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Reducing uncertainty associated with CO₂ injection and brine production in heterogeneous formations

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Abstract

Spatial heterogeneity and variability across many orders of magnitude are two properties of formation permeability that are challenging to effectively capture in subsurface flow models. With regard to geological CO₂ storage, heterogeneity affects storage capacity, plume migration, pressure build-up around injection wells and, if utilized, the possibility of early breakthrough at brine extraction wells. Faced with under-characterized heterogeneity and an information-poor environment, the challenge is to make as much use as possible of the available data in reducing uncertainty associated with model prediction of a CO₂ injection operation. The two types of data used here to inform models are point permeability measurements from each well and interference tests between wells; these are both obtained from a synthetic permeability distribution approximating a hypothetical CO₂ storage formation. These data are used to reduce uncertainty in predictions of CO₂ injection, brine and CO₂ production rates, and CO₂ breakthrough times obtained from simulations of five-spot CO₂ injection/brine production performed on >600 conditional permeability realizations. First, assuming the underlying permeability field exhibits long-range correlation and a log-normal permeability distribution, a Bayesian analysis was undertaken using the point permeability measurements to reduce the likely magnitude of permeability heterogeneity. Comparison of realizations drawn from the prior and posterior indicate that the data were sufficient to exclude extreme scenarios with very rapid or very slow CO₂ transport and breakthrough at brine production wells. Thirty-year prediction envelopes for net CO₂ retention, brine and CO₂ production were reduced by 40, 45 and 72%, respectively. In the second stage, simulated interference tests for each of the posterior realizations were compared against interference tests simulated for the synthetic “true” permeability field. Weighting functions derived from these comparisons are used to further refine predictions, providing additional reductions of uncertainty by 38 and 69% for brine and CO₂ production rates, respectively. Predictions of CO₂ breakthrough are especially sensitive to analysis of interference tests, with a good estimate of the correct time obtained in three out of four cases.

Keywords

CO₂ geologic storage; permeability; heterogeneity; Bayesian; interference test

1 Introduction

Geological storage of carbon dioxide is one strategy for reducing emissions of greenhouse gases. One proposed method is the injection of liquid or super-critical CO₂ into deep formations, displacing the saline brine currently in place. Displaced brines are much less compressible than CO₂; consequently, injection is likely to be accompanied by increases in brine pressure at great distances from the CO₂ plume (Birkholzer et al., 2009). There are concerns that the overpressured brine may be displaced into freshwater aquifers at shallower depths (Oldenburg and Rinaldi, 2011; Keating et al., 2013), trigger earthquakes on critically-stressed faults (Cappa and Rutqvist, 2011; Zoback and Gorelick, 2012), or otherwise reduce the effectiveness of the CO₂ injection operation (Buscheck et al., 2012).

53 Recently, several methods have been proposed to manage reservoir overpressure through extraction of
54 some part of the saline brine. Active CO₂ reservoir management (Buscheck et al., 2012) suggests limiting
55 both the spatial extent and magnitude of the overpressured region by deploying brine production wells
56 at the periphery of the injection well-field. Numerical simulations of this approach at a 1:1 injection-
57 extraction ratio demonstrate the proposed reductions in pressure build-up, as well as an improvement
58 of the CO₂ injection rate (for fixed wellhead pressure). As an extension of this method, Dempsey et al.
59 (2014) suggested a zero-overpressure target for the reservoir and showed that this could be achieved
60 through brine production, a marching well configuration, and management of the surface wellhead
61 pressure (WHP) for CO₂ injection; however, this approach required much greater brine extraction ratios
62 than simulated by Buscheck et al. (2012), at least greater than 1:1.7. In contrast, Birkholzer et al. (2012)
63 proposed that brine extraction could be minimized by deploying wells to satisfy local performance
64 criteria, e.g., to provide pressure shielding for a known critically-stressed fault. In situations where
65 pressure-sensitive features are well-characterized, this method is particularly favorable for minimizing
66 the costs of brine treatment and disposal – variously estimated between \$0.40 and \$8.02/ton (Bourcier
67 et al., 2011; IEAGHG, 2012; Sullivan et al., 2013).

68 In any system with concurrent CO₂ injection and brine production, there will be some additional impetus
69 for the CO₂ plume to migrate in the direction of the low pressure zone created around the extraction
70 well. Eventually, the plume may impinge upon the extraction well and CO₂ would then be co-produced
71 along with the brine, reducing the efficiency of the storage operation. A particularly detrimental
72 scenario would be one in which the drilled injection and production wells both intersected the same
73 highly conductive feature, e.g., a fault or fracture zone. In this case, CO₂ breakthrough at the production
74 well may occur much more rapidly than expected, possibly requiring that the well be shut-in or
75 abandoned. Therefore, the issue of permeability heterogeneity is of economic significance to geologic
76 CO₂ storage in general, and pressure management schemes in particular.

77 In recent years, several studies have been published on the implications of permeability heterogeneity
78 for the effectiveness of CO₂ sequestration strategies. For the purposes of this overview, it is useful to
79 distinguish three types of heterogeneity (following Lengler et al. (2010)): structural, facies, and inter-
80 facies (the latter two are classified stratigraphic heterogeneity in Lengler et al. (2010)). Structural
81 heterogeneity is derived from faults or folds that impose permeability contrasts. For example, faults and
82 anti-clinal folds limit the lateral and vertical extent of a natural CO₂ reservoir at the Springerville-St.
83 Johns Dome in eastern Arizona (Stevens et al., 2001). Here also, structural permeability facilitates slow
84 leakage of CO₂ to the surface, as evidenced by travertine deposits along the fault trace (Gilfillan et al.,
85 2011) and elevated concentrations of dissolved CO₂ in the shallow groundwater (Moore et al., 2005;
86 Keating et al., 2014). Pasala et al. (2013) used numerical simulations to investigate end-member barrier-
87 and conduit-type faults; they found that reservoir compartmentalization by the barrier-types had a
88 positive impact on sequestration efficiency whereas the high-permeability conduits allowed the plume
89 to bypass parts of the reservoir and access overlying strata.

90 Heterogeneity at the facies level is related to the geometric and spatial distribution of high- and low-
91 permeability deposits (e.g., sand channels, muddy floodplains) in a sedimentary environment. At this
92 scale, it is often necessary to assume each facies is homogeneous and assign it a characteristic

permeability that may be common to all instances of that facies (Deng et al., 2012; Han et al., 2014) or drawn from a distribution (Flett et al., 2007). For instance, Flett et al. (2007) investigated heterogeneous permeability fields generated using indicator geostatistics and containing varying fractions of permeable sand and impermeable shale. They showed that with increasing shale content, lateral plume migration was promoted over vertical, and that residual trapping was impeded but CO₂ dissolution enhanced. Deng et al. (2012) also applied indicator geostatistics to generate 42 different permeability realizations, each comprised of 11 reservoir or seal facies, approximating conditions at the Rock Springs Uplift, Wyoming. Simulation of fixed pressure injection into 16 wells for a period of 50 years suggested potential CO₂ storage of between 420 and 700 Mt with corresponding displaced brine volumes between 340 and 630 Mt.

Han et al. (2014) investigated vertical and lateral migration of injected CO₂ through sequences of low permeability lenses. Similar to the approach adopted here, they first constructed a true permeability field (referred to as the deterministic case by Han et al. (2014)) and then supposed this field to be sampled at discrete locations by a series of drilled wells, as might occur in a field setting. Fifty permeability realizations, conditioned on the well data, were generated and a CO₂ injection scenario simulated for each. Prediction envelopes of mass distribution at various depths were constructed from the simulations and in most cases these were shown to bound the true – or deterministic – outcome. This approach demonstrated how sparse information from a particular site – such as might be obtained from well logging – can be incorporated into numerical simulations to provide a realistic bracket on the range of outcomes a particular sequestration operation might encounter.

The smallest-scale of permeability heterogeneity considered here is that occurring within a single facies. For instance, Lengler et al. (2014) investigated CO₂ transport within a sandy interval of the Stuttgart formation at the Ketzin injection site, Germany. They generated 29 permeability realizations for five different parameter sets, varying correlation length, standard deviation of the permeability population, and other parameters. In accordance with the findings of Flett et al. (2007), they observed enhanced rates of CO₂ dissolution as more of the reservoir was accessed by the plume. Contrasting these results against an equivalent homogeneous model, they found that storage capacity is underpredicted under the assumption of homogeneity but that CO₂ arrival at a nearby observation well was adequately predicted.

Of course, spatial heterogeneity is not the exclusive province of permeability; it is likely to be of varying importance to other material properties relevant for geological CO₂ storage, including: mechanical properties controlling damage, fracturing or fault failure; drainage curves and capillary trapping (Saadatpoor et al., 2010); and the lithological or brine composition relevant to CO₂-rock and CO₂-brine geochemical interaction. The study presented here will not consider these forms of heterogeneity.

