Optimizing CO_2 Injection Rates in CCS: A Bayesian Approach for Realistic Business Efficiency

Introduction

The adoption of Carbon Capture and Storage (CCS) technology is crucial for reducing CO_2 emissions, combating climate change and transitioning to a carbon-neutral future (Jarvis and Samsatli 2018). Endorsed by prominent institutions such as the International Energy Agency (IEA) and the Global CCS Institute, CCS plays a pivotal role in mitigating emissions from existing energy infrastructure, hard to abate industries and advancing low-carbon hydrogen production.

At its core, CCS technology involves the permanent geological storage of captured CO_2 in deep rock formations such as saline aquifers (Ji X. & Zhu C. 2015) and depleted oil or gas fields (Hannis S. et al. 2017). However, large-scale deployment in these locations requires a meticulously planned and executed storage Field Development Plan (FDP). This includes decisions on the location of CO_2 injection wells and potentially brine producers, balancing the injection schedule (CO_2 injection rate/brine production rate) while ensuring the integrity of the storage site and addressing complexities (Ismail I. & Gaganis V. 2023). Key risks include pressure buildup and geomechanical complications such as reactivated faults. If not managed properly, these risks can compromise the main objective of carbon sequestration, which is to ensure long-term containment and maintain cost-effective permanent storage (Rutqvist J. et al. 2007).

The current approach to address these challenges involves engineers conducting multiple simulations runs. These simulations consider sensitive parameters such as well location and injection/extraction rates for each CO_2 injector and water producer. Each run checks constraints (e.g., carbon storage mass within a specified injection interval) and adheres to subsurface technical policies (e.g., pressure buildup) while factoring in economic considerations to maintain project viability. Decisions regarding the current configuration and designing subsequent trials rely heavily on engineers' expertise and the time dedicated, as simulation is time-consuming .

To automate and improve the FDP, which must adhere to operational, managerial and economic constraints, automated optimization techniques are essential. This is particularly crucial for determining optimal well locations (Fotias et al., 2024) and designing efficient injection/production schemes. Subsurface flow optimization has proved to be very complex and cannot be resolved within a classical optimization framework by simply defining an objective function and using gradient methods. This complexity arises from the increased non-linearity of the problem and the imposition of technical policy constraints, such as preventing CO_2 migration beyond designated boundaries, which depend on various reservoir factors, including the formation's physical properties (e.g., local heterogeneity). The challenges increase when incorporating economic factors and market fluctuations, such as CO_2 market price variations and capture costs, potentially affecting project feasibility and economic viability. These factors can significantly impact project feasibility and economic viability, necessitating sophisticated optimization approaches that integrate technical, operational, and economic considerations seamlessly.

Various optimization methods have been explored to address the complexity of FDP design factors, using both derivative-based and derivative-free approaches. For example, Cihan et al. 2015 optimized well locations and pumping rates for pressure management in saline aquifers using a Constrained Differential Evolution (CDE) algorithm, successfully estimating optimal solutions for brine extraction wells in the reservoir and limiting local pressure along faults to a prescribed threshold. Similarly, Cameron and Durlofsky 2012 optimized injection well locations and strategies by minimizing the long-term fraction of mobile CO_2 trapped underground using a non-invasive gradient-free Hooke-Jeeves direct search method. Santibanez-Borda et al. 2017 and 2019 used the (non-linear) Simplex method to optimize injection strategies with surrogate models, achieving a significant increase in CO_2 storage capacity.

Despite advancement in computing power available, subsurface reservoir complexity makes running (typically fully implicit) simulations challenging, therefore even a single objective function evaluation is hard to get. Gradient-based methods require multiple evaluations per estimate due to the lack of an explicit expression of the objective function, while evolutionary algorithms need numerous evaluations as they rely on recent objective function values only. The high non-linearity of the system response, the abundance of local optima and the imposition of operational constraints has led the research community towards derivative-free optimization methods like Genetic Algorithms and Particle Swarm Optimization, unavoidably combined with various heuristics to achieve some moderate result.

On the other hand, proxy modeling serves as the optimal compromise between the two approaches. Clearly, a sequential design strategy for optimizing such a black-box objective function - without assuming any predetermined functional form – while exploiting the information from all preceding iterations emerges as the appropriate option. Bayesian optimization stands out as the suitable method for optimizing costly functions, such as CCS design, akin to its successful application in tunning hyperparameters of various Machine Learning (ML) models (regression, classification, and reinforcement learning), where each training exercise may require significant CPU time. Instead of providing a distinct solution, the Bayesian approach offers a (multi-dimensional) probability density function (pdf) of the objective function for all possible solutions, selecting the one with the highest probability. Once the pdf has been estimated, the optimal solution is obtained by applying rapidly any classic optimization method on the developed surrogate model of the objective function.

