

Optimization Under Geological Uncertainties for CO₂ Injection in CCUS: A Case Study from the Lusitanian Basin

Introduction

The PilotSTRATEGY project, funded by the European Union's Horizon 2020 programme, focuses on advancing Carbon Capture, Utilization, and Storage (CCUS) technologies to mitigate CO₂ emissions. This study investigates optimizing CO₂ injection in the Q4-TV1 prospect of the Lusitanian Basin, offshore Figueira da Foz, Portugal.

The Lusitanian Basin's geological framework, characterized by Lower Cretaceous siliciclastic reservoirs capped by Upper Cretaceous limestones, offers promising conditions for CO₂ storage. However, the presence of a legacy well and intersecting faults poses risks, such as potential CO₂ leakage and reservoir pressure build-up, which necessitate advanced modelling and optimization strategies to ensure both safety and efficiency.

A high-resolution 3D static model, covering 1925 km² with a grid resolution of 250 m horizontally and 10 m vertically, was constructed in Aspen SKUA software using seismic data and information from legacy wells (Pereira et al., 2024). This research integrates the 3D static model, at the Q4-TV1 prospect location, into the dynamic modelling framework with Bayesian optimization under geological uncertainties.

Methodology

The work was undertaken in three phases to select and assess the optimal well location that provides the greatest CO₂ mass injection total while addressing the associated risks i.e., the long-term containment and safety of CO₂ injection in the Q4-TV1 prospect.

In the first phase, the Big LoopTM (Jonet et al., 2024) approach was executed to link the static and dynamic modelling domains in a unified framework, via a developed macro, utilizing the Aspen SKUA and Aspen Tempest ENABLE software. Then, a Bayesian optimization algorithm (Bordas et al., 2020) was also used with an objective function of maximizing the total injection mass of CO₂ over a 30-year injection period. The optimization process aimed to determine the maximum injected mass of CO₂ achievable by optimizing the X and Y coordinates of the injection well and perforation interval depth. To account for subsurface heterogeneity, at each well location, 16 geological uncertainties were varied, including statistical parameters from the interlinked porosity-permeability reservoir models, dependent on lithofacies variations, and two major faults intersecting the seabed, which were identified as potential risks for CO₂ leakage. These faults were modelled to evaluate their dual roles as barriers and conduits for CO₂ migration. In addition, the bottom hole pressure of the injection well was constrained to 165 bar to prevent reservoir fracturing. The optimization process simulated numerous simulation models, and those models where the CO₂ plume migrated to the legacy well and faults were disqualified even if they produced maximum injection totals. Phase one concluded with the selection of an optimal well location and perforation depth that maximised total injected CO₂ mass while maintaining the plume migration far from the legacy well and faults.

In phase two a further 450 appraisal simulations are run at the optimum well location varying all 16 geological uncertainties to better identify the uncertainty in total injected mass of CO₂. In addition and importantly, as part of Phase 2, the selected optimal scenario is modelled for an extended up to 1000-

years period to determine long-term containment and safety of the CO₂ plume, ensuring the plume stays away from the faults, and the legacy well.

In phase three, a sensitivity analysis is conducted on the optimal scenario derived from phases 1 and 2, to evaluate the impact of varying a set of parameters, including key parameters such as simulation bottom hole pressure target, anisotropy of reservoir permeability, and perforation interval.

Results

The performance of the Big Loop™ and Bayesian optimization processes resulted in a set of 948 scenarios. All scenarios were analysed to meet the defined criteria. This analysis underscores the variability of injection performance under geological uncertainties while affirming the stability and efficiency of the selected optimal scenario within the modelled constraints. The scenario Refine 200 shown in Figure 1 was considered as the optimal scenario, with a perforation length of 50m at the depth interval between 1177–1227 m. This strategic location (**Erro! A origem da referência não foi encontrada.**), situated 11.7 km from the legacy well and 8.7 km from faults, effectively minimizes the risks associated with fault interactions and potential leakage, ensuring the long-term stability of the CO₂ plume.

The probability distribution of total injected mass of CO₂, found from Phase 2, is shown in Figure 2, from which the P₁₀, P₅₀ and P₉₀ values were extracted. The P₅₀ percentile for total injected mass of CO₂ is 8.8 million tons with a maximum total injection mass of approximately 24 million tons.

