2021-2022 Grand Challenge Award Final Report

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Research Award Title: **Decarbonatization While Increasing Oil Production Using CO_2**

Research Summary

Carbon capture utilization and storage (CCUS) provides a key opportunity to reach climate change goals and enhance US energy security. One example of such projects is PetraNova, Texas. PetraNova has installed post combustion CO_2 capture on a 240 MW coal fired unit at the Parish power plant near Houston, Texas where 80 MMcf/d of captured CO_2 is transported and used for Enhanced Oil Recovery (EOR) at the West Ranch oil field. There is an estimate of 1.6 MM tonnes/year CO_2 emission captured and stored with over 60MM bbls of oil produced in one year.

The ability to efficiently model and predict the storage capacity and oil recovery potential will have a monumental impact in the future CCUS projects. We have the modeling capabilities to demonstrate the feasibility of storage and co-optimize the stored volume and produced oil recovery for specific geological storage sites. A summary of results is provided below.

Bayesian Optimization for Field Scale Geological Carbon Storage

We present a framework that couples a high-fidelity compositional reservoir simulator with Bayesian optimization (BO) for injection well scheduling optimization in geological carbon sequestration. This work represents one of the first attempts to apply BO and high-fidelity physics models to geological carbon storage. The implicit parallel accurate reservoir simulator (IPARS) is utilized to accurately capture the underlying physical processes during CO_2 sequestration. IPARS provides a framework for several flow and mechanics models and thus supports both stand-along and coupled simulations. In this work, we use the compositional flow model, which includes a hysteretic three-phase relative permeability model, accounts for thee major CO_2 trapping mechanisms: structural trapping, residual gas trapping, and solubility trapping.

Furthermore, IPARS is coupled to the International Business Machines (IBM) Corporation Bayesian machine learning algorithm - the Gaussian process regression, and then uses an acquisition function that leverages the uncertainty in the surrogate to decide where to sample. The IBM Bayesian Optimization Accelerator (BOA) addresses the three weaknesses of standard BO that limits its scalability in that IBM BOA supports parallel (batch) executions, scales better for high-dimensional problems, and is more robust to internalizations. We demonstrate these merits by applying the algorithm in the optimization of the CO_2 injection schedule in the Cranfield site in Mississippi, USA using field data. The optimized injection schedule achieves 16% more gas storage volume and 56% less water/surfactant usage compared with the baseline. The performance of BO is compared with that of a genetic algorithm (GA) and a covariance matrix adaptation (CMA)-evolution strategy (ES).

The results demonstrate the superior performance of BO, in that it achieves a competitive objective function value with over 60% fewer forward model evaluations.

The FluidFlower CO_2 International Benchmark Study

Successful deployment of geological carbon storage (GCS) requires an extensive use of reservoir simulators for screening, ranking, and optimization of storage sites. However, the time scales of GCS are such that no sufficient long-term data is available yet to validate the simulators against. As a consequence, there is currently no solid basis for assessing the quality with which the dynamics or large-scale GCS operations can be forecasted. To meet this knowledge gap, we have conducted a major GCS validation benchmark study. To achieve reasonable time scales, a laboratory-sized geological storage formation was constructed (the "FluidFlower"), forming the basis for both the experimental and computational work.

A validation experiment consisting of repeated GCS operations was conducted in the FluidFlower, providing what we define as the true physical dynamics for this system. Nine different research groups from around the world provided forecasts, both individually and collaboratively, based on detailed physical and petrophysical characterization of the FluidFlower sands.

The major contribution of this paper is a report and discussion of the results of the validation benchmark study, complemented by a description of the benchmarking process and the participating computational models. The forecasts from the participating groups are compared to each other and to the experimental data by means of various indicative qualitative and quantitative measures. By this, we provide a detailed assessment of the capabilities of reservoir simulators and their users to capture both the injection and post-injection dynamics of the GSC operations.

Offshore Long-term Storage of Carbon Dioxide as Hydrates

Carbon Capture and Storage (CCS) is a key technology to achieve net-zero energy systems. However, current carbon sequestration practices face significant challenges to ensure the safety of operations and minimize the probability of leakage. The formation of gas hydrates immobilizes CO_2 in the subsurface and reinforces long-term retention. The objective of this paper is to analyze the technical feasibility of sequestering CO_2 in the form of hydrates in offshore environments. A numerical study is conducted to simulate the evolution of CO_2 plume in saline formations under high-pressure and low-temperature conditions. In addition to hydrate formation, the study quantifies the effects of trapping mechanisms including structural, capillary, dissolution, and mineralization. The numerical model is based on non-isothermal, reactive transport, and compositional multiphase flow formulations. It employs an iteratively coupled non-isothermal pressure concentration scheme with geochemistry and phase behavior. The governing equations and solution schemes are provided.

