Evaluating large-scale saline aquifers: Unlocking CO_2 storage in the Santos Basin through consistent multiscale analysis

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Summary

Regional-scale saline aquifers are promising candidates for geological CO_2 storage but present significant modeling challenges due to their vast extent, heterogeneity, and limited subsurface data. This study introduces a multiscale modeling framework that was applied to assess CO_2 storage in the Ponta Aguda saline aquifer (Santos Basin, Brazil, 40,000 km² area). Consistency of the multiscale models is checked by combining boundaries conditions for pressure match and verification of trapping mechanisms representativity. Four different methods were evaluated regarding the trapping mechanisms accuracy in coarse models: Local Grid Refinement, Effective Values, and Algebraic Dynamic Multilevel. Compositional simulations conducted with CMG-GEM and DARSim2 demonstrate that coarse-scale models systematically overestimate CO_2 trapping due to numerical artifacts, particularly in solubility and hysteresis behavior. These artifacts arise from mismatched CO_2/brine volumes in large cells, leading to artificially enhanced trapping efficiency. Among the evaluated methods, Algebraic Dynamic Multilevel delivers the most reliable predictions, providing a general solution that aligns closely with fine-scale reference simulations while remaining computationally feasible. The results show the importance of scale-consistent modeling approaches for accurate CO_2 storage assessment and highlight the risks of relying on overly simplified coarse models in the design and optimization of carbon storage projects in large saline aquifers.

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Introduction

Large-scale, regional saline aquifers, spanning through hundreds of kilometers, could be ideal candidates for CO_2 storage. However, for these giant fields, any quantitative assessment which requires detailed modelling and simulation of the process is significantly challenging due to the size of the heterogeneous formation. These include quantification of the storage capacity, near wellbore injectivity, CO_2 plume transport and trapping, and the security of the structural seals. Beside the scale of the system, the properties of these giant fields are quite unknown, due to the lack of commercial interests. As such, designing an optimal storage strategy from injection (location, number of wells, and their flow rates) to migration and distribution (heterogeneities and seals) and certainly to abandonment is a significantly challenging task. This becomes even further pronounced when highly nonlinear and hysteretic physics of the CO2 / brine / rock system is considered (Krevor et al. 2023, Wang et al. 2023, Lyu and Voskov, 2023, Hampson et al. 2023).

One of the most relevant requirements for an effective CO2 storage design is to adequately quantify the dominant trapping mechanisms that occur during the lifetime of the project. The simplest description includes the solubility of CO2 in brine, the residual trapping of immobile CO2 in a porous space, and the structural/stratigraphic trapping (Krevor et al., 2015). These mechanisms interact with each other, producing complex dynamics that is easily overlooked by the various types of simplification, from rock properties to fluid physics (Zhang et al. 2025). This effect is even more pronounced by the "*difficulties in characterizing and upscaling small-scale geologic heterogeneities*" (Zhang et al. 2025), leading to increased uncertainties and lower reliability of the quantitative analyses. Indeed, a typical approach in the literature has been to impose coarse grid blocks to be able to simulate the dynamics of the system in a timely feasible manner. However, during the development of coarse-scale 3D flow simulations, there is clear evidence of overstating the solubility and residual trapping mechanisms (Pickup, Kiatsakulphan and Mills, 2010; Ukaegbu et al. 2009; Doughty and Pruess, 2003). Unfortunately, these previous studies did not provide applicable solutions to resolve the simulation accuracy-efficiency trade-off. In fact, providing consistent results on coarse-scale models is a significant challenge for CO2 storage simulations, resolving which is relevant to all types of reservoirs but absolutely essential for regional giant saline aquifers.