The objective of this paper is similar to Han et al. (2014), in that, methods will be presented for incorporating site data to reduce outcome uncertainty for injection/production in a heterogeneous permeability environment. In contrast to Han et al. (2014), who investigated heterogeneity at the facies-level, here we confine our study to heterogeneity within a formation. This paper is organized as follows. Section 2 introduces two mathematical models for permeability heterogeneity and then discusses the

Fractional Brownian motion (FBM) concepts specifically applied in this study. At this stage, the particular permeability realization, k_{true} , to be used as an approximation to reality and for evaluating the efficacy of the developed methods, is introduced. Section 3 introduces our methodology, including details of the numerical model for CO₂ injection and brine production (3.1), Bayesian analysis of the permeability distribution (3.2), and the use of simulated interference tests for weighting model realizations (3.4). Section 4 discusses simulation results, beginning with simulated outcomes of the CO₂ storage operation for k_{true} (4.1), which are both the predictive goal and yardstick for success in this study. Two methods for reducing uncertainty and improving predictive accuracy are demonstrated: the first (4.2) contrasts predicted CO₂ injection and brine production rates, and CO₂ breakthrough times for a set of 324 Bayesian prior and 336 posterior realizations; the second (4.3) investigates the same outcomes when posterior realizations are weighted by a similarity measure between true and simulated interference tests. A summary of the developed methods, their advantages and limitations, is given in Section 5.

2 Permeability heterogeneity

For subsurface flow, permeability is the most important, most variable and least well-constrained material parameter (Matthews and Russell, 1967; Ingebritsen et al. 2010). Observations of permeability span many orders of magnitude depending on depth, lithology, measurement scale or degree of fracturing (Brace, 1980; Evans et al., 1997; Manning and Ingebritsen, 1999; Townend and Zoback, 2000). Importantly, permeability is heterogeneous, i.e., it is a spatially variable field. Permeability is also anisotropic, although this particular property is not investigated here.

Permeability heterogeneity is a rich field of study that has spawned advances in geostatistics (Johnson and Dreiss, 1989), analogue (Zhang et al., 2005) and numerical modeling (Kitanidis and Vomvoris, 1983), and uncertainty quantification (Lu and Zhang, 2004), while borrowing from fields as diverse as earthquake physics (Heffer, 2007), signal processing (Molz et al., 1997), and Bayesian statistics (Coptý et al., 1993). Permeability is said to be spatially correlated; this means that two permeability measurements, separated by a distance, L , are not independent of one another unless L is greater than the correlation length, L_{max} . Two common empirical models for quantifying this heterogeneity assume that L_{max} either has a finite value or that it is infinite, i.e., there is no correlation length. A commonly employed example of the latter is Fractional Brownian motion (Molz et al., 1997).

The correlation length, L_{max} , is often determined by fitting an exponential model to the variogram of geospatial permeability data; a finite correlation length is indicated by a plateau of the variogram. In situations where no plateau is observed, this indicates that either (1) L_{max} is finite, but the spatial extent of the data is not sufficient to reveal the correlation length (variogram plateau), or (2) L_{max} is infinite (FBM) and no plateau will be observed, even if additional data are gathered. While of considerable academic interest, this distinction is not practically important if investigations are confined to a domain of study that has dimensions less than the correlation length. FBM concepts can be developed and applied without penalty in such investigations, as will be done here.

2.1 A true, heterogeneous permeability field

Our intent is to develop methods that reduce uncertainty when injecting CO₂ into, or producing brine from, a formation with some underlying, but unknown, heterogeneous permeability distribution. For the purposes of assessing the accuracy of the methods developed here, it is useful to work with a synthetically-generated “true” permeability field, k_{true} , that might be an acceptable approximation to some real permeability distribution, k_{field} , at a given CO₂ injection site. As for k_{field} , k_{true} can be sampled at discrete locations by “drilling” wells and can be further interrogated by simulating well interference tests. However, unlike k_{field} , k_{true} is known completely and, therefore, the outcome of a CO₂ injection operation into k_{true} is easily obtained by numerical simulation. The disadvantage is that any assumptions built into the synthetic generation of k_{true} may not necessarily be true for every k_{field} .

In generating the particular k_{true} used in this study (Figure 1A), the following assumptions were made:

1. Permeability is spatially correlated for distances less than ~3 km; this is sufficient to constrain a domain of study that includes a generic 5-spot well pattern for which CO₂ injection and brine production will be simulated. In an analogue modeling study of scaled depositional environments in sedimentary basins, Zhang et al. (2005) demonstrated spatial correlation over distances of 3 km in 8 out of 10 sampled regions, so this assumption is not unreasonable. Note, this neither precludes nor endorses a view that k_{field} is spatially correlated at lengths greater than 3 km, i.e., whether L_{max} is, or is not, finite.
2. A histogram of all permeability values has a log-normal distribution (Figure 1B). This is a commonly-observed feature of many compiled permeability datasets (Snow, 1970; Leary and Al-Kindy, 2002).
3. A power spectrum, $S(f)$, computed from the Fourier transform of k_{true} (Figure 1C) has a power-law dependence on spatial frequency, f , i.e., $S(f) \sim f^{-\beta}$ where β is the spectral slope (in this case set equal to 1.4). Such spectral methods are often used to analyze FBM permeability distributions (Molz et al., 1997; Zhang et al., 2005) and compiled permeability datasets indicate that frequently $1 < \beta < 2$.

The particular permeability field, k_{true} , shown in Figure 1A was selected from an infinite set of permeability fields satisfying the above assumptions. We selected k_{true} based on the qualitative assessment that a five-spot well pattern would sample a variety of permeability conditions – high and low local permeability, high and low connectivities between wells – thus allowing us to demonstrate both the advantages and limitations of the methods developed in this paper for a variety of drilling outcomes. Here, high connectivity between wells implicitly refers to the presence of high permeability pathways that connect the wells and favors rapid flow between them.

Several features of k_{true} are derived from data for the Weber Sandstone formation at Rock Springs Uplift (RSU), Wyoming. RSU is the site of a proposed CO₂ injection operation and the Weber Sandstone would be one of the primary storage formations (Deng et al., 2012). Based on these data, we have assigned the log-normal permeability distribution (Figure 1B) a mean of -15 and a standard deviation of 0.91; however, we emphasize that advance knowledge of these parameters is not a requirement of the approach demonstrated here. Finally, following Deng et al. (2012), we assign porosity as a linear function of log-permeability, i.e., $\log(k) = 0.1937\phi - 1.2911$.

3 Methodology

The objective is to constrain as well as possible operational outcomes of economic significance for a CO₂ injection operation in which concurrent brine production is used to manage reservoir overpressure. The specific operational outcomes addressed here are: (1) the stabilized CO₂ retention and brine production rates at given operating wellhead pressure (WHP); (2) the timing of CO₂ breakthrough at brine production wells; and (3) the rate of CO₂ co-production after breakthrough occurs. The CO₂ retention rate is defined as the difference between rates of injected and co-produced CO₂. Each of these outcomes impacts the economic decision-making around the use, or not, of brine production wells.

For the heterogeneous permeability field designated k_{true} (Section 2.1), we consider a traditional five-spot scenario with CO₂ injection into a central well and brine production from four peripheral wells 1 km distant. In a practical CO₂ injection operation, siting of new wells would involve weighing specific geological, engineering or economic considerations. Furthermore, brine wells may be present in equal or fewer numbers to the CO₂ injection wells. Nevertheless, the five-spot configuration, with a high number of brine production wells, is conceptually simple and has the advantage of demonstrating a multitude of breakthrough outcomes, e.g., rapid versus slow. The methodology introduced here is not specific to any particular well pattern, although the degree of uncertainty reduction will depend on the number of wells drilled and the area they cover.

For the case of sequestration within a depleted oil or gas reservoir, existing wells are likely to be prioritized over the drilling of new ones. In this case, data on the production history of the field would be invaluable in characterizing permeability heterogeneity and the uncertainty quantification process. However, this scenario is fundamentally different to the one considered here: CO₂ injection into a deep saline formation for which previous utilization has been minimal or non-existent and consequently no wells or previous production history are available.

Injection and production are simulated for a period of 30 years. Operational outcomes (1)-(3) (defined at the beginning of this section) for the CO₂ storage simulation using k_{true} represent the goal of the developed predictive methods and thus also serve as a yardstick to quantitatively assess the efficacy of those methods. In all figures presented, operational outcomes obtained using k_{true} are denoted by thick red lines.

In a practical CO₂ injection operation, some limited information about k_{field} can be gathered; we assume the same information is available for k_{true} :

1. Point measurements of permeability at the locations where injection (k_0) and the four brine production wells (k_1 , k_2 , k_3 and k_4) intersect the storage formation. These measurements may be derived from either experiments on extracted core or by field-testing of the well, e.g. a push-pull pump test. In practice, they would be associated with an error; however, this is not accounted for in the methodology developed here. Furthermore, it is important to note that permeability observations depend on the scale of measurement; here, it is assumed that measurement of $k_0, \dots k_4$ is appropriate for the lateral scale of the grid-block to which it is assigned (~25×25 m). For the permeability field, k_{true} , the five point measurements are given in Figure 1A.