The study analyzes different field injection strategies that mimic offshore depositional environments. The results from a 2D numerical model are benchmarked against an identical case in a commercially available reservoir simulator. A series of scenarios are presented to demonstrate the long-term offshore sequestration of CO_2 in the presence of hydrate formation. The first strategy simulates the injection of CO_2 into the hydrate stability zone after

water production. When the injection of CO_2 re-pressurizes the zone, hydrate formation occurs and traps the CO_2.
The second strategy simulates the injection of CO_2 at a depth below the hydrate stability zone. At this depth, CO_2 remains in the liquid phase due to the geothermal gradient. This allows CO_2 to travel upward into the hydrate stability zone, where it is trapped as hydrates.
The third strategy simulates a water-alternating-gas scenario below the hydrate stability zone, which establishes a convective system to maximize the capillary and dissolution trapping mechanisms.
For all strategies, the results support that CO_2 hydrates provide safe, long-term storage of CO_2 and favorable storage capacity in offshore environments. Additionally, the water-alternating-gas scenario achieves the highest amount of trapped CO_2 in the marine subsurface. This work demonstrates a capability to evaluate advanced large-scale CO_2 storage strategies in untapped environments. The novelty of this work also lies in the ability to model and quantify complex physicochemical processes for offshore carbon sequestration.

Publications

- Xueying Lu, Kirk E. Jordan, Mary F Wheeler, Edward O Pyzer-Knapp, and Matthew Benatan, “Bayesian Optimization for Field-Scale Geological Carbon Storage”, Journal of Computer Methods in Applied Mechanics and Engineering, 2022.
- Xueying Lu, Kirk E. Jordan, Mary F. Wheeler, Edward O Pyzer-Knapp, and Matthew Benatan, ”Bayesian Optimization for Field-Scale Geological Carbon Sequestration”, SPE Reservoir Simulation Conference, 2021.
- Bernd Flemisch, Jan N. Nordbotten, Martin Ferno, Ruben Juanes, Holger Class, Mojdeh Delshad, Florian Doster, Jonathan Ennis-King, Jacques Franc, Sebastian Geiger, Dennis Glaser, Christopher Green, James Gunning, Hadi Hajibeygi, Samuel Jackson, Mohamad Jammoul, Jiawei Lli, Stephan Matthai, Qi Shao, Catherine Spurin, Hamdi Tchelepi, Xi-aoming Tian, Denis Voskov, Yuhand Wang, Michiel Wapperom, Mary F. Wheeler, Andrew Wilkins, Abdallah Youssef, and Ziliang Zhang, ”The FluidFlower International Benchmark Study: Process, Modeling Results, and Comparison to Experimental Data”, under review, Journal of Transportation in Porous Media, 2023.
- Mohamad Jammoul, Mary F. Wheeler, and Mojdeh Delshad, ”Numerical Modeling of CO_2 Storage: Applications to the FluidFlower Experimental Setup”, under review, Journal of Transport in Porous Media, 2023.
- Tri Pham, Mohamad Jammoul, Mojdeh Delshad, Mary F. Wheeler, Tan Bui, and Quoc P. Nguyen, ”Offshore Long-term Storage of Carbon Dioxide as Hydrates”, abstract submitted, Annual Technical Conference and Exhibition, 2023.
- Mohamad Jammoul, Mary F. Wheeler, and Mojdeh Delshad, ”Field-Scale Modeling of Geological Carbon Storage”, Siam News, December 1, 2022.

Presentations made

- Mary F. Wheeler, Xueying Lu, Mohamad Jammoul, Kirk E. Jordan, Edward O Pyzer-Knapp, and Matthew Benatan, ”Bayesian Optimization for Field Scale Geological

Carbon Sequestration", in AAPG's Carbon, Capture, Utilization, and Storage Conference, 2021.

- Mohamad Jammoul, Mojdeh Delshad, and Mary F. Wheeler, "Numerical Modeling and Uncertainty Quantification of Geological CO_2 Storage", SPE Workshop: Oil and Gas Technology for a Net-Zero World, Austin, TX, January 24, 2023.