One of these giant aquifers is the Ponta Aguda aquifer of the Santos Basin (Brazil), which is selected for the assessment of a carbon dioxide storage prospect and is hence our demonstration test case for the development of a novel framework applicable to model CCS in large-scale, regional aquifers. The total area of the aquifer is approximately 40,000 km^2. Within this area, a 400 km2 localized acreage must be characterized in detail. This smaller area is a prospect for a cluster of wells that are set to receive 5% of the regional emissions (6 million tons/year, or 240 million tons in 40 years). This would be a first phase for CCS development, with the potential to scale-up the project to store 25% of regional industrial emissions (30 million tons/year, or 1.2 billion tons in 40 years), by expanding the injection to a storage hub with an area of 4,000 km2.

Producing reservoir engineering models for such a huge area, including modeling the dynamics of CO_2 storage processes, is a significantly challenging multiscale problem. Modeling and understanding the overall behavior of the pressure in the entire aquifer is necessary, while detailed observation of plume transport and trapping must be generated at the project scale with high resolution around the wells. Global parameters, such as pressure and stress, are required to be assessed at the entire reservoir domain with high sensitivities to the boundary conditions. Transport, being a local parameter, requires sharp fronts, which demand for high resolution grids. Thus, it is necessary to develop a multiscale simulation strategy which is consistent on a regional (global) and localized scales.

Method

To maintain consistency across scales (Figure 1), three different strategies were applied to improve the representation of the trapping mechanisms, forming our basis for comparing multiscale results with the reference fine-scale solutions. Firstly, the Localized Grid Refinement (LGR) approach was employed, which is a well-established method for dealing with complex systems (Barbosa Machado, Delshad and Sepehrnoori, 2024; Syrakos et al. 2012) - here we extend it to CCS applications. Then, the Effective Value (EV) strategy was extended to CCS applications, which is based on tuning the parameters in the coarse scale, based on a fine scale solution (Durlofsky, 1991; King and Mansfield, 1999). Finally, the Algebraic Dynamic Multilevel (ADM) modeling approach, which has been originally developed for multiphase immiscible systems (Cusini, van Kruijsdijk and Hajibeygi, 2016), was extended to account for complex thermodynamics and compositional effects that control the migration of the CO2 plume in aquifers.

Simulations of CO_2 injection for storage in brine are performed by a compositional flow simulation (brine and CO_2 phases), on a consistent set of four models at different scales (using CMG-GEM software, version 2024.10 (CMG, 2024) in a 64-node computational cluster). The solubility of CO_2 in brine is computed by K-values equilibrium ratios, and it is assumed that there is no brine dissolved in the CO_2 phase. The residual trapping is modeled as a process derived from the relative permeability curves hysteresis. From these simulations, the participation of the trapping mechanisms after a migration period equal to the injection period is extracted. This period was assumed to be 40 years. The predicted CO_2 plume on the global scale is presented in Figure 1. Despite the wide range of results that can be extracted from simulating the models on different scales, this work will focus solely on analyzing the trapping mechanisms.

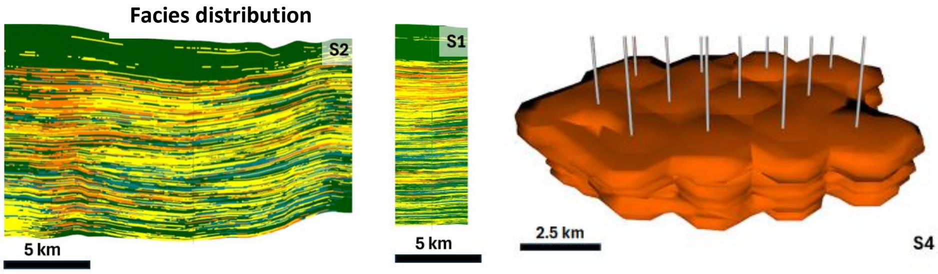

Figure 1. *Snapshot of geological heterogeneity on detailed scales (left) and global (S4) simulation results for CO2 plume evolution after 240 million tons injected (right).*

In addition to the CMG-GEM simulations, a representative 2D section and a homogeneous model were defined and simulated in the “DARSim2” flow simulator (https://gitlab.tudelft.nl/darsim ; Cusini, van Kruijsdijk and Hajibeygi, 2016) to ensure that the same behavior is found in different flow simulators and whether it occurs even in simplistic scenarios (homogeneous case), as well as the effect of the Algebraic Dynamic Multilevel (ADM) method on predictions, since this method was not implemented in CMG-GEM. The solubility and residual trapping by hysteresis in DARSim2 are modeled by the same principles as CMG-GEM.