2. The average permeability between two wells can be estimated by conducting an interference test. In this case, each brine production well would be produced at a constant rate and the pressure drop at the shut-in, central injection well recorded with time. Once again, measurement error associated with this test is not accounted for in the developed methods.
3. The mean permeability, $\bar{k}_{true}$, of the formation (or, rather, the area enclosed by the five-spot pattern) can be estimated by combining the four interference tests, any other interference tests between production wells, and the five point permeability measurements. This measure is used to center the log-normal permeability distribution given in Figure 1B and any subsequent realizations. Any discrepancy between the measured and actual $\bar{k}_{true}$ is not accounted for in the developed methods.

There is one final parameter that affects operational outcomes of interest but is at present only weakly constrained: the standard deviation of the log-normal permeability distribution, σ_{true} (Figure 1B). As an approximation to σ_{true} , we have the sample standard deviation, σ_{smp} for the permeability point measurements $k_0, \dots, k_4$.

In the limit that $\sigma_{true}=0$, the log-normal permeability distribution (Figure 1B) becomes a delta function and the permeability field is homogeneous; under such circumstances, operational outcomes can be calculated with a high degree of confidence. However, it is generally recognized that formations are heterogeneous and that $\sigma_{true} \neq 0$. One consequence of this is the possible existence of fast pathways, e.g., between the injection well and brine production well 1 in Figure 1A. Importantly, the magnitude of σ_{true} tells us how fast these fast pathways potentially are.

3.1 Numerical model

Computer simulations presented here are performed using the Finite Element Heat and Mass transfer code [Zyvoloski, 2007]. FEHM uses a control volume approach to solve heat and mass flow of multi-phase mixtures of water and CO₂, and provides a variety of sub-models for specifying relative permeability and complex material property distributions. It also uses finite elements to solve for mechanical deformations coupled to the flow solution; however this capability is not required here.

The model comprises three layers: a single, horizontal storage formation, bounded above and below by impermeable aquitards ($k=10^{-19}$ m²). The storage formation comprises a single layer of grid nodes with vertical thickness 20 m; therefore buoyancy effects and vertical stratification between the CO₂ and brine are neglected. This allows us to maximize horizontal resolution, which is important for capturing permeability heterogeneity at different length scales as well as lateral plume migration – the two issues of primary interest. We use a linear relative permeability relationship with zero capillary pressure, consistent with analytical modeling studies for CO₂ plume evolution (e.g., Nordbotten et al., 2005). This simplification facilitates rapid forward modeling and multiple model realizations; however, such assumptions may not be appropriate in all situations (e.g., Court et al., 2012). In the methodology developed here, use of more complex physical models is not discouraged, although consideration of performance trade-offs is a necessity when performing multiple model realizations. While in actuality brine is here simulated as pure water, the term is retained for sake of convention. Model results are not expected to be significantly different for higher density brines.

Horizontally, the model grid spans $10 \times 10 \text{ km}^2$ and contains a $2 \times 2 \text{ km}^2$ area of high resolution ($24 \times 24 \text{ m}^2$) at its center. Initial formation conditions are 30 MPa and 100°C . At the lateral boundaries, pressures are maintained at initial conditions with any inflow occurring at 100°C . Both CO_2 injection and brine production are modeled as fixed pressure sources either 5 MPa above or below ambient pressure, respectively. In a practical situation, it may be required that the mass flow rate of the source, rather than pressure, be fixed (e.g., a fixed CO_2 stream from an emitter); however, under some operational circumstances fixed pressure injection may be unavoidable, such as when pumps operate at their maximum pressure due to pressure increase/drawdown around the well or when regulatory considerations impose a safe operating limit for pressures within the reservoir. In any case, for the simulations presented here, injection and production rates rapidly stabilize to near constant mass flow rates over a short period of time (< 1 year) compared to the simulation length (30 years).

Simulation of CO_2 injection and brine production for the permeability field k_{true} provides the set of true operational outcomes to be used in evaluating the predictive methods of this study. In addition, we perform a simulation for the equivalent homogeneous formation ($k = \bar{k}_{true}$) and for 660 different permeability realizations (denoted $k_{rlz,i}$, where $i = 1, \dots, 660$) that are, to greater or lesser extents, approximate representations of k_{true} .

3.2 Bayesian constraint of heterogeneity

As discussed previously, one challenge in devising representations of k_{true} is the poor constraint on the degree of heterogeneity, as parameterized by the population standard deviation, σ_{true} . The sample standard deviation, σ_{smp} gives us some information about σ_{true} ; however, before obtaining the permeability measurements $k_0, \dots, k_4$ from which σ_{smp} is derived, our expectations about σ_{true} must necessarily be constrained by prior experience, perhaps at different sites or for different formations or lithotypes. These expectations are expressed probabilistically as the Bayesian prior.

The Bayesian prior used in this study is a transformed gamma function (Figure 3A; see also Appendix A). It reflects an expectation that permeability probably varies by “some orders of magnitude” and the likelihood of a totally homogeneous formation is vanishingly small. The relatively wide nature of this prior reflects our ignorance of the likely value of σ_{true} ; however, as discussed by Gauch (2003), the “ignorance” prior is a versatile choice for calculating a Bayesian posterior.

While a uniform distribution is often used as an ignorant prior due to the fact that it is the maximum entropy distribution with support on a finite interval, we have elected to use a gamma distribution instead. Like the uniform distribution, the gamma distribution can also be characterized as a maximum entropy distribution (Park and Bera, 2009). In addition to the maximum entropy property, the gamma distribution was chosen for two reasons: (1) since we cannot provide reliable upper or lower bounds for the degree of heterogeneity, the prior distribution should have positive likelihood for any $\sigma_{true} > 0$; and (2) since there will certainly be some heterogeneity, the likelihood for $\sigma_{true} = 0$ should be zero.

From the five permeability measurements $k_0, \dots, k_4$ we obtain a sample standard deviation, σ_{smp} , for k_{true} of 0.73, which is less than the true (but, in practice, unknown) population standard deviation of 0.91. Nevertheless, this information can be used to update our prior expectations (the Bayesian prior)

about the distribution of σ_{true} . The resulting distribution, expressed now as a histogram of samples, is the Bayesian posterior (Figure 3A); calculation of the Bayesian posterior is detailed in Appendix A. Variances for the prior and posterior distributions are 0.69 and 0.18, respectively.

There are several notable features of the Bayesian posterior: (1) the central moment is much lower than that of the prior; essentially, our observation of such a low value for σ_{smpl} is not consistent with our prior expectation of high heterogeneity; (2) the width of the posterior is somewhat less than that of the prior, which reflects less uncertainty – less “ignorance” – due to the incorporation of observational data; (3) finally, our prior conviction that k_{true} is very unlikely to be homogeneous remains intact; it is reflected in the posterior as low probability at $\sigma_{true}=0$.

To highlight the value of a wide “ignorance” prior, Figure 3B plots the posterior incorporating the same Bayesian analysis of $k_0, \dots k_4$ with a prior that reflects a strongly held, but incorrect, belief about the likely range of σ_{true} . This “incorrect” prior is relatively narrow and centered on a value of 1.8, approximately twice the value of σ_{true} . Displacement of the calculated posterior toward σ_{smpl} is very small, largely due to the strength of the prior belief. The variance of both prior and posterior distributions is 0.041.

3.3 Constructing permeability realizations

We wish to construct a series of representations, $k_{rlz,i}$, of the underlying, but unknown, permeability distribution, k_{true} , that incorporates all that is assumed, known and inferred about k_{true} . This includes the three assumptions made in Section 2.1 ($L_{max} > 3$ km, log-normality of k_{true} , and $\beta = 1.4$), the known permeabilities $k_0, \dots k_4$ at the locations of the wells (Figure 1A), and the inferred probability distribution of σ_{true} (Figure 3A). Each of these realizations is constructed using Fourier transformations and a technique called random-bridging (Benson et al., 2013). The method generates spatially correlated fields ($\beta = 1.4$) conditioned on the known geospatial permeability data ($k_0, \dots k_4$); each realization has a log-normal permeability distribution whose center is fixed at $\log(\bar{k}_{true}) = -15$ and whose standard deviation is randomly sampled from either the prior (324 samples) or posterior (336 samples). The properties of these realizations are summarized in Figure 3A, C-E. For each realization, the CO₂ storage simulation described in Section 3.1 was performed.

3.4 Interference testing

Knowledge of permeability at two locations does not necessarily provide a good indication of the permeability structure between those two points. For instance, production wells 1 and 2 (Figure 1A) sample areas of nearly equal permeability ($\log(k_1) = -13.6$ and $\log(k_2) = -13.7$) and yet the connectivity of each to injection well 0 is substantially different (well 1 has much greater connectivity). Nevertheless, an indication of the connectedness between wells can be derived from an interference test, and this information used to improve prediction of operational outcomes.

