the modified JBN method provided detailed permeability curves for water and gas across all models. As evident from the figures (Figures 13-15), as the structure of the pores becomes more complex, the relative permeability of water increases, while the relative permeability of gas decreases. However, the relative permeability of gas does not exhibit significant changes, and the difference in relative permeability of gas is the same across all three models. Additionally, the graphs indicate that with increasing wettability, the relative permeability of water increases, and the relative permeability of gas decreases, which aligns with findings from previous studies. Specifically, the relative permeability of water in the realistic model at a wettability of 30 degrees and water saturation of 0.7 is 0.3623, while at the same saturation and a wettability of 75 degrees, it is 0.4156. The small variation in the relative permeability changes of gas and water may be attributed to the assumption of a water-wet medium and the relatively small differences in wettability, which result in minimal differences in the relative permeability of water and gas across the models. Furthermore, due to the ease of movement of carbon dioxide gas in all three structures, the relative permeability curve of gas appears nearly linear. However, since not all fluid is displaced from the medium, the sum of the relative permeabilities of gas and water at any saturation does not equal 1.

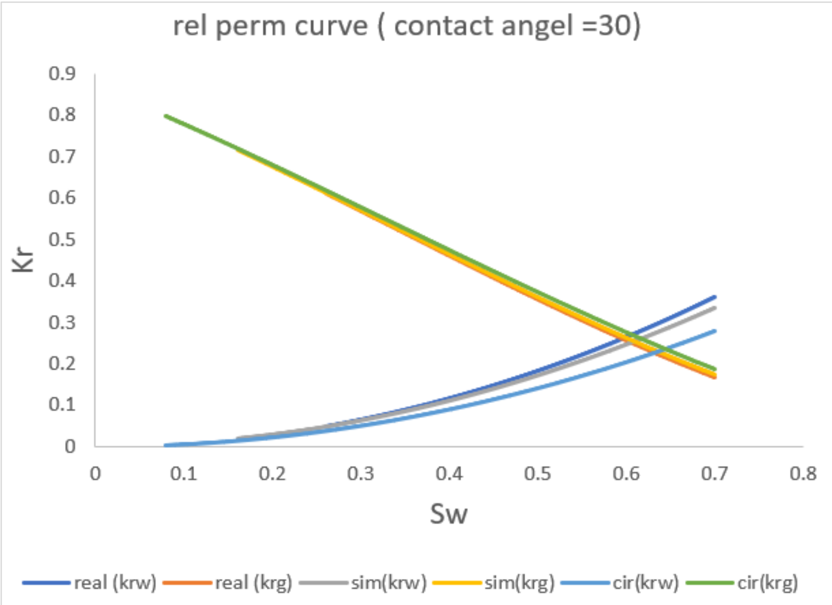

Figure 13. *Relative Permeability of Three Models at contact angle 30.*

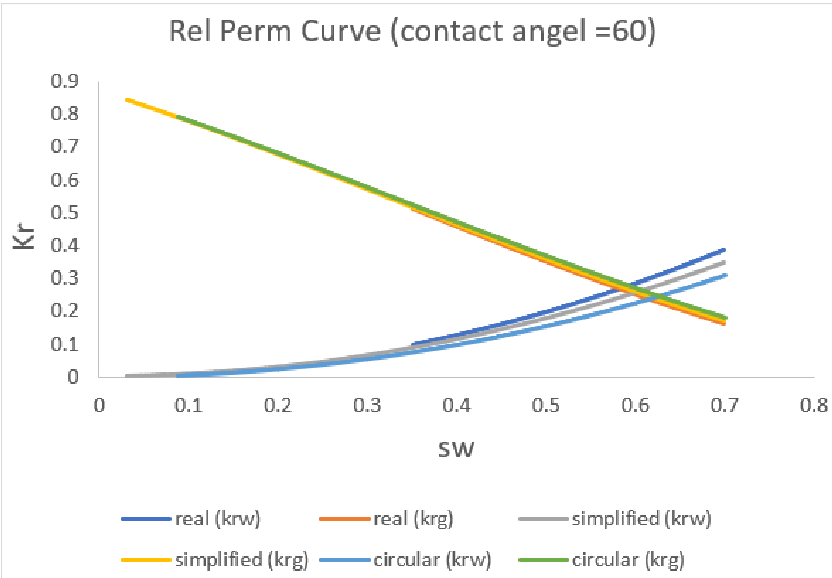

Figure 14. *Relative Permeability of Three Models at contact angle 60.*

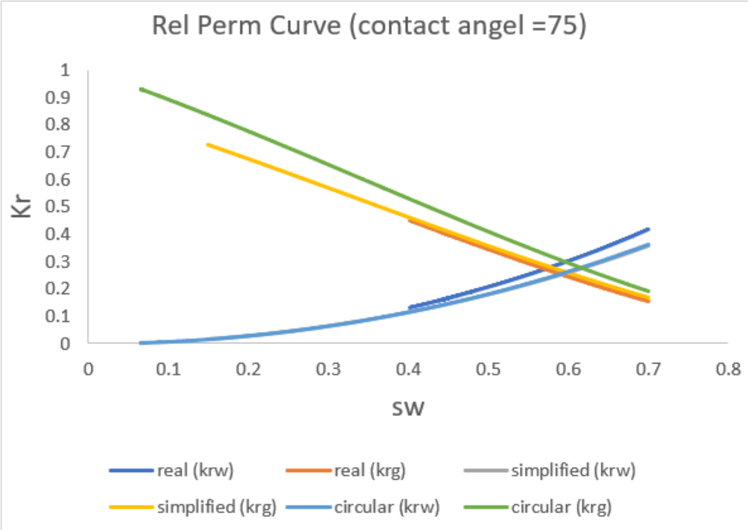

Figure 15. *Relative Permeability of Three Models at contact angle 75.*

4. Discussion

The findings of this study illuminate the critical roles of pore structure and wettability in governing CO_2-water displacement and relative permeability in porous media, addressing the research question of how these factors influence fluid dynamics at the pore scale. The observed trend of increasing breakthrough time and decreasing water recovery with greater pore complexity underscores the impact of structural heterogeneity on fluid trapping, likely due to elevated capillary pressures in intricate pore networks. Conversely, the homogeneous model's near-piston-like displacement suggests that uniform pore structures facilitate more efficient fluid flow, enhancing recovery efficiency. The increase in water relative permeability with higher wettability angles indicates that water-wet conditions promote water mobility, while reducing gas permeability, which aligns with (Green & Willhite, 2018). These results highlight the practical importance of tailoring CO_2 injection strategies to reservoir-specific pore characteristics, offering theoretical insights into optimizing enhanced oil recovery (EOR) and CO_2 sequestration by accounting for microscale fluid behavior.