When simulating a set of models constructed in different scales, it is important that at some point the results between scales must be checked for consistency, since the simulations are applied for different scales independently. The saturation distribution operates on a local scale, while the pressure distribution operates on a regional scale, so the information from both simulated scales must be connected (Hajibeygi, Lee and Lunati, 2012). This connection is made by defining boundary conditions to define the pressure dissipation on smaller scales accordingly to the pressure dissipation observed on larger scales. This consistency check step is called here a loosely coupled solution, as only the average pressure match is aimed through a volume flow instead of a full volumetric pressure distribution.

Results

There is a general bias in the representation of the trapping mechanism when using upscaled models: coarser grids lead to an overestimation of the solubility and residual CO_2 mechanisms, reducing the total amount of free CO_2 migrating in the reservoir (Figure 2). This is a relevant issue, since it would lead to an overoptimistic estimative in simplified models, which is the opposite of a best (robust) design practice.

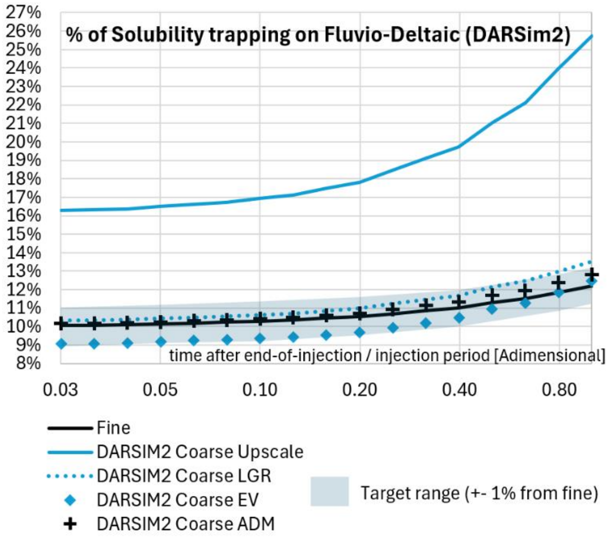

Figure 2 *Comparison of trapping mechanisms on fine grids vs different simplification strategies*.

This coarse grid effect is a numerical artefact that overstates the relevance of trapping mechanisms and has been observed by other authors in other specific scenarios (Pickup, Kiatsakulphan and Mills, 2010; Ukaegbu et al. 2009; Doughty and Pruess, 2003): It was confirmed even for a homogeneous scenario by this work. These artefacts are produced because larger cells combine a relatively small mass of CO2 and extensive porous rock volume, as soon as the injection started and enters the cell. These unbalanced volumes result in anomalous fast and effective trapping mechanisms as a numerical result of low CO_2 contents in contact with much larger volumes of water (solubility mechanism) and rock pore volumes (hysteresis mechanism), without the possibility of reaching saturation concentration that limits solubility. The overestimation of residual trapping seems higher on the larger scales because the facies are upscaled, which might produce a different spatial distribution of the facies.

Conclusions

Giant saline aquifers are naturally important candidates for CO_2 storage, but there are no tools available to produce the results needed for decision making in the correct resolution for each design question. The optimistic bias on typically imposed coarser models is a serious concern, since it challenges the reliability of the trapping assessments. Development of a generic and consistent multiscale approach is essential for these fields. A multiscale approach that seeks to only match the pressure distribution will fail to resolve the challenge of a reliable trapping assessment. Here, we develop and compare different multiscale scenarios. Among these, the ADM provides both generic and accurate trapping analysis framework which match fairly well with those obtained with the fine-scale reference simulations. As such, it is the method of choice for giant saline aquifers in which considerations of the reservoir multiscale heterogeneity and complex physics of CO2 are essential for reliable assessments.

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