An interference test is performed by shutting in one well (the observation well) and producing another well at a fixed flow rate (Theis, 1935). Given information about flow rates, separation between the wells, pumping time and other aquifer properties, the average permeability sampled by flow between the

wells can be calculated from the pressure drop at the observation well. However, for the purposes of this study, the pressure drop profile with time will be sufficient.

In this study, we take pressure responses of simulated interference tests for the realizations $k_{rlz,i}$ and compare these against those obtained from k_{true} . Based on the goodness-of-fit, a weight is assigned to the realization representing the degree of confidence its predictions should be assigned. In this case, we are attempting to match the data using a random permeability field, albeit informed by previous point permeability measurements $k_0, \dots k_4$ through use of a Bayesian posterior.

An alternative approach in reservoir simulation is to insert geological features, e.g., high conductivity fractures, flow barriers, and to calibrate the permeability of these features to achieve a good match with the interference test data. The inclusion of such features must be motivated by geological or geophysical observation and thus this approach involves a degree of interpretation. Other approaches for incorporating pressure measurements into conditioned permeability realizations might also be applied. For instance, the use of an Ensemble Kalman Filter allows sequential observations of pressure to be used to refine a heterogeneous permeability field (Lu et al., 2008). A comparative study of these methods is not the objective of this paper, although a comprehensive site analysis would benefit from multiple perspectives on uncertainty quantification.

For the five-spot injection/production operation considered here, the connectivities of interest are the outer brine production wells to the central injection well. Four 100-day interference tests were simulated, using k_{true} , by producing brine at each of the four production wells and monitoring the pressure response at the shut-in injection well (Figure 1D). The relative magnitude of the plotted pressure response for each pair qualitatively matches expected differences in connectivity based on inspection of k_{true} in Figure 1A. For instance, wells 1 and 2 are, respectively, well-connected and poorly-connected as indicated by large and small pressure responses, respectively.

The length of the interference test was necessary to produce a response at the observation well; for closer spaced wells or more permeable formations, shorter tests would suffice. Interference tests can be performed concurrently (Matthews and Russell, 1967), although this is a needless complication for this study.

3.4.1 Weighting of interference tests

For each of the 324 prior and 336 posterior permeability realizations, an interference test for each of the four production wells was simulated. Goodness of fit between these simulated pressure drops and the true pressure drop (which, here, also happens to be simulated) tells us how good a representation of reality that particular realization is. Goodness of fit can be assessed on the basis of one interference test, or some average of the suite of four.

To quantify the misfit between two profiles, here we use the integrated difference between the profiles normalized by the integral of the observed pressure drop profile, P_{obs} , e.g., for the i^{th} permeability realization, and the j^{th} production well,

$$\Delta_i^j = \int P_{rlz,i}^j - P_{obs}^j dt / [\int P_{obs}^j dt],$$

where if Δ_i^j falls outside the range $[-1, 1]$ it is shifted to the nearer of these two values. For example, if $P_{rlz,i}^j$ overpredicts the true pressure drop, P_{obs}^j , then $\Delta_i^j > 0$, and vice versa. Weighting functions can be derived from the Δ_i^j ; the three used here are

1. $w_i^j = (1 - |\Delta_i^j|)^n$ – this weight reflects the goodness of fit for the j^{th} production well but, in taking an absolute value, it makes no distinction between over or underprediction of the pressure profile. The exponent n is a parameter that, when set >1 , assigns comparatively less weight to realizations further from reality.
2. $W_i = \frac{1}{4} \sum_j w_i^j$ – this weight reflects the average goodness of fit for the realization, based all four production wells and again makes no distinction between over or underprediction.
3. $\omega_i^j = (1 - \Delta_i^j)^n$ – this directional weight is used to either increase or decrease the predicted production rate of the j^{th} well. For example, if $P_{rlz,i}^j$ overpredicts P_{obs}^j , then $0 < \omega_i^j < 1$ indicating production rates from this well (brine or CO₂) may also overpredict. Whereas the original simulated brine production rate is $Q_i = \sum_j Q_i^j$ (total from four wells), the modified brine production rate becomes $Q_i' = 4 \sum_j \omega_i^j Q_i^j / \sum_j \omega_i^j$.

The results presented here use an exponent, $n = 5$, which yielded a reasonable uncertainty reduction (see Section 4.3). Other values for n or alternative weighting methods may yield improved predictions. Following the Generalized Likelihood Uncertainty Estimation (GLUE) method of Beven and Binley (1992), the weighting terms calculated here are later applied to the ensemble of model predictions to yield a weighted set of modeled operational outcomes, from which uncertainty bounds are extracted. As a final note, due to measurement error, P_{obs} is an uncertain estimate of the true pressure drop, P_{true} . However, we have elected not to account for sources of measurement error in the current treatment.

4 Discussion of results

In this section, we discuss numerical simulation results and two methods used to improve the predictive accuracy of these results. Attention is focused on the operational outcomes defined in Section 3: (1) CO₂ retention and brine production rates; (2) timing of CO₂ breakthrough at production wells; and (3) rate of CO₂ co-production after breakthrough. Improved prediction of these outcomes is gained through the incorporation of permeability data into a Bayesian posterior (Section 4.2) and use of interference tests to weight the relative likelihood of each realization (Section 4.3).

4.1 Effects of heterogeneity

It is useful to contrast forward models of the CO₂ injection operation under assumptions of permeability homogeneity versus the true distribution (k_{true}). For both cases, Figure 2 summarizes for a 30 year simulation, retention and production curves of interest as well as the position of the plume at ~5 and 20 years after injection has commenced.

Although the injection well samples a region with permeability very similar to the mean – $\log(k_0) = -15.1$ whereas $\log(\bar{k}_{true}) = -15$ – much of the region between brine wells 1 and 3 has above average

permeability. As a consequence, injection and production flow rates and the rate of CO₂ retention within the storage formation (Figure 2A) is appreciably higher than that predicted by a homogeneous model. At 5.7 years, the areal extent of the plume is greater in the heterogeneous case and is laterally biased in the direction of wells 1 and 3 (Figure 2D). The fast pathways conducting the plume in these directions are responsible for CO₂ breakthrough, first at well 1 (~9 years) and then at well 3 (~11 years); in contrast, in the homogeneous case, no breakthrough occurs at any of the wells at the end of the 30 years simulation. This result supports our contention that fast pathways pose a risk to the brine production side of a CO₂ injection operation. The rate of CO₂ co-production increases linearly after breakthrough to nearly equal the CO₂ retention rate at the end of the 30 year simulation.

4.2 Predictive improvements using Bayesian posterior

The purpose of the Bayesian analysis conducted in Section 3.2 is to constrain the degree of permeability heterogeneity, parameterized by the distribution's standard deviation, σ , that is likely to be encountered in $k_{rlz,i}$ during the CO₂ storage operation. To quantify any reductions in predictive uncertainty this step confers, we performed the CO₂ storage simulation for 324 permeability realizations with σ drawn from the prior and 336 simulations with σ drawn from the posterior (Figure 3A). For both the prior and posterior sample sets, ensembles of predicted operational outcomes are summarized in Figure 4.

For predictions of the rate of CO₂ retention or CO₂/brine production, one useful output is the envelope that encloses a given percentage of ensemble realizations (here we use 90%). Ideally, this envelope will be accurate enough to contain the true operational outcome while at the same time narrow enough that a prohibitively large uncertainty is not implied. Under this definition, use of a Bayesian posterior has been advantageous if the size of the predictive envelope is reduced (compared to the prior) while at the same time still containing the true outcome.

Prior and posterior predictive envelopes for the long-term, stabilized CO₂ retention rate are presented in Figure 4A. By the previously defined measure, predictive uncertainty has been improved by the Bayesian posterior; the envelope area has been reduced by 40% while still containing the true CO₂ retention rate near the lower margin. Envelope reduction occurs by excluding the very low and very high injection rates admitted by a Bayesian prior that permits many orders of magnitude variability in permeability, both very high and very low.

Results are similar for the brine production rate (Figure 4B) except in this case the true brine production rate lies very near the bottom posterior prediction envelope. Envelope reduction is still achieved (by 45%); however, unrealistically high production rates are suggested.

Finally, the CO₂ co-production envelopes exhibit a similar behavior to the CO₂ retention envelopes, with a 72% reduction in uncertainty and the true outcome contained near the bottom of the posterior envelope. Reduction here has largely been achieved by excluding permeability realizations that produce very rapid breakthrough times and therefore very high CO₂ co-production.

For all three of the previously discussed operational outcomes (Figure 4A-C), the true outcome was contained within the prediction envelope but was somewhat less than the median. Because these three

outcomes are not independent, we cannot establish whether this implies systematic overprediction, a bias toward heterogeneity in the prior, or is simply the result of random chance. Nevertheless, in the next section, we will present a second method for envelope reduction, which, as a second consequence, also displaces the envelopes so as to more centrally straddle the true outcome.