In this study, we investigate the application of Bayesian optimization (BO) to optimize the rate of CO_2 injection and brine withdrawal in CCS operations. This work builds on our previous research (Fotias et al. 2024), where BO optimized well locations. In that study, producers and injectors operated under group control policies, leading to a novel approach in applying the kernel function of the Gaussian Process, the surrogate model typically used in BO. Our focus now extends to optimizing injection and production wells rates. Building on those results, this work focuses now on optimizing the injection and production rates, addressing two critical issues to develop realistic storage schemes applicable at field level. Firstly, ensuring a constant total injection rate guarantees uninterrupted CO_2 injection as contracted with emitters, minimizing the need for intermediate storage. Secondly, producers no longer operate under group control policies. Instead of a constant, intuitively estimated target production rate based on the expected Voidage Replacement Ratio, producers in this study dynamically and independently adjust their target rates, thus guaranteeing the utilization of more degrees of freedom, necessary for achieving the goal of constant injection rate and establishing maximum CO_2 storing result. Apart from efficiently and realistically handling the black-box nature of the CCS design problem, the new approach constitutes a fully automated method which can be easily coded and embedded in commercial software solutions.

Methodology

Surrogate modelling aims at generating a predictive model through analytical expressions tuned to queried values of the hard to evaluate objective function. In this work, a stochastic surrogate modelling approach is used, the Bayesian Optimization (BO), which offers a robust framework for quantifying aleatoric uncertainty, arising from data collection noise or discrepancies between the actual reservoir and its digital twin, and epistemic uncertainty, stemming from a lack of data. BO is a global optimization method which efficiently constructs and updates stochastic surrogate models, most commonly Gaussian Processes (GP), making it suitable for CCS optimization.

Research in BO has focused on developing new acquisition functions, combining kernel functions, using gradient information, handling multiple objectives, and applying BO to discrete spaces. In our previous work (Fotias et al., 2024), a modified permutation invariant kernel function was developed to optimize CCS well placement under group control. Each time a new simulation was run to evaluate a test wells position configuration, the newly obtained objective function value (total CO_2 amount stored) was utilized to update the posterior distribution of the GP describing the black box objective function. Subsequently, the acquisition function approach was explored to identify the next configuration which should be tested to provide maximum improvement on the knowledge of the objective function, hence its optimum. As shown in Figure 1, although this solution led to optimal storage results, it did not achieve a constant (or at least periodically constant) total injection rate, which was shown to decay after 25 years of operation. Such a condition cannot be accepted by the emitters who contract a fixed amount of CO_2 to be transported and eventually stored on a yearly basis.

We build upon these foundations, to explore the optimization of well injection and production rates in this work. Firstly, the user is allowed to define the total injection rate schedule of their own according to the contracted amount and clients' availability. Subsequently, BO is utilized to optimally split this amount to all available injection wells over time, provided that the maximum bottom hole pressure is not violated. The producers are controlled by a group policy which lets them remove as much brine as needed to avoid excessive pressure buildup. In theory, huge amounts of CO_2 could be injected in a reservoir provided that producers keep withdrawing fluids. However, the amount of CO_2 permanently

stored would be limited since CO_2 breakthrough would appear very soon and recycling would kill the project. To account for that effect, the objective function in our approach penalizes the CO_2 amount returned to surface through recycling. This way, unrealistically high storage schedules are penalized and the method only provides the maximum amount of CO_2 which can be safely stored while honoring the emitters' schedule and minimizing recycling. Simply speaking, the method answers the question "how should we distribute among the injecting wells the CO_2 arriving on site while honoring the contracted amount and eliminating, or at least minimizing the recycled gas".
The rate of each producer doesn't depend on any predefined target, but it is rather defined to automatically control the developed pressure under additional, realistic constraints such as minimum bottom hole pressure (due to excessive production).
Various stochastic models of the unknown objective function which can be used in BO rather than classic GPs, are examined. Such models are Bayesian Neural Networks (BNNs) and models that are approximate Bayesian. BNNs can flexibly represent the non-stationary behaviour typical of the optimization objectives under study, discover similarity measures through representation learning for higher-dimensional inputs, and naturally handle multi-output objectives. Additionally, Monte Carlo acquisition functions, which only require posterior samples, significantly lower the barrier to using non-GP surrogates that do not provide closed-form predictive distributions.