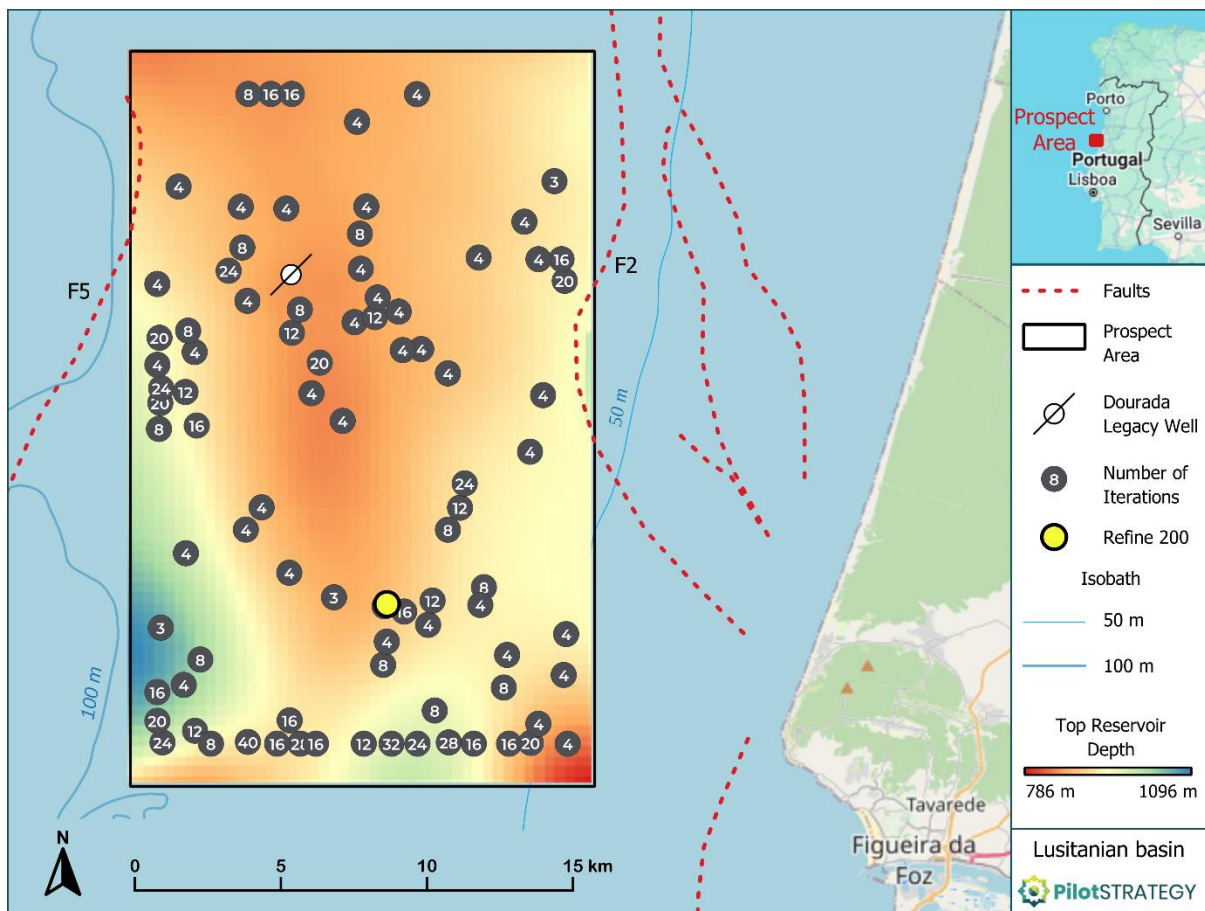


Figure 1 Map of the area of interest showing 948 scenarios for CO₂ injection well locations. Grey dots represent overlapping optimal scenarios for well placement. Scenario Refine 200, with a capacity of 24

million tons (optimal well location), is positioned further from the legacy well and faults, enhancing safety. The map also illustrates the depth of the top reservoir (shown in colour gradient).

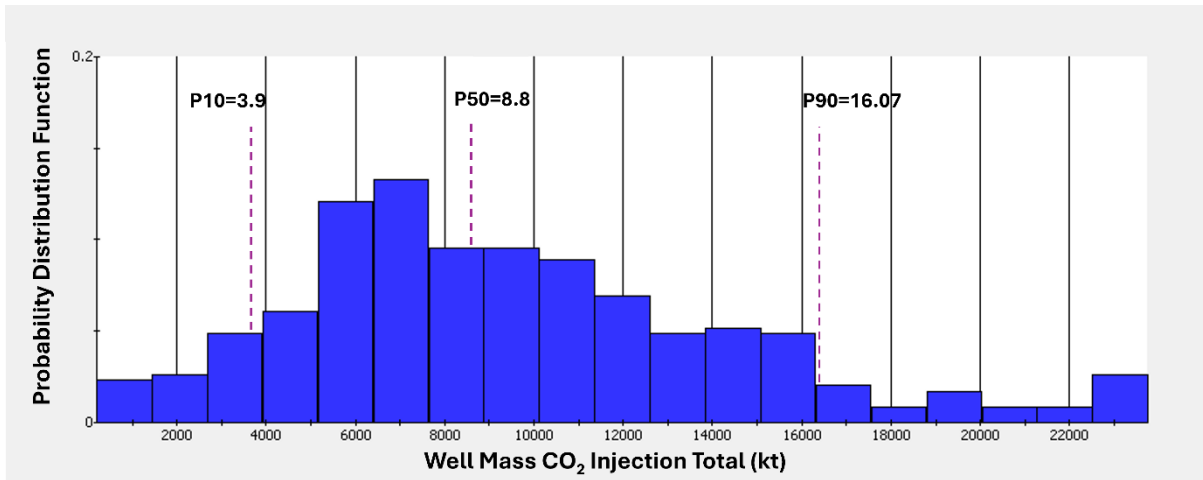


Figure 2 Probabilistic outcomes of CO₂ injection modeling showing the Well Mass Injection Total (wmassit) over a 30-year period. Key statistical values include Max: 23.7 million tons, P90: 16.07 million tons, P50: 8.8 million tons, P10: 3.9 million tons, and Min: 0.204 million tons.