Figure 4D-G shows histograms of CO₂ breakthrough times at each of the four brine production wells. Compared with the true breakthrough time at each, the predictions, both prior and posterior, are of varying quality. Individual discussions for the four wells are given below:

1. The prior distribution of breakthrough at well 1 comprises a large number of very short and very long times. The median breakthrough corresponds well with the true breakthrough at ~8 years; this successful prediction is probably due to random chance. The posterior distribution shows substantial reduction at both tails and is more centrally distributed about the true breakthrough.
2. Both prior and posterior distributions for well 2 are extremely similar to those for well 1; however, in this situation, the true breakthrough (>30 years) is poorly predicted. The similarity in distributions occurs because the permeabilities at wells 1 and 2 (k_1 and k_2) with which both prior and posterior realizations are conditioned, are nearly identical (-13.6 and -13.7, respectively). The method has no information about permeability between the wells which it might use to distinguish these two cases; this deficiency will be addressed in the next section with interference testing.
3. Both prior and posterior distributions for well 3 have a heavy tail at breakthrough > 30 years; the true value is much earlier, at ~ 11 years. The median prediction is somewhat improved for the posterior, but at 20 years still substantially overpredicts the true breakthrough time.
4. Both prior and posteriors for well 4 agree with the true prediction that CO₂ breakthrough will occur after more than 30 years.

The main consequence of using an updated posterior for predicting CO₂ breakthrough times is to eliminate extreme values associated with very fast and very slow pathways. While reducing uncertainty, this does not appear to confer a consistent improvement in accuracy.

4.3 Predictive improvements using interference tests

Section 3.4 discussed how simulated interference tests could be used to distinguish which realizations, $k_{rlz,i}$, are a better approximation to k_{true} than others. Figure 5A plots the simulated pressure response at the observation well for the 336 posterior realizations; the goodness of fit between these curves and the true pressure response (red line) is quantified by the first weighting function described in Section 3.4.1. For wells 1, 3 and 4, these weights, when plotted against the corresponding CO₂ breakthrough time at the well (Figure 5B), tend to cluster around the true breakthrough time. Thus, the higher the weight, the more likely the predicted breakthrough time for that realization is to be close to the true breakthrough time.

Realization weights are combined with the breakthrough time frequencies in Figure 4D-G to create a weighted histogram of per-well breakthrough times, as described in Beven and Binley (1992). The height of each bin is no longer the total number of realizations in that bin, but now the sum of the weights of those realizations. The weighted histogram is scaled to have the same area as the unweighted version

and plotted below it for comparison (Figure 5C). Individual discussions for the four wells are given below:

1. The median breakthrough time prediction for well 1 is not significantly altered for the weighted distribution; it remains a good estimate of the true breakthrough time. The distribution has been displaced to higher values and is better centered on the median. The range of breakthrough times, i.e., the uncertainty on this prediction, has been reduced (Figure 6).
2. The unweighted distribution for well 2 was similar to that for well 1, despite lower connectivity with the injection well. The weighted distribution has no clear peak. The median prediction has been increased from 8 to 16 years but still falls well short of the true value (> 30 years). Overall this is an improvement.
3. The median breakthrough time prediction for well 3 (10 years) has been significantly reduced for the weighted distribution; it is now quite a good estimate of the true breakthrough time (11 years). As for well 1, the uncertainty on this prediction has also been reduced.
4. The median prediction for well 4 remains in excess of 30 years and a good estimate of the true value. Here too, uncertainty has been reduced.

In general, weighting of the breakthrough time distributions against the simulated interference tests has yielded positive gains both for predictive accuracy and uncertainty. However, the method is not perfect, still failing to provide a good estimate for breakthrough at well 2.

Interference test weights have been used to further improve the prediction envelope for CO₂ retention. The second weighting function described in Section 3.4.1 is used here. The original envelope bounded the 5th and 95th percentile outcomes after simulation of 336 posterior realizations (Figure 4A). The new envelope is calculated from an expanded simulation set constructed by duplicating the posterior simulation results in proportion to their relative weight, e.g., a realization with weight of 0.5 has five times as many duplicates as a realization with weight 0.1. The new envelope is once more bounded by 5th and 95th percentile outcomes (Figure 5D).

Uncertainty reduction of the CO₂ retention rate is relatively small; an 8% decrease in envelope area. The true retention rate remains within the prediction envelope but is still at the low prediction end. These modest gains are probably due to the necessary averaging of interference tests for this particular operational outcome. Unlike brine production or CO₂ co-production, CO₂ retention cannot be deconstructed into components attributable to individual production wells with each then weighted accordingly.

Comparatively greater improvements to the prediction envelopes for brine production and CO₂ co-production are achieved by considering the interference weights for individual wells. Here we make use of the third, directional weighting function discussed in Section 3.4.1. For a given realization, the brine or CO₂ streams from each well are multiplied by that well's weighting term (restricted within a range of [0.2, 5]); the sum of the four streams is the new estimate of total brine or CO₂ production. These estimates are compiled for the 336 posterior realizations and the 5th and 95th percentile outcomes used to construct the prediction envelope (Figure 5E and F).

Substantial gains in both the accuracy and uncertainty of the predicted brine production are achieved by this method. The interference weighted envelope is 38% smaller than the unweighted envelope, while the center has been translated downward to better contain the true brine production profile. Similar gains are made in the prediction of CO₂ co-production, with envelope reduction of 69%.

4.4 Comparison of median predictions and true flow rates

For the particular reality investigated here (k_{true}), median predictions of CO₂ injection, brine production and CO₂ co-production – whether using prior, posterior or weighted posterior distributions – generally overestimate the actual quantities. Stated differently, true flow rates (red profiles in Figures 4A-C and 5D-F) tend to sit in the lower half of prediction envelopes.

This occurs because the mean permeability of the ensemble, $k_{rlz,i}$ is slightly higher than the true mean permeability, $\log(\bar{k}_{true}) = -15$; this is evident in Figure 3C and D, where the true distribution (red profile) is displaced slightly to the left of the ensemble. While $\log(\bar{k}_{true})$ was used in the construction of permeability realizations, $k_{rlz,i}$, the conditioning algorithm introduces a bias towards the mean of the conditioning values, $k_0, \dots, k_4$, which in this case, at -14.5 , is slightly higher than $\log(\bar{k}_{true})$.

5 Conclusion

Spatial heterogeneity and variability across many orders of magnitude are two long-recognized challenges for characterizing and simulating subsurface permeability. For the geological CO₂ storage scenario considered here, heterogeneity results in uncertainty of the productivity of drilled wells and the potential for rapid breakthrough of CO₂ at brine production wells. The objective of this study was to reduce this uncertainty by using information plausibly obtainable from a given site to constrain the heterogeneity.

Our approach involved simulating CO₂ injection/brine production for many different realizations of a heterogeneous permeability field and taking the ensemble result as an uncertain bracket for the true outcome. We incorporated two sources of data – point permeability measurements, and interference tests between wells – in two different methods to reduce the predictive envelopes of CO₂ retention, brine production and CO₂ co-production rates, and CO₂ breakthrough at production wells (Figure 6). These methods were applied to a synthetic “true” permeability realization – representing a hypothetical sequestration site – so that predictive envelopes could be compared against actual outcomes.

In most cases, uncertainty associated with predictions was reduced by incorporating data – this is reflected as a general trend toward more compact box-plots in Figure 6. Bayesian analysis of point permeability measurements was used to constrain the magnitude of permeability heterogeneity, as parameterized by the population standard deviation, σ_{true} . Compared to an “ignorant” prior that admitted a wide spectrum of possibilities for σ_{true} , uncertainty envelopes for CO₂ retention, and brine and CO₂ production are between 40 and 72% smaller due largely to the rejection of very high or very low permeability realizations. Improvement of predicted CO₂ breakthrough time at each of the four production wells was mixed (Figure 6B); this is because our Bayesian posterior was informed by permeability measurements at wells, but not between them.

Interference tests, which interrogate the permeability distribution between wells, were simulated for each of the permeability realizations. Various schemes to weight the realizations based on their correspondence with the real interference test provided further uncertainty reduction. Prediction envelopes for brine and CO₂ co-production rates were reduced 38 and 69%, respectively. For CO₂ breakthrough, in three of the four cases, prediction envelopes were narrower and included the true CO₂ breakthrough. However, for well 2, which happened to sample a small permeable zone in a larger impermeable region, breakthrough continued to escape prediction; clearly the developed methods require further refinement to improve predictions of such heterogeneity scenarios.