The study's findings both corroborate and diverge from existing literature, enriching the understanding of two-phase flow in porous media. The higher water recovery in homogeneous models aligns with Ayatollahi et al. (2016), who reported reduced capillary trapping in uniform pore structures, suggesting that simplified geometries enhance displacement efficiency. Similarly, the increase in water relative permeability with wettability is consistent with Di et al. (2018), who found that water-wet systems favor water flow at higher contact angles. However, the unexpectedly higher recovery in the simplified model at 60° and 75° wettability angles deviates from Basirat et al. (2017), who noted consistent recovery declines with increasing wettability in complex media. This discrepancy may stem from the two-dimensional nature of the simulations could misrepresent three-dimensional flow dynamics. By systematically comparing three pore structures, this study extends prior research by Rokhforouz et al. (2019), offering a nuanced perspective on how structural complexity interacts with wettability to shape permeability and recovery, thus refining models used in reservoir simulations.

The study's reliance on two-dimensional pore-scale simulations presents a notable limitation that three-dimensional models would better capture the spatial complexity of real reservoirs, potentially altering recovery and permeability outcomes. The assumption of constant wettability throughout the simulations oversimplifies real-world conditions, where wettability may vary dynamically during CO_2 injection (Maaref et al., 2017). Additionally, the limited range of wettability angles (30°–75°) restricts insights into oil-wet systems, which are prevalent in some reservoirs. The potential numerical errors in the Level Set method, particularly affecting the simplified model's recovery trends, further highlight the need for robust computational validation. Future research should prioritize three-dimensional simulations to enhance accuracy and incorporate dynamic wettability models to reflect reservoir conditions more realistically. Exploring a broader range of wettability angles and grain shapes could further elucidate their impacts on fluid dynamics, advancing the predictive capabilities for EOR and CO_2 sequestration strategies.

