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Perspective

Advances in the microscopic and mesoscopic simulation technologies developed for subsurface gas storage

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Abstract:
Subsurface gas storage refers to the practice of storing natural gas or other gases in underground reservoirs. It plays a crucial role in ensuring a stable and reliable supply of energy, especially during periods of high demand or supply disruptions. This work collectively highlights the significance of the microscopic and mesoscopic reservoir simulation techniques developed for subsurface gas storage. Specific technology progresses are demonstrated for a better storage of hydrogen and carbon dioxide, which meets well with the current focus on carbon reduction. In particular, molecular dynamics simulations can provide insight for the microscopic mechanisms affecting the adsorption and leakage of stored gas. Pore-network model generated using the advanced algorithm can determine the geological scenario for further flow and transport simulations.

1. Introduction

Subsurface gas storage is a critical component in the energy sector, providing a reliable way to balance supply and demand, especially with the integration of renewable energy sources (Pozo et al., 2023). As of the latest data, there are over 600 underground gas storage facilities worldwide, with significant capacity in North America and Europe (Caglayan et al., 2020). This represents a significant increase from previous years, indicating the ongoing expansion and importance of these facilities in energy management. The main types of subsurface gas storage include depleted oil and gas reservoirs, aquifers, and salt caverns (Wan et al., 2023). Depleted reservoirs are the most common due to their existing infrastructure and proven containment capabilities. Aquifers, though less common, provide large storage capacities. Salt caverns, while offering excellent sealing properties and high withdrawal rates, are geographically limited (Liu et al., 2023b). Natural gas storage is primarily used to manage seasonal demand fluctuations. During periods of low demand (typically summer), excess gas is injected into storage, and during high demand periods, the stored gas is withdrawn to meet consumption needs. This system ensures a steady supply and stabilizes prices.

Hydrogen is gaining attention as a carbon-free fuel alternative (Zhang et al., 2022). Large-scale hydrogen storage is primarily demonstrated in salt domes, but not all regions have suitable geological formations. Currently, hydrogen storage is being tested for its potential to provide long-term energy storage solutions that can balance intermittent renewable energy sources like wind and solar (Liu et al., 2023a). This involves storing surplus energy produced during peak generation periods and releasing it during periods of low generation research is focused on assessing the feasibility of using depleted gas reservoirs and developing technologies to mitigate risks associated with hydrogen storage (Liu et al., 2024). Specific challenges include understanding material compatibility and

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microbial interactions, and leveraging advanced technologies like sensors and reservoir simulators (Zhang et al., 2024). In addition, CO_2 geological storage, a key component of carbon capture and storage technologies, involves injecting captured CO_2 into deep geological formations such as saline aquifers, depleted oil and gas fields, or unmineable coal seams (Wei et al., 2023).

This work discusses the latest developments in the multi-scale modeling and algorithms that can be used for ensuring the safety and integrity of subsurface gas storage. Both the microscopic mechanism analysis of hydrogen leakage and pore-scale pore-network construction are presented to overcome the regulatory and technical challenges of hydrogen and carbon dioxide storage.

2. Lattice Boltzmann method simulation of gas flow in rock

Multiphase flows in porous media are commonly modeled using macro-scale simulations. These simulations solve the continuity equation in conjunction with momentum and species balances, utilizing constitutive equations such as Darcy's law. However, these models, which are predicated on the validity of constitutive relationships like the multiphase extension of Darcy's Law, require semiempirical parameters such as relative permeability. They also struggle to account for heterogeneity and the complexity of pore interconnectivity and morphologies. Consequently, macro-scale simulations may not always accurately represent effects associated with the microscale structure in multiphase flows. In contrast, pore-scale simulations can effectively capture heterogeneity, interconnectivity, and non-uniform flow behavior, such as various fingerings, which are challenging to resolve at the macroscopic scale. Furthermore, pore-scale simulations can provide detailed local information on fluid distribution and velocity, facilitating the development and validation of new models or constitutive equations for macroscopic scales.

Pore-network models serve as a practical and computationally efficient tool for comprehending multiphase flows at the pore scale. However, their predictive capability and accuracy are limited due to their reliance on simplified representations of the intricate pore geometry.

The lattice Boltzmann method (LBM) differs from traditional computational fluid dynamics methods, which rely on the resolution of macroscopic variables such as velocity, pressure, and density (Zhao et al., 2023). LBM is a pseudo-molecular method that monitors the evolution of the particle distribution function within a molecular assembly, grounded in microscopic models and mesoscopic kinetic equations. Macroscopic variables are derived from the moment integration of the particle distribution function. In LBM multiphase flow simulations, the fluid-fluid interface is not a sharply defined material line, but a diffuse interface of finite width. The effective slip of the contact line results from the relative diffusion of the two fluid components near the contact line. Consequently, there are no singularities in the stress tensor in LBM simulations of moving contact-line problems, while the no-slip condition is maintained. Unlike traditional computational fluid dynamics methods, LBM does not require complex interface tracking, capturing, or reconstruction techniques. Instead, the formation, deformation, and transport of the interface emerge from the simulation results. Moreover, LBM computations involve only local variables, enabling highly efficient parallel implementations based on simple domain decomposition. With the advent of more powerful computers, it has become possible to perform detailed simulations of flow in artificially generated geometries and tomographic reconstructions of sandstone samples.