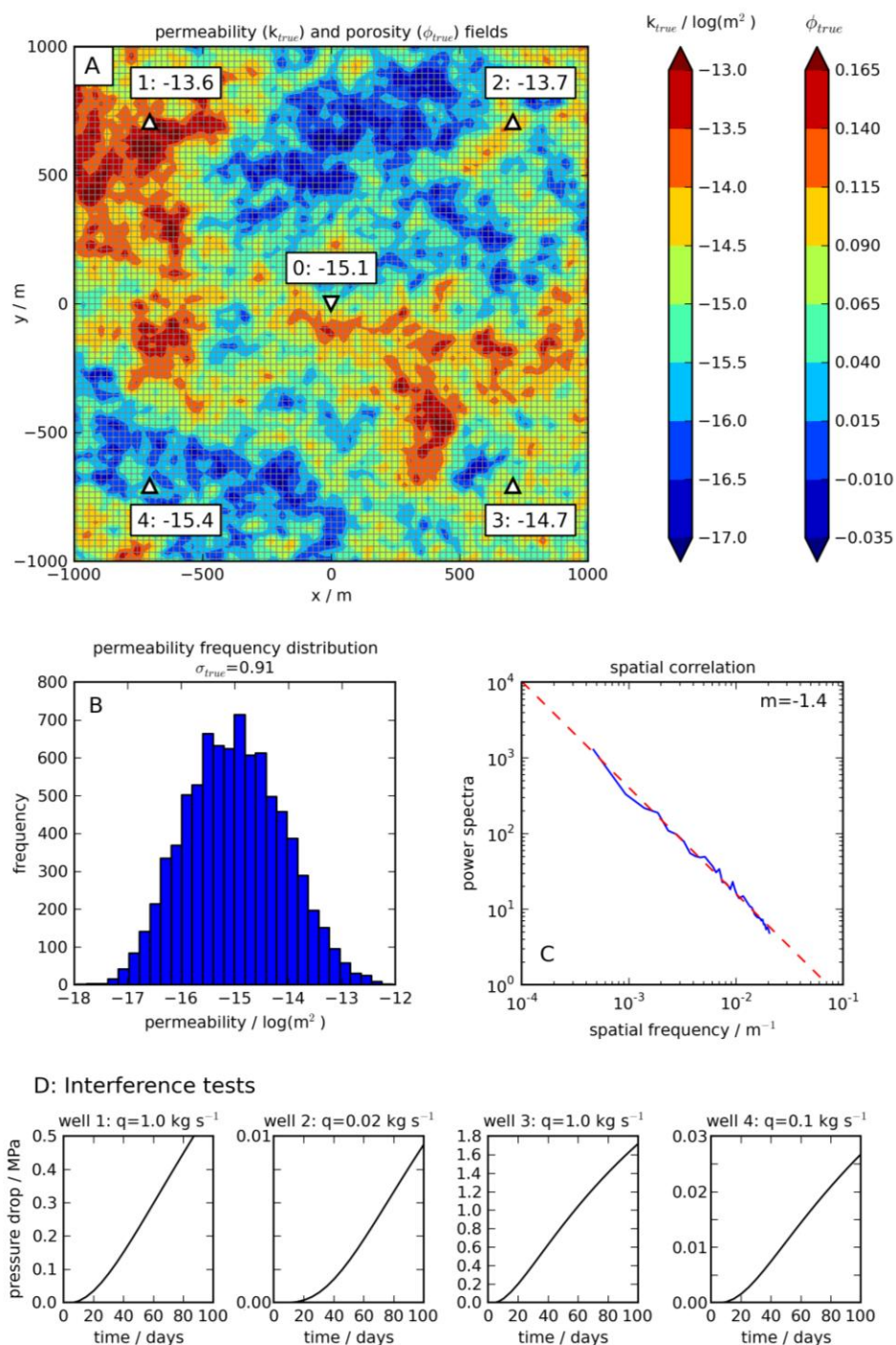
In demonstrating the value of data in reducing uncertainty, our approach also emphasizes the value of ongoing data collection: in pre-site characterization, during the injection phase, and during post-site monitoring. As new wells are drilled, additional permeability measurements acquired and interference tests performed, the analysis described here can be updated to further reduce the width of prediction envelopes. Dynamic uncertainty reduction through assimilation of new data is central to this Bayesian approach.

As a final note, it is important to stress that the approach taken here is independent of the conceptual and model assumption made either in constructing permeability realizations or performing forward simulations. Many of these assumptions may be regarded as controversial, e.g., long-range spatial correlation at least larger than the domain size, neglect of lateral plume migration. However, the intent of this study is not to wade into the debate over which models are the best representation of reality; indeed, the more-appropriate interpretation at one site may be less accurate than a competing interpretation at a different one. In the situation where several models are deemed plausible, a full and thorough accounting would require the simulation procedure be repeated for each assumption set with the final prediction envelope some amalgamation of all possibilities. Alternatively, future studies might investigate the error introduced when constructing the realizations, $k_{rlz,i}$, due to inaccurate assumptions regarding k_{true} .

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613 Figures and figure captions



614

615 **Figure 1: Summary of the true permeability realization, k_{true} .** A. Log-transformed permeability and porosity fields contoured
 616 in the horizontal plane. The positions of the injection (well 0) and four production wells (1-4) are indicated by downward and
 617 upward pointing triangles, respectively. The permeability at the location of each of these wells is indicated. The
 618 computational mesh is overlaid in grey. B. Histogram of all permeability values in k_{true} . The standard deviation of this
 619 distribution, σ_{true} , is 0.91. C. Power spectrum showing the spatial correlation of k_{true} . The spectral slope, β , is 1.4. D.
 620 Pressure decline at the shut-in injection well for a 100-day interference test simulated for each of the injection/production
 621 well pairs in A. The produced flow rate, q , at each production well is given in the title.

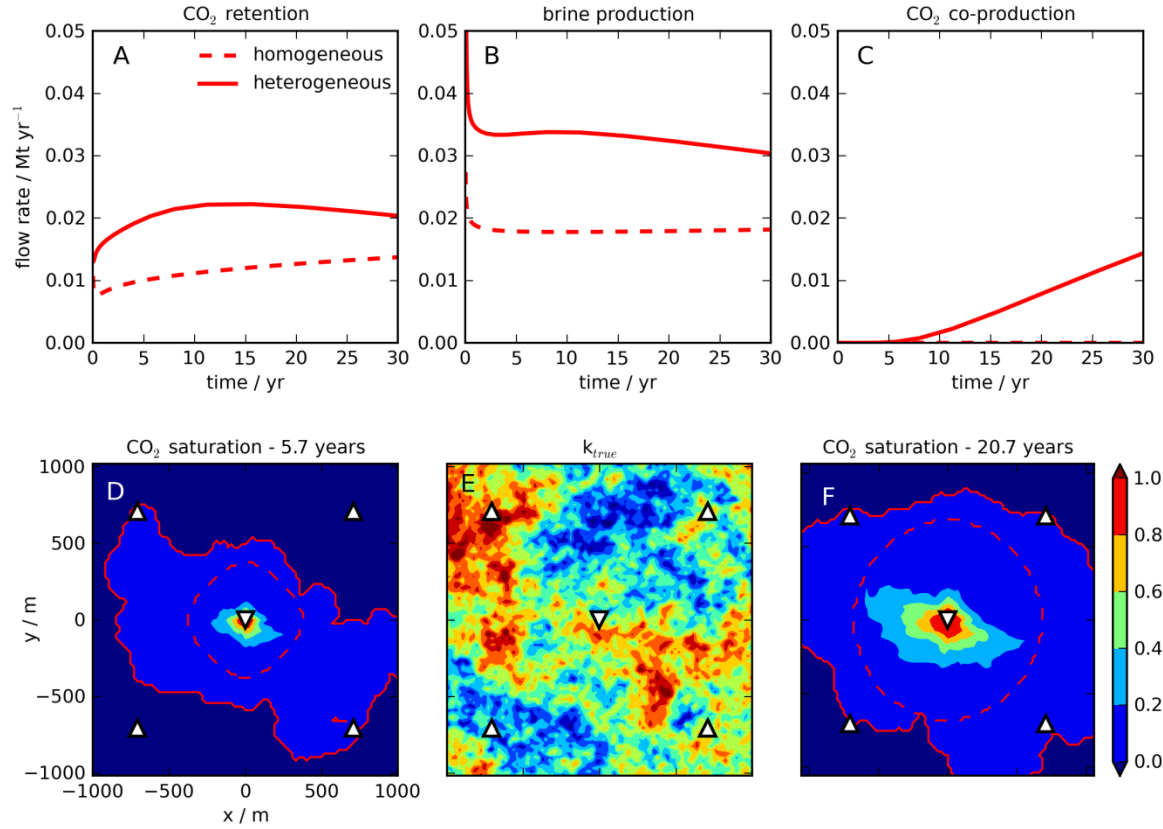


Figure 2: Comparison of CO₂ injection/brine production simulations using homogeneous ($k = \bar{k}_{true}$, red dashed lines) vs. heterogeneous ($k = k_{true}$, red solid lines) permeability distributions. A. CO₂ retention rate (injection less co-production) over time. B. Total brine production rate from wells 1-4. C. Total CO₂ co-production rate at brine wells. D. Distribution of CO₂ plume (by saturation) after 5.7 years of injection into the heterogeneous formation. Red solid and dashed lines define the plume extent for heterogeneous and homogeneous simulations, respectively. Injection and production wells are indicated by downward and upward pointing triangles respectively. E. Heterogeneous permeability distribution, from Figure 1A, for reference. F. As for D, but after 20.7 years of CO₂ injection.

