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## Journal of Sustainable Mining

journal homepage: <http://www.elsevier.com/locate/jsm>

Research paper

## Impact of the capillary pressure-saturation pore-size distribution parameter on geological carbon sequestration estimates

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## ARTICLE INFO

## Article history:

Received 11 January 2017

Received in revised form

24 July 2017

Accepted 5 September 2017

Available online xxx

## Keywords:

Geological carbon sequestration

Numerical modeling

Capillary pressure

Saturation

Cost estimate

## ABSTRACT

Cost estimates for geologic carbon sequestration (GCS) are vital for policy and decision makers evaluating carbon capture and storage strategies. Numerical models are often used in feasibility studies for the different stages of carbon injection and redistribution. Knowledge of the capillary pressure-saturation function for a selected storage rock unit is essential in applications used for simulating multiphase fluid flow and transport. However, the parameters describing these functions (e.g., the van Genuchten  $m$  pore size distribution parameter) are often not measured or neglected compared to other physical properties such as porosity and intrinsic permeability. In addition, the use of average instead of point estimates of  $m$  for numerical simulations of flow and transport can result in significant errors, especially in the case of coarse-grained sediments and fractured rocks. Such erroneous predictions can pose great risks and challenges to decision-making. We present a comparison of numerical simulation results based on average and point estimates of the van Genuchten  $m$  parameter for different porous media. Forward numerical simulations using the STOMP code were employed to illustrate the magnitudes of the differences in carbon sequestration predictions resulting from the use of height-averaged instead of point parameters. The model predictions were converted into cost estimates and the results indicate that varying  $m$  values in GCS modeling can cause cost differences of up to hundreds of millions dollars.

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## 1. Introduction

Anthropogenic emissions of CO<sub>2</sub> are rapidly changing the gaseous composition of the atmosphere, and contributing to global climate change due to the demands for power production. Assuming the continued use of fossil fuels, geologic carbon sequestration (GCS) is considered to be the most promising storage option for the CO<sub>2</sub> produced, due to its high potential volume of sequestration, combined with manageable life cycle cost (Herzog, 2001; Ennis-King & Paterson, 2002; Herzog & Golomb, 2004; Pacala & Socolow, 2004; Bickle, 2009; Szulczewski, MacMinn, Herzog, & Juanes, 2012; Rogelj, McCollum, Reisinger, Meinshausen, & Riahi, 2013; Scott, Gillan, Markusson, Chalmers, & Haszeldine, 2013). The main geologic storage units are confined saline aquifers,

coal beds, depleted oil reservoirs, shales, and other reactive rocks that facilitate carbonate precipitation. Scientists and engineers around the world from countries including Australia, Canada, Japan, China, the United Kingdom, and many other member states of the European Union, are working on pilot projects and conducting research to develop economically acceptable full-scale facilities in the near future (Clean Energy Ministerial, 2012).

The Carbon Storage Program of the U.S. Department of Energy (DOE) aims to develop and advance technologies that will significantly improve the efficacy of GCS, reduce the cost of implementation, and lay the foundations for widespread commercial deployment between 2020 and 2030. Over the past few years, DOE alone has committed millions of dollars in funding to research in order to evaluate, improve, and engineer GCS for future full-scale operations (DOE, 2009; DOE, 2010; DOE, 2011; DOE, 2012). The first demonstration-scale test to inject 1 million metric tons (~32 kg/s) of carbon dioxide at a depth of 7000 feet in a saline formation over a three-year period began in Illinois in November 2011. The target saline formation, Mt. Simon Sandstone, is the

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thickest and most widespread saline reservoir in the Illinois Basin, which has an estimated CO<sub>2</sub> storage capacity of 11–151 billion metric tons (Illinois State Geological Survey, 2011).

Numerical simulations are important tools in evaluating the feasibility of GCS, and the design and operation of future storage systems (Birkholzer, Zhou, & Tsang, 2009; Gherardi, Xu, & Pruess, 2007; Han, Kim, Esser, Park, & McPherson, 2011; Jiang, 2011; Juanes, Spiteri, Orr, & Blunt, 2006; Nordbotten, Celia, Bachu, & Dahle, 2005; Obi & Blunt, 2006; Oldenburg & Doughty, 2011; Pruess & Garcia, 2002; Pruess et al., 2002; Wigand, Carey, Schutt, Spangenberg, & Erzinger, 2008). Among the four trapping mechanisms of CO<sub>2</sub> in the subsurface (structural, capillary, solubility, and mineral trappings), capillary or residual-phase trapping of CO<sub>2</sub>-rich fluids in pores is particularly important for geologic sequestration in dipping aquifers that do not have structural closure (Hesse, Orr, & Tchelepi, 2008; MacMinn, Szulczewski, & Juanes, 2011). After CO<sub>2</sub> injection stops, plumes of CO<sub>2</sub> gas begin to migrate into the adjacent water/brine saturated rocks, where the hysteresis of relative permeability can be important (Juanes et al., 2006; Oostrom, White, Porse, Krevor, & Mathias, 2016). Predicting the behavior of these CO<sub>2</sub> plumes depends upon our knowledge of the petrophysical parameters for CO<sub>2</sub> gas displacing water or brine in geologic materials (Doughty, 2007). However, estimates of these input parameters are limited and can vary across a wide range depending on the rock type of the target reservoir. Researchers and policy makers need accurate parameter estimates to evaluate the total amount of carbon that can be stored in a particular rock formation and to predict the redistribution of CO<sub>2</sub> following injection (Cheng et al., 2013; Doughty, 2007; Schnaar & Digiulio, 2009). Along with total porosity and intrinsic permeability, parameters describing the functional relationship between liquid saturation,  $S$ , and capillary pressure,  $P_c$ , are essential for modeling gas-liquid displacements (i.e. the prediction of the relative permeability functions for the wetting and non-wetting phases) in porous media. Because of their dependence upon interfacial tension and contact angle, these parameters vary depending on the particular combination of displacing and displaced fluids under different temperatures and pressures, and can change drastically.