Erro! A origem da referência não foi encontrada. 3 illustrates the gas phase saturation for Refine 200 after a 30-years injection period (Phase 1) and 1000-years continuous modelling (Phase 2), showcasing the CO₂ plume is stored according to the defined criteria. This outcome highlights the effectiveness of the proposed optimization and modelling strategy in achieving both operational efficiency and long-term safety in CO₂ storage.

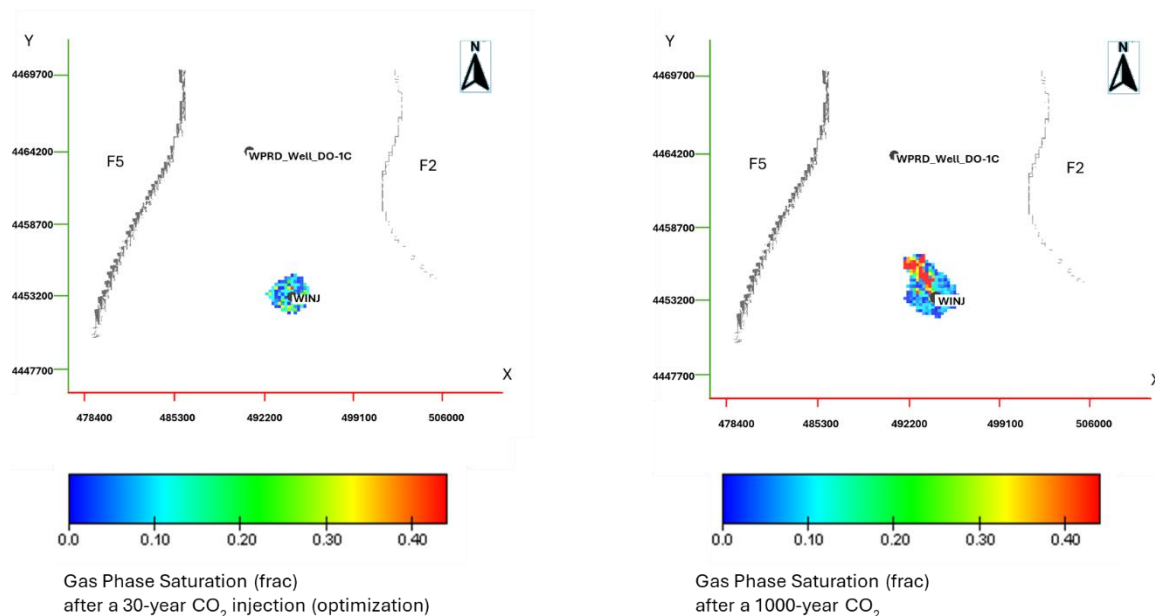


Figure 3 Gas phase saturation for Refine 200 after a 30-year CO₂ injection (optimization) period, indicating effective containment of the CO₂ plume away from the legacy well Do-1C and faults F2, and F5.

In the phase 3, a sensitivity analysis was undertaken . The sensitivity analysis indicated that the total injected mass was most sensitive to the bottom hole pressure target and perforation depth but also showed significant dependence on some of the key geological uncertainties.

Conclusions

The study successfully demonstrated the utility of Bayesian optimization integrated within the Big Loop™ approach for addressing geological uncertainties in CCUS projects. By incorporating static and dynamic uncertainties into a comprehensive probabilistic framework, this methodology enabled the exploration of multiple configurations and scenarios, leading to the identification of optimal solutions. The integration of stochastic modelling with advanced simulation techniques provided a robust and scientifically sound approach for enhancing CO₂ storage strategies in geologically complex settings.

The sensitivity analysis aids in identifying critical parameters that significantly impact injection performance, providing information for making informed decisions during the planning and execution phases of CO₂ storage projects. By focusing on parameters with the highest positive influence, operators can enhance the overall performance and efficiency of CO₂ storage, ensuring safety and effectiveness.

The findings of this work contribute significantly to the broader understanding of CO₂ storage optimization under geological uncertainty. The successful application of Bayesian optimization in the Lusitanian Basin underscores its global potential for advancing CCUS initiatives. The dynamic modelling and optimization framework developed here serves as a valuable reference for addressing similar challenges in other geological contexts, highlighting the critical role of data-driven, multidisciplinary approaches in the progression of CCUS technologies and the mitigation of climate change impacts.

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