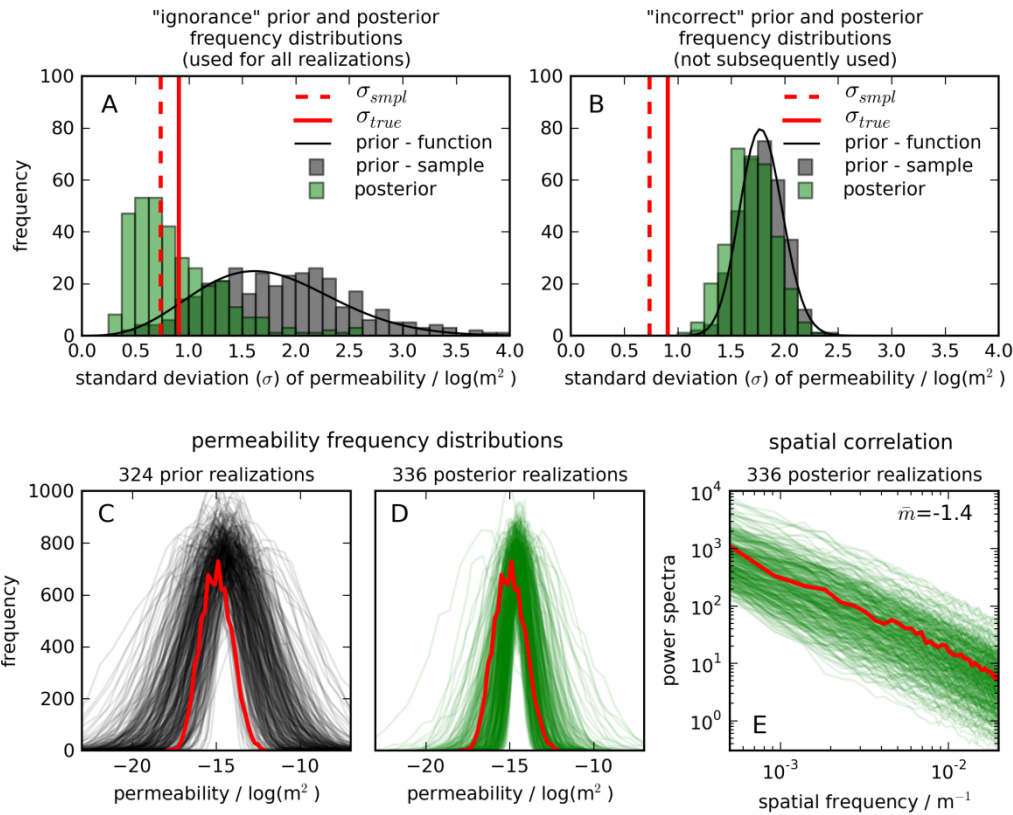
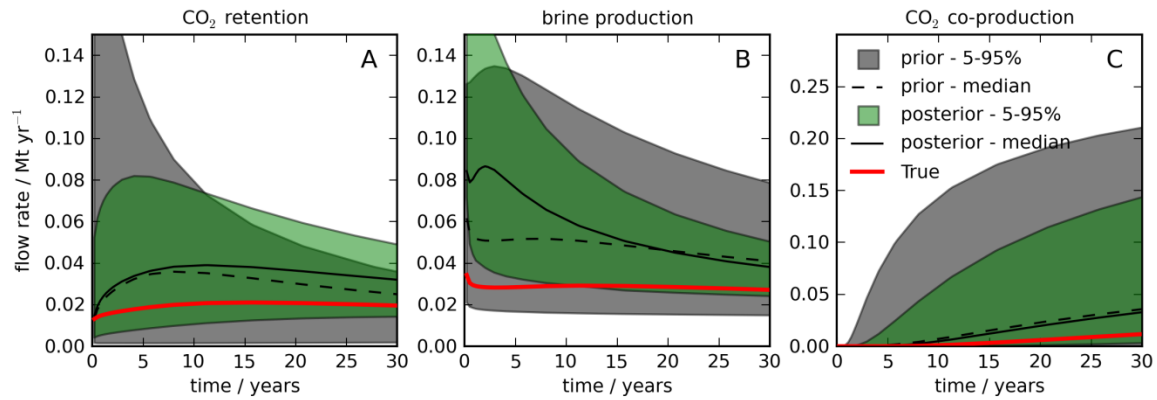


Figure 3: Summary of permeability realizations drawn from the prior (grey, black) and posterior distributions (green). A. The "ignorance" prior (black line) is a relatively wide, transformed gamma function (see Appendix A) from which 324 samples have been selected (grey histogram). The histogram of 336 posterior samples (green) has been displaced toward the measured sample standard deviation, σ_{simpl} (red dashed line), which is an approximation of the true standard deviation, σ_{true} (red solid line). B. As for A, but using a different "incorrect" prior distribution. C. Stacked outlines of permeability histograms for the prior samples in A, with the true histogram (Figure 1B) overlain as a solid red line. D. As for C, but for the posterior samples in A. E. Stacked power spectra for the posterior samples in A. The mean slope, $\bar{m}$, of these spectra is -1.4.

Ensemble flow rates - prior and posterior



Breakthrough time distributions (2% CO₂ production)

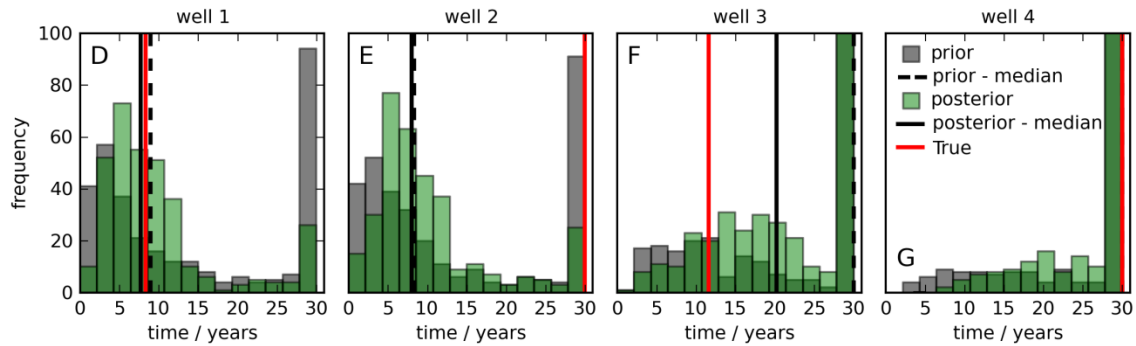


Figure 4: Summary of predicted operational outcomes for prior (grey) and posterior (green) realizations compared to “true” outcomes (red). A. CO₂ retention rate (injection less co-production) over time. The solid grey and green areas enclose 90% prediction intervals for the prior and posterior realizations with corresponding median profiles given by dashed and solid black lines, respectively. B. Total brine production rate from wells 1-4. C. Total CO₂ co-production rate at brine wells. D-G. Histograms of CO₂ breakthrough time at each of the four production wells for the prior (grey) and posterior (green) realizations. CO₂ breakthrough is defined as the time at which CO₂ co-production exceeds 2% (by mass). The breakthrough time for k_{true} is indicated in red and median values for the prior and posterior by dashed and solid lines, respectively. Note, in (G), the true and prior/posterior median values are 30 years, although only the true value is shown.