5. Conclusions

This study successfully addressed the research question of how pore structure and wettability influence CO_2-water displacement and relative permeability in porous media at the pore scale. The simulations revealed that homogeneous pore structures yield the highest water recovery and shortest breakthrough times, while complex real models exhibit the lowest recovery and longest breakthrough times. Increasing wettability angles from 30° to 75° consistently delayed breakthrough and enhanced water relative permeability, with minimal impact on gas permeability across all models. The modified JBN method effectively quantified relative permeability, providing robust data on fluid dynamics in varied pore configurations. These findings confirm the significant role of structural complexity and wettability in governing two-phase flow, offering a clear empirical foundation for understanding fluid behavior in reservoir systems.

The outcomes of this research hold substantial implications for optimizing enhanced oil recovery (EOR) and CO_2 sequestration strategies, as they highlight the need to account for pore-scale characteristics in reservoir management. Practically, the higher recovery rates in homogeneous structures suggest that reservoirs with uniform pore networks may be prioritized for efficient CO_2 injection, potentially reducing operational costs and enhancing carbon storage efficiency. Theoretically, the study advances pore-scale modeling by demonstrating the utility of COMSOL Multiphysics in capturing nuanced fluid interactions, contributing to more accurate predictive models for reservoir performance. Future research should focus on three-dimensional simulations to better replicate real-world reservoir conditions and explore dynamic wettability changes to enhance applicability to diverse reservoir types (Jia et al., 2019). Investigating a wider range of wettability conditions, including oil-wet systems, and incorporating varied grain shapes could further refine these insights, paving the way for more sustainable and effective EOR and CO_2 storage practices.

Abbreviations

JBN	Johson Bossler Neumann
EOR	Enhanced Oil Recovery
CT scan	Computed Tomography Scan
MATLAB	Matrix Laboratory

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Dr. Masihi, a wise and erudite professor who has guided me in the pursuit of knowledge and understanding, and as the instructor of courses on fractured reservoirs and geostatistics, I have learned a great deal from them.

Author Contributions

Mohsen Masihi: Conceptualization, Resources, Validation, Supervision.

Abuzar Abdollahi: Data curation, Methodology, Formal Analysis, Investigation, Writing – review & editing.

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Data Availability Statement

The data is available from the corresponding author upon reasonable request.

Conflicts of Interest

The authors declare no conflicts of interest.

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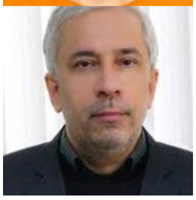
Biography

Abuzar Abdollahi atani is a graduate of Petroleum Engineering from Sharif University of Technology at the bachelor's level. He achieved the top rank in the university entrance exam for master's (2020) and doctoral programs (2024) and has also authored a book in the field of petroleum engineering.



Mohsen Masihi is a Professor of Petroleum Engineering at Sharif University of Technology in Tehran, Iran. He has established himself as a prominent academic and researcher in the field of petroleum and reservoir engineering, with a focus on areas such as reservoir modeling, fractured reservoir engineering, and statistical analysis for reservoir characterization. Academic Background: (1) BSc: Earned a Bachelor of Science degree with first-class honors and an award in 1993. (2) msc: Completed a Master of Science degree with an honor degree in 1995. (3) PhD: Received a full scholarship from the Ministry of Science, Research and Technology of Iran for PhD studies in Petroleum Engineering at Imperial College London, which he pursued in 2003. He ranked second in the national examination for PhD studies in Iran in 2002

Research Field

Abuzar Abdollahi: Petroleum Engineering, Reservoir Engineering, Enhanced Oil Recovery, Fluid Flow Simulation, Wettability Alteration.

Mohsen Masihi: Petroleum Engineering, Reservoir Engineering, Fractured Reservoirs, Enhanced Oil Recovery, Fluid Flow Simulation, Wettability Alteration, Reservoir Characterization, Spontaneous Imbibition.