Developing and Validating Simplified Predictive Models for CO₂ Geologic Sequestration

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Abstract

The objective of this study is to develop and validate a portfolio of simplified modeling approaches for CO₂ sequestration in deep saline formations – based on simplified physics and statistical learning – for predicting injection well and formation pressure buildup, and lateral CO₂ plume migration. Such computationally-efficient alternatives to conventional numerical simulators can be valuable assets during preliminary CO₂ injection project screening, serve as a key element of probabilistic system assessment modeling tools, and assist regulators in quickly evaluating geological storage projects. Detailed numerical simulation of such processes generally requires extensive reservoir characterization data and computational burden. In this context, validated simplified models can be valuable as they have minimal data and computational requirements in comparison. Simplified models that are based on the most relevant physical processes and validated against full-physics simulators are thus being sought after as efficient and useful alternatives for rapid screening and evaluation of CO₂ sequestration projects.

In the simplified-physics based approach, only the most important physical processes are modeled to develop and validate the predictive models. The system of interest is a single vertical well injecting supercritical CO₂ into a 2-D layered reservoir-caprock system with variable layer permeabilities. A set of well-designed full-physics compositional simulations is used to understand key processes and parameters affecting pressure propagation and buoyant plume migration. Based on these simulations, correlations have been developed for dimensionless injectivity as a function of the slope of CO₂-water fractional-flow curve and the variance of layer permeability values. The same variables, along with a modified gravity number and the nature of vertical permeability arrangement, can be used to develop a correlation for the total storage efficiency within the CO₂ plume footprint. Correlations are also developed to predict the average pressure buildup within the injection reservoir, as well as the pressure buildup within the caprock. These correlations are generally found to have good predictive ability. The predictive model formulations are also validated using results from two different simulations that were not used to develop the correlations.

In statistical-learning based modeling, two approaches are compared for building a statistical proxy model (meta-model) for CO₂ geologic sequestration from the results of full-physics compositional simulations. The first approach involves a classical Box-Behnken or Augmented Pairs experimental design with a quadratic polynomial response surface. The second approach uses a space-filling maxmin Latin Hypercube sampling (LHS) or maximum entropy design with the choice of five different meta-modeling techniques: quadratic polynomial, kriging with constant and quadratic trend terms, multivariate adaptive regression spline (MARS) and additivity and variance stabilization (AVAS). Simulations results for CO₂ injection into a reservoir-caprock system with 9 design variables (and 97 samples) are used to generate the data for developing the proxy models. The fitted models are validated with using a multi-fold cross-validation approach for three different
performance metrics: total storage efficiency, CO$_2$ plume radius and average reservoir pressure. The Box-Behnken–quadratic polynomial meta-model and the maximin LHS–kriging meta-model are found to perform almost the same.

One of the intended applications of simplified models is for performance assessment calculations, where the analyses are typically carried out in a probabilistic framework to deal with model and parameter uncertainty. It is therefore important to ensure that the simplified models are also capable of reproducing the full spectrum of uncertainty and sensitivity analysis results from detailed numerical simulators. A 97-run LHS design with the full-physics numerical model is used to generate the reference cumulative distribution function (CDF) of two key outcomes: plume radius and average pressure buildup in the reservoir. This is compared against CDFs from 10,000-run LHS designs with three different simplified models: (a) response surface from a Box-Behnken design and quadratic meta-model, (b) response surface from a maximin LHS design and kriging meta-model, and (c) simplified physics based methodology. The differences are quantified using two statistical measures: (1) Earth-movers distance and (2) Kolmogorov-Smirnov statistic. The statistical learning-based simplified models are found to provide a more robust representation of the reference CDF, particularly with respect to outliers.

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