Optimal Model Complexity in Geological Carbon Sequestration: A Response Surface Uncertainty Analysis

Award Number: DE-FE0009238

Prime Performer:
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Project Duration:
10/01/2012 – 09/30/2016

Performer Location:
Laramie, Wyoming

Program:
Carbon Transport & Storage

Project Summary:

The project aimed to investigate fundamental model complexity in representing coupled physical and chemical processes that accompany carbon storage operations in hierarchical subsurface geologic media. Specifically, the research focused on developing a simulation and upscaling methodology that is generally applicable to sedimentary environments that are characterized with multiple scales of permeability, heterogeneity, and diverse mineralogies. This included investigation of the effect of increasing reservoir permeability variance and depth on the uncertainty outcomes including optimal heterogeneity resolution(s) and investigation of the effect of mineral reactions occurring in the subsurface in geologic storage systems, including mineral volume fractions, reactive rate constants, reactive surface areas, and the impact of different geochemical databases.

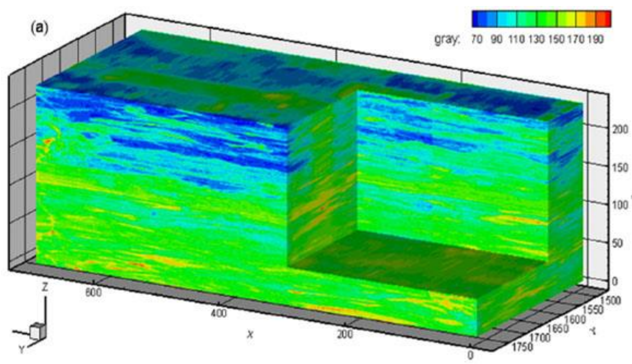

Figure 1: A large model with 3.25 million grid cells. Only the reservoir portion is shown. A region of the model is cut away to reveal its internal structure. Color represents the grayscale of the image obtained from the sediment experiment, with higher grayscale values indicating higher sand content and vice versa.

Project Outcomes:

In this study, an intermediate approach was proposed based on the Design of Experiment and Response Surface methodology, which consisted of using a limited number of numerical simulations to estimate a prediction outcome as a combination of the most influential uncertain site properties. The method was tested and verified on modeling long-term carbon dioxide (CO_2) flow, non-isothermal heat transport, and CO_2 dissolution storage by coupling two-phase flow with explicit miscibility calculation using an accurate equation of state that gives rise to convective mixing of formation brine variably saturated with CO_2. Geological carbon sequestration simulation was performed, yielding insights into the level of parameterization complexity that is needed for the accurate simulation of reservoir pore pressure, CO_2 storage, leakage, footprint, and dissolution over both short (i.e., injection) and longer (monitoring) time scales. Important uncertainty parameters that impact these key performance metrics were identified for the stratigraphic models as well as for the heterogeneous model, leading to the development of reduced/simplified models at lower characterization cost that can be used for the reservoir uncertainty analysis. To accurately model CO_2 fluid-rock reactions and resulting long-term storage as secondary carbonate minerals, a modified kinetic rate law for general mineral dissolution and precipitation was proposed and verified that is invariant to a scale transformation of the mineral formula weight. This new formulation will lead to more accurate assessment of mineral storage over geologic time scales.

Presentations, Papers, and Publications

Final Report: **Optimal Model Complexity in Geological Carbon Sequestration: A Response Surface Uncertainty Analysis** (December 2016) – Ye Zhang