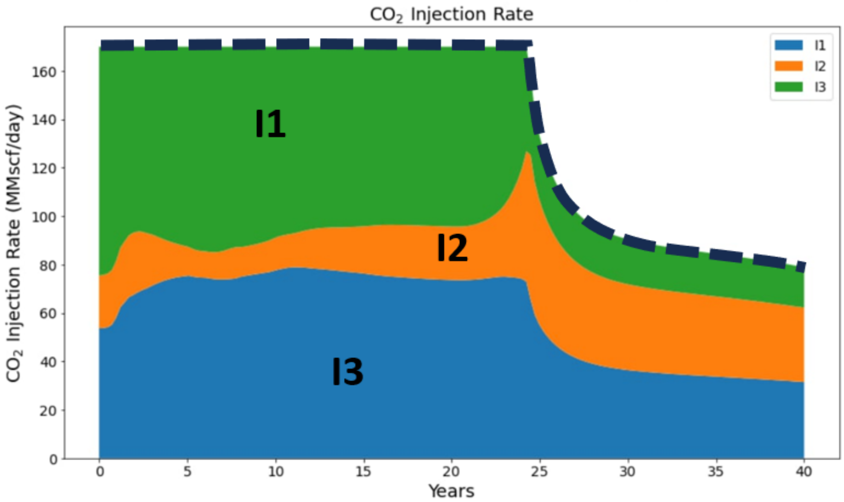

Figure 1: Maximum, time varying total CO_2 injection rate achieved using BO

Examples
The model of an inhomogeneous depleted oil field containing 3 injectors and 8 producers, with their location optimized following the guidelines in (Fotias et al. 2024), was used to further optimize the storage result after 40 years of continuous CO_2 injection. Given that 6 out of the 8 producers were located very close to each other, they were replaced by a single one lying in the middle to remove unnecessary degrees of freedom. Subsequently, the developed optimization method was run repeatedly to identify the maximum constant total injection rate which could be injected while leading to an affordable CO_2 recycling (up to 5%).
Despite the reduction on the number of the producers, the total number of decision variables was increased since they now include the target injection rate of each well at each selected timestep. When comparing the applicability of BNNs vs GPs, we were able to capture equally efficient solutions, although the former surrogate models are much simpler than the latter. Therefore, by further increasing the proxy complexity, it is expected that they will perform much better than GPs. The total injection rate remained constant throughout the period and all surrogate models successfully converged to a solution. Despite the reduction in the number of producers to three, we were still able to keep the injection rate constant. This successful result can be attributed to the newly acquired degrees of freedom resulting from the relaxation of the group control policy as well as the controlled CO_2 breakthrough. Figure 2 illustrates the CO_2 saturation (plume) after 40 years of storage, highlighting the optimal well locations determined by the initial BO run.

Conclusions

In this work, optimization of well injection and production rates in Carbon Capture and Storage (CCS) projects using Bayesian Optimization (BO) was explored. We expanded upon our previous research where a modified permutation invariant kernel function was developed for optimizing CCS well placement. Here, two key enhancements were investigated: tuning the target injection rates of injectors and removing the group control constraint on producers. Our findings demonstrated that by readjusting the injection rates from a fixed value, the optimization routine was allowed to explore alternative solutions, thus achieving improved results. This flexibility, coupled with relaxations on additional constraints on CO_2 breakthrough, led to improved performance of the CCS system.

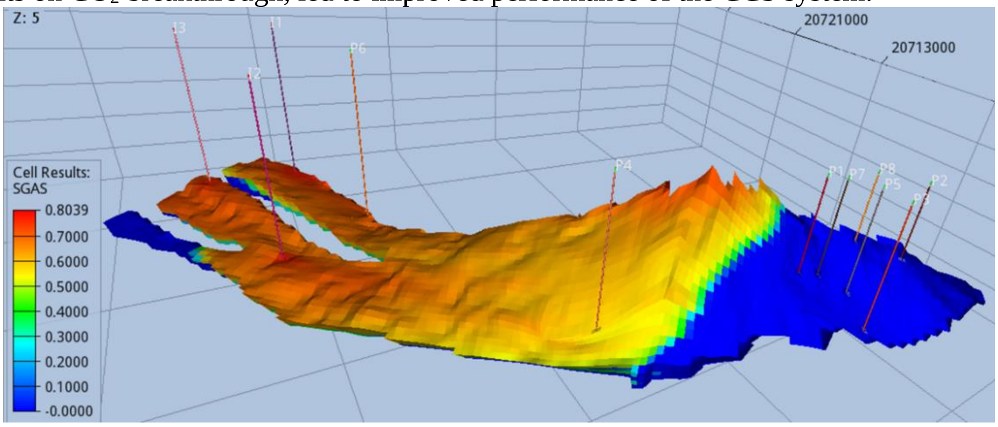

Figure 2: Gas saturation at the end of 40 years continuous injection

Moreover, alternative stochastic models were examined within the BO framework. BNNs, in particular, demonstrated promising results when it came to the increase of the number of the decision variables. Our results indicated that the optimized well locations and injection rates led to successful convergence of all surrogate models. Notably, despite the reduction in the number of producers from six to three, the production rates converged to viable solutions while meeting all Operator's constraints. These findings underscore the business value of leveraging BO for optimizing CCS operations, ensuring efficient resource allocation and operational excellence in carbon management strategies.

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