



Probabilistic modeling and global sensitivity analysis for CO₂ storage in geological formations: a spectral approach



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ABSTRACT

This work focuses on the simulation of CO₂ storage in deep underground formations under uncertainty and seeks to understand the impact of uncertainties in reservoir properties on CO₂ leakage. To simulate the process, a non-isothermal two-phase two-component flow system with equilibrium phase exchange is used. Since model evaluations are computationally intensive, instead of traditional Monte Carlo methods, we rely on polynomial chaos (PC) expansions for representation of the stochastic model response. A non-intrusive approach is used to determine the PC coefficients. We establish the accuracy of the PC representations within a reasonable error threshold through systematic convergence studies. In addition to characterizing the distributions of model observables, we compute probabilities of excess CO₂ leakage. Moreover, we consider the injection rate as a design parameter and compute an optimum injection rate that ensures that the risk of excess pressure buildup at the leaky well remains below acceptable levels. We also provide a comprehensive analysis of sensitivities of CO₂ leakage, where we compute the contributions of the random parameters, and their interactions, to the variance by computing first, second, and total order Sobol' indices.

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1. Introduction

Carbon capture and storage (CCS) is an important topic related to the reduction of CO₂ pollution in the atmosphere. In general, CCS is process of capture and long-term storage of CO₂. Different variants for CO₂ storage are being explored, with the storage in deep underground formation such as oil fields, gas fields, abandoned mines, and saline formations being of highest interest. Various risks exist in CO₂ sequestration in deep underground formations, the most important being (i) CO₂ leakage through caprock failure, faults, and abandoned wells; (ii) structural failure due to large pressure peaks; and (iii) brine displacement and infiltration into drinking water aquifers. Quantification of the risks is of paramount importance for

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decision makers when evaluating the storage approaches before this technology can be implemented on large scale projects. In the case of deep geological storage of CO₂, there have been significant research efforts dealing with mathematical and numerical models for simulating the CO₂ injection processes into geological formations. Nordbotten et al. [1–3], presented in a series of papers the development of a semi-analytical model to describe the space and time evolution of CO₂ plumes and the leakage through abandoned wells. A reduced spatial dimension model based on vertical equilibrium was discussed by Nilsen et al. [4]. Ebigbo et al. [5] set up benchmark examples in order to compare different modeling approaches such as numerical and semi-analytical models, for the problem of CO₂ leakage. Class et al. [6] published a benchmark study, comparing a number of mathematical and numerical models with different complexities for problems related to CO₂ storage in geologic formations.

CO₂ sequestration is a complex multiphysics process, in which multiphase multicomponent flows play a critical role. The fact that the CO₂ should be stored for many thousands of years implies that full scale experiments are not possible, and computer simulation is the main approach for exploring the feasibility of different CO₂ storage options. However the mathematical models of underground CO₂ storage involve many sources of geological uncertainties [7,8]. These uncertainties are due to the limited knowledge about reservoir properties such as porosity and permeability. These sources of uncertainty lead to large variabilities in the predictive modeling of subsurface processes. Hence, one needs to propagate such uncertainties throughout the calculations to quantify their impact on results of computer simulations. This requires the use of stochastic modeling approaches.

Survey of literature on uncertainty quantification (UQ) for CO₂ storage. In [9] the authors utilize a stochastic response surface method for assessment of leakage detectability for CO₂ sequestration, by parameterizing the spatially heterogeneous reservoir permeability using Karhunen–Loève expansion. However, they used the analytical solution developed by Nordbotten et al. [2] to generate the pressure distribution at the injection zone, which is then used to calculate the leakage flux into a confined aquifer using Darcy's law. The analytical solution in [2] assumes that the phase saturations and fluid viscosities are constant within each zone, that the capillary effects are small, and that vertical equilibrium applies to the entire flow system. In [10], the authors use polynomial chaos (PC) expansions for probabilistic analysis of the CO₂ leakage rate in the CO₂ benchmark presented by Class et al. [6]. In that article, the authors use a number of simplifying assumptions to set up the mathematical model: fluid properties such as density and viscosity are constant, all processes are isothermal, CO₂ and brine are immiscible phases, capillary pressure is negligible and mutual dissolution is neglected.

The article [11] provides estimates of the risk of brine discharge into freshwater aquifers following CO₂ injection into geological formations and resultant salt concentrations in the overlying drinking water aquifers using arbitrary PC expansions combined with the probabilistic collocation method of [12]. Other works include [13,14] where the authors develop a screening and ranking method and a certification framework based on effective trapping for geologic carbon sequestration, for selecting suitable storage sites on the basis of health, safety, and environmental (HSE) risk resulting from CO₂ or brine leakage. Similarities and differences between radioactive waste disposal and CO₂ storage for performance assessment have been discussed in [15]. We also mention the paper [16] that presents a simple analytical method for the quick assessment of the CO₂ storage capacity in closed and semi-closed systems to assess the expected pressure buildup and CO₂ storage capacity in such potentially pressure-constrained systems.

Spectral methods for UQ. In the present work, we rely on spectral UQ methods to build a surrogate model for the nonlinear function that maps the uncertain model parameters to the model observables. In particular, we utilize PC expansions to build such surrogates. PC expansions, whose theory goes back to the late 30's and 40's [17,18], have become an increasingly popular tool in recent years as they provide efficient means for performing UQ in computationally intensive mathematical models; see e.g., [10,19–30] for a nonexhaustive sample of research contributions to numerical methods for UQ using PC expansions and applications of these methods to real world problems.

PC methods employ an approximation of the model variables in terms of a spectral expansion in an orthogonal polynomial basis. Once available, the PC representations can be used to efficiently approximate the statistical properties of the model outputs. Generally, there are two approaches for computing a PC expansion: (1) intrusive methods (see e.g. [19–24]) and (2) non-intrusive methods (see e.g., [24,25,31]). Intrusive methods require a reformulation of the original uncertain partial differential equations (PDEs) that govern the system, through a Galerkin projection onto the PC basis [32,33]. This entails the need for rewriting the existing deterministic solvers. Subsequently, one has to solve a larger system for the time/space evolution of the PC coefficients. Non-intrusive methods, on the other hand, provide a means to compute the spectral representation via a sampling of the existing deterministic solvers. In this paper, we will follow a non-intrusive approach to compute the coefficients in the PC expansion.

Our approach and contributions. Existing analyses of uncertainties in CCS using PC expansions, either rely on simplified physical models or do not rigorously establish the accuracy of the PC representations of the model observables used for uncertainty analysis. The goal of this article is to further the understanding of the impact of parametric uncertainties in the physical processes involved in CCS by using a more comprehensive physical model, a rigorous numerical study of the accuracy of the computed PC representations for the quantities of interest, and a comprehensive analysis of the impact of parametric uncertainties in the physical processes involved in CO₂ storage, in the benchmark geological structure under study.

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