3. Pore-scale pore-network models and their efficient construction

Pore-network models are helpful and easy to implement for studying fluid flow in porous media (Zhao et al., 2023). Traditional methods, like the maximal ball and medial axis methods, depend heavily on image resolution, affecting accuracy and computational cost. A novel pixel-free pore-network extraction method, called the Flashlight Searching Medial Axis (FSMA) algorithm, is proposed to better describe the geological information for reservoir simulations of subsurface gas storage. The FSMA algorithm overcomes these issues by operating in a pixel-free manner, providing a more efficient and resolution-independent approach.

The FSMA algorithm comprises several key steps. It starts with capturing medial axis characteristics. The medial axis is identified by the local maxima in the distance map, where the distance from a point in the void space to the nearest solid phase is maximized. This approach identifies critical points, which define the medial axis. The algorithm uses a steepest descent method to find the initial pore center and employs a flashlight searching technique in a fan-shaped region to update critical points along the medial axis, determining pore centers and throats. Similar to the two-dimensional approach but uses a cone-shaped searching region. The algorithm projects a cube onto a sphere for better discretization, identifying medial surfaces and axes more accurately. FSMA significantly reduces computational complexity compared to traditional methods.

Unlike pixel-based methods, FSMA is not affected by image resolution. Dimensionality reduction techniques significantly lower computational requirements. Besides, it accurately identifies pore centers and throats in both two-dimensional and three-dimensional porous media, handling complex shapes and structures effectively.

4. Molecular mechanism analysis of hydrogen leakage

Subsurface hydrogen storage is gaining attention due to increasing clean energy demands and the need for seasonal energy storage. It leverages physical and chemical methods to store hydrogen, with depleted oil and gas reservoirs being potential sites for such storage. A significant challenge in subsurface hydrogen storage is the potential leakage of hydrogen through the caprock, a layer intended to seal the storage reservoir (Yu et al., 2023). Hydrogen's small molecular size (< 1 Å) makes it particularly susceptible to leakage through nanopores in the caprock.

A molecular dynamics (MD) model and a combined MD-Monte Carlo algorithm are developed to investigate hydrogen leakage. These techniques provide detailed insights at the molecular level, allowing for the assessment of interactions and diffusion behaviors under different conditions. The simulations focus on caprock, a type of rock typically used to seal underground gas storage sites. Caprock samples are analyzed under conditions of varying moisture levels and the presence of residual gases like methane. The simulations are carried out to understand how hydrogen and methane molecules interact with the mineral components of caprock. This includes adsorption (how gases stick to surfaces) and diffusion (how gases move through materials). It can be also examined that whether different scenarios including dry and wet conditions, mimicking realistic underground environments where water presence can significantly affect gas behavior.

Understanding these molecular mechanisms provides valuable insights for designing more secure and efficient underground hydrogen storage systems, which are crucial for future energy solutions. Increasing water content in hydrogen storage projects can help mitigate leakage. The diffusion rates of hydrogen and methane through caprock were measured, which indicates that hydrogen tends to diffuse faster than methane under similar conditions. The presence of moisture significantly impacts diffusion rates. Wet samples exhibited diffusion coefficients approximately half of those observed in dry samples. This suggests that water within the caprock can impede the movement of hydrogen, potentially enhancing storage integrity. It has also been observed that hysteresis occurs in the adsorption and desorption processes of hydrogen. This means that the pathway of hydrogen entering the caprock differs from that of hydrogen leaving, which can affect the predictability of storage performance over time. By comparing hydrogen and methane behaviors, the MD study provides valuable insights for predicting the performance of gas storage systems. Methane's slower diffusion suggests it might be less prone to leakage, but hydrogen's higher diffusivity means that storage systems must account for its more mobile nature.

5. Conclusions

This study underscores the importance of microscopic mechanism analysis for subsurface gas storage. Understanding how hydrogen interacts with caprock under various conditions helps in developing strategies to mitigate leakage risks and ensure the long-term viability of hydrogen storage. The comparative analysis with methane also aids in transferring knowledge from natural gas storage practices to hydrogen storage applications. LBM has gained popularity as a tool for calculating flow in complex geometries, such as porous media. Beyond single-phase simulations, which, for instance, enable precise quantification of a porous sample's permeability, there are numerous LBM extensions available. These extensions facilitate the study of multiphase and multicomponent flows at the pore scale. A new pore-network construction method called FSMA algorithm represents a significant advancement in pore-network extraction methods, offering a more efficient, accurate, and resolution-independent approach. Its validation in various scenarios highlights its potential for large-scale applications in the subsurface gas storage scenarios.

Conflict of interest

The authors declare no competing interest.

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