## 2. Materials and methods

Capillary pressure-saturation function parameters are essential for modeling the geological storage of carbon dioxide, where brine is the wetting phase, and the supercritical CO<sub>2</sub> is the non-wetting phase. Parameter estimates need to be obtained by fitting equations to experimentally-determined data (Doughty, 2007; Heath, Kobos, Roach, Dewers, & McKenna, 2012). The van Genuchten (VG) (van Genuchten, 1980) and Corey equations (Brooks & Corey, 1996; Corey, 1954; Mualem, 1976) are commonly used in fitting experimental data and extracting the saturation function parameters (White & Oostrom, 2003):

$$S^* = \left(1 + \alpha(P_c)^{1/(1-m)}\right)^m \quad (1)$$

$$K_{rw} = (S^*)^{0.5} \left\{1 - \left[1 - (S^*)^{(1/m)}\right]^m\right\}^2 \quad (2)$$

$$K_{rn} = [1 - (S^*)^2] \cdot [1 - (S^*)^2] \quad (3)$$

where  $S^*$  is the normalized water saturation,  $m$  is an empirical pore-size distribution parameter,  $\alpha$  is the inverse of the entry pressure for the non-wetting fluid,  $K_{rw}$  is the relative permeability of the wetting phase, and  $K_{rn}$  is the relative permeability of the non-

wetting phase. Estimates of the parameters in Eq. (1) depend upon the height of the column used in the experiments. As a result, inverse modeling must be used to extract unique parameters for a physical point (Cropper, Perfect, van den Berg, & Mayes, 2011). The uncorrected parameters are non-unique and are referred to as height-averaged. Significant difference in the cumulative drainage of a sample column can be observed for variably-saturated flow simulations in response to step changes in applied pressure with point and average capillary pressure-saturation parameters (Fig. 1). Variations in the van Genuchten  $m$  pore-size distribution parameter on the capillary pressure-saturation and relative permeation functions can be very significant as shown in Fig. 2.

To the authors' knowledge, only a few experimental  $S$  versus  $P_c$  data sets are available for CO<sub>2</sub> gas or supercritical CO<sub>2</sub> displacing water or brine in porous media. Chalbaud, Lombard, Martin, and Robin (2007) used x-ray imaging in carbonate rock to quantify water saturation profiles during multi-rate unsteady flow experiments, and then employed an inverse history matching approach to estimate  $P_c$  at all locations where  $S$  was measured yielding multiple point estimates of the drainage capillary pressure-saturation curve. The  $S$  versus  $P_c$  curves for CO<sub>2</sub> differed from those obtained for N<sub>2</sub> displacing water depending on the wettability of the rocks. Plug and Bruining (2007) used unconsolidated quartz sand with a pressure cell combined with dynamic flow conditions to measure the average saturation at different fluid pressures and temperatures during CO<sub>2</sub> injection and imbibition. The resulting hysteretic average saturation versus capillary pressure curves were compared to those obtained using immiscible N<sub>2</sub> and exhibited a pronounced pressure dependency. Their data suggests that the indirect approach can be applied to predict drainage curves, but that rewetting curves do not scale according to the interfacial tension when temperature and pressure change. The Stanford University group has used X-ray CT scanning to measure relative permeability functions for CO<sub>2</sub> and water systems, but no capillary pressure-saturation parameters were reported (Krevor, Pini, Li, & Benson, 2011; Pini, Krevor, & Benson, 2012).

As the number of projects evaluating GCS has grown, journal publications on numerical modeling of GCS are appearing at a rate of approximately 7–9 per month in comparing to 5–6 per month before 2013. Searching the Web of Science with the keywords “carbon dioxide”, “geological”, “storage”, and “modeling” returned

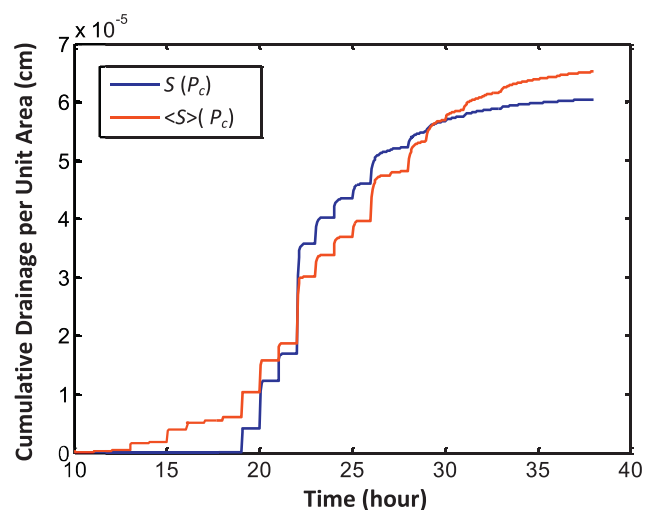


Fig. 1. Cumulative drainage of sample column in response to step changes in applied pressure simulated using both point,  $S(P_c)$ , and average,  $\langle S \rangle(P_c)$ , capillary pressure-saturation parameters in the STOMP numerical model for variably-saturated flow.

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