



Global Climate & Energy Project
STANFORD UNIVERSITY

A Numerical Simulation Framework for CO₂ Sequestration in Subsurface Formations

Investigators

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Objective

The objective of this project is to build a numerical simulation framework that allows for the design, management and optimization of subsurface CO₂ sequestration operations. Using scaling analysis and high resolution simulation techniques, the dominant physical mechanisms associated with CO₂ injection and long-term storage in subsurface formations will be identified. Based on that knowledge, a numerical simulation platform will be developed. This platform will be modular and object-oriented, which will enable future extensions to be accomplished efficiently. The emphasis will be on numerical algorithms that are accurate and computationally efficient. This includes multi-scale methods capable of resolving the length and time scales that govern the complex interactions between the fluid system and the heterogeneous porous formation. In addition, adjoint-based procedures for the optimization of injection and long-term storage operations, which account for geologic uncertainty, will be developed.

Background

Several general-purpose simulation codes have been proposed as vehicles for the study of CO₂ sequestration in subsurface formations, especially in deep saline aquifers [1, 2, 3, 4]. An important example is the TOUGH2 family of codes, which are based on a general-purpose numerical approach for non-isothermal flow of multi-component multiphase fluids in porous and fractured media [2]. It has been extended to study CO₂ disposal into saline aquifers [5, 6].

Extension of compositional reservoir modeling capabilities to include processes of specific interest in subsurface CO₂ sequestration has been an active area of recent research. A prominent example is GEM [7, 8], which is an advanced equation-of-state compositional reservoir simulator. Using the GEM simulator, Kumar *et al.*, [9] found that trapping of CO₂ as a residual phase during the injection and post injection periods can be a very significant sequestration mechanism. They also concluded that the time scales for the key geochemical reactions are quite long - hundreds or even thousands of years.

Much work is needed, both in terms of developing a fundamental understanding of the physics and also in translating that understanding into a practical simulation framework for the design and optimization of large-scale CO₂ sequestration operations.

Approach

Physical Models: During the injection period, a number of effects are likely to be important, including convection, buoyancy, dispersion, dissolution and precipitation. The post-injection period also includes several interesting effects. These include: (1) very long time scales (compared to the injection period), (2) convection may not be a dominant mechanism of flow and transport in the post-injection period, (3) diffusion and dispersion effects may have to be modeled explicitly, (4) detailed understanding of density driven instabilities and the interactions with diffusion, geochemical reactions, dissolution, and solids precipitation is needed, and (5) the

effects of permeability heterogeneity must be quantified. A detailed scaling analysis of the CO₂ sequestration process will be performed covering both the injection and post-injection periods. The importance of the various mechanisms in the parameter space of practical interest will be delineated using high resolution numerical methods for flow and transport.

Adaptive Implicit Method: The adaptive implicit method (AIM) offers an excellent compromise between Implicit Pressure, Explicit Saturations (IMPES) and Fully Implicit Methods (FIM). AIM combines the large timestep size of FIM with the low computational cost of IMPES [10]. The approach is based on the observation that, in most cases, for a particular timestep, only a small fraction of the total number of cells in the simulation model requires fully implicit treatment, and that a simpler mixed implicit treatment (e.g., IMPES) is adequate for the great majority of cells. For each timestep in an AIM simulation, the variables (e.g., pressure, saturation, composition) are labeled implicit or explicit on a cell by cell basis. A stability analysis can be used to balance the size of the timestep with the target fraction of cells with FIM treatment [11].

Multiscale Finite-Volume Formulation: The multiscale character of the properties of natural porous media makes the problem of predicting flow and transport in such systems a natural target for multiscale methods, which have been an active area of interdisciplinary research. In this project we will employ and further develop adaptive multi-scale finite-volume (MSFV) methods for multiphase flow and transport in highly heterogeneous reservoirs. The MSFV framework would allow for accurate and scalable simulation of CO₂ sequestration processes in large-scale highly heterogeneous geologic porous formations. Currently, the MSFV approach is being extended to account for compressibility effects in nonlinear multiphase flows, buoyancy-driven miscible and immiscible counter-current flows, and the presence of wells in the domain. Further extensions will account for the physical mechanisms found to be of relevance to CO₂ sequestration. The MSFV should permit investigations into multiscale interactions (between, for example, flow instabilities and formation properties) with high resolution.

Optimization under Uncertainty: History matching (i.e., solution of the inverse problem) and optimization techniques have been shown to provide a prototype for real-time “smart” production operations in oil fields. These optimization procedures are able to account for geological uncertainty. The objective is to extend adjoint-based optimization methods for CO₂ sequestration and investigate the use of smart wells for the injection and storage periods. Smart wells could be used, for example, to optimize injection schedules or to maintain desired pressure or flow rate ranges within the formation. They also might enable CO₂ injection operations in favorable parameter ranges (and to avoid problematic flow regimes). In addition, optimization procedures could be used in the long-term storage period to effectively “stir” the *in-situ* CO₂ via targeted injection and production. Such a process might be able to alter the pressure and composition in a manner conducive to enhanced long-term storage.

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