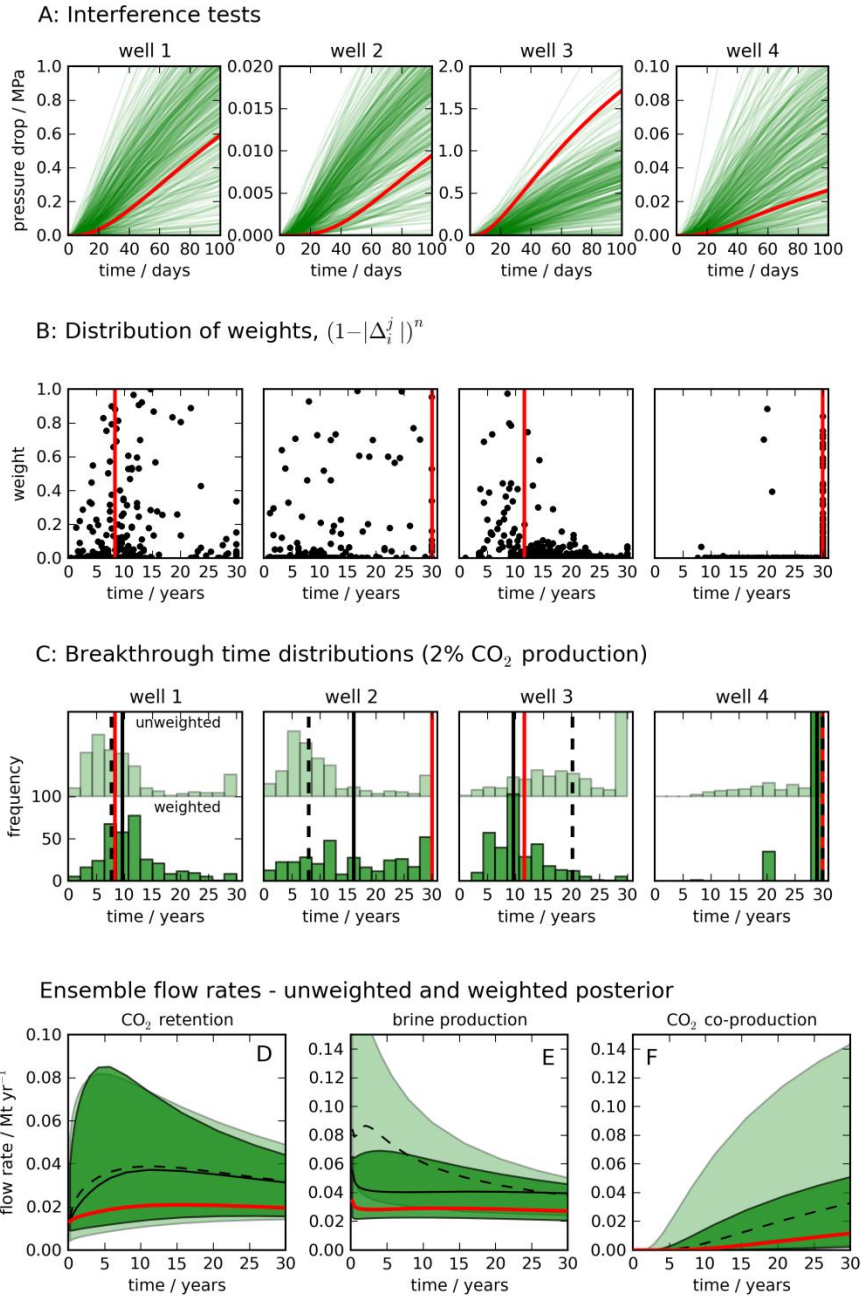


Figure 5: Effect on predicted operational outcomes by weighting against simulated interference tests. A. Stacked pressure responses for simulated interference tests at each production well for 336 posterior realizations. The true pressure response is indicated by a solid red line. B. For each well, the realization weight based on goodness of fit between simulated and “true” interference test plotted against the corresponding CO₂ breakthrough time. C. Histograms of CO₂ breakthrough time at each of the four production wells for 336 posterior realizations and the same data weighted by the values in B. The true breakthrough time is given by a red line, while median values for the unweighted and weighted histograms are given by dashed and solid black lines respectively. D. Envelopes for predicted CO₂ retention (5-95 percentile) from 336 posterior realizations, unweighted (light green) and weighted (dark green) by realization average of values in B. Medians for the unweighted and weighted distributions are given by dashed and solid black lines respectively. E. As for D, but for brine production. The weighting function modifies the component brine stream from each well according to method described in Section 3.4.1. F. As for E, but for CO₂ co-production.

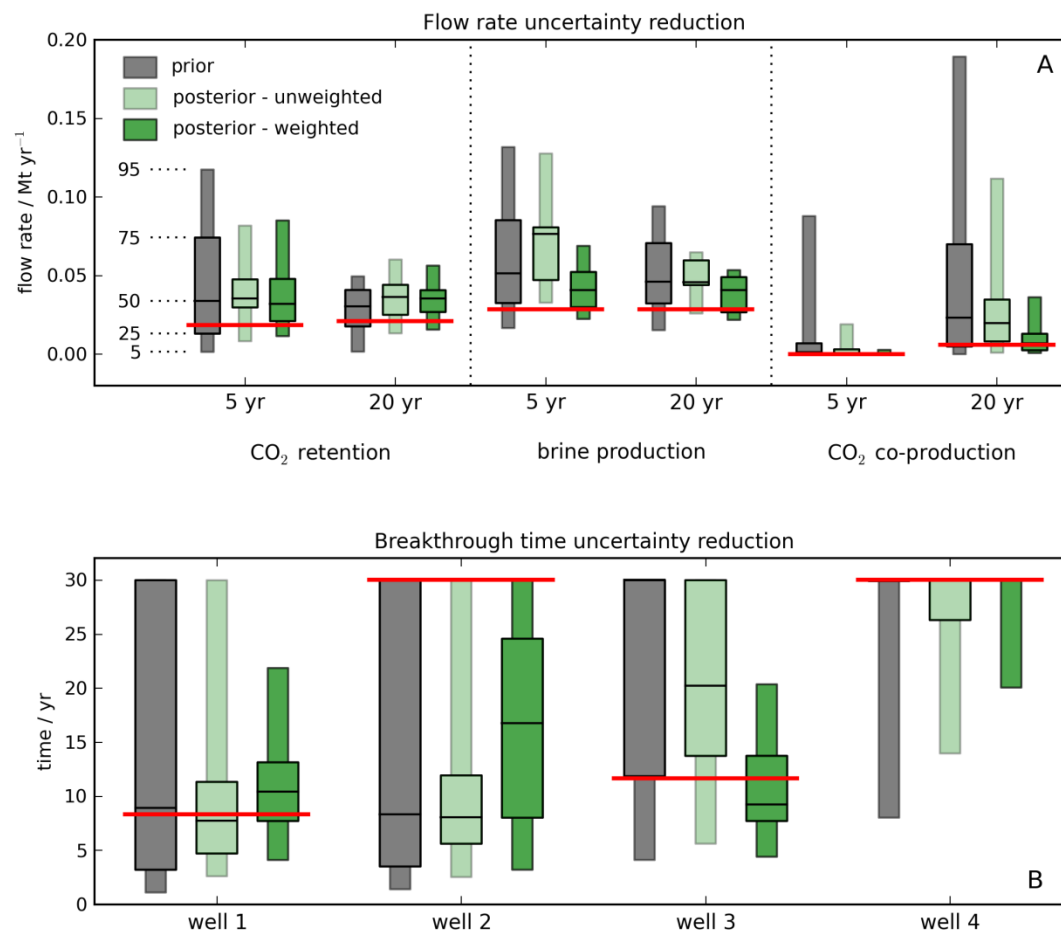


Figure 6: Summary of (A) flow and (B) breakthrough predictions for the prior (grey), posterior (light green), and posterior distribution weighted by the goodness-of-fit of simulated interference tests (dark green). True outcomes are indicated by a solid red line. For the three flow outcomes (CO₂ retention, brine production and CO₂ co-production), the predictions for 5 and 20 years after the start of injection are shown. Percentile demarcations common to all box-plots are indicated on the prior distribution for 5 year CO₂ retention rate.

Appendix A

The probability density/likelihood function for a fractional Brownian field is

$$f_{BBF}(\mathbf{y}; \sigma^2, H, \mu) = \frac{\exp(-(\mathbf{y} - \mu)^T \Sigma^{-1} (\mathbf{y} - \mu)/2)}{\sqrt{(2\pi)^n |\Sigma|}},$$

where $\mathbf{y} = (y_0, y_1, \dots, y_n)$, y_i is the value of the field at the point x_i , $n = 4$, and Σ is the covariance matrix given by

$$\Sigma_{i,j} = \frac{\sigma^2}{2} (\|x_i\|^{2H} + \|x_j\|^{2H} - \|x_i - x_j\|^{2H}),$$

where H is related to the spectral slope β by $\beta = 2H + 1$. For the Bayesian analysis, the log-permeability field is treated as a fractional Brownian field with known values of μ and H , but the value of σ^2 is uncertain. As stated previously, $\mu = -15$ and $H = 0.2$ (corresponding to $\beta = 1.4$). The statement of Bayes' theorem for continuous random variables is

$$f_X(\mathbf{x}|\mathbf{Y} = \mathbf{y}) \propto f_Y(\mathbf{y}|\mathbf{X} = \mathbf{x})f_X(\mathbf{x})$$

where $f_X(\mathbf{x}|\mathbf{Y} = \mathbf{y})$ is the so-called posterior distribution of $\mathbf{X}$ and $f_X(\mathbf{x})$ is the prior distribution of $\mathbf{X}$. The constant of proportionality is chosen so that the integral of the posterior distribution is equal to 1. The uncertainty in the value of σ^2 is encoded in the prior distribution, and the posterior distribution is conditioned on the permeabilities at wells 0-4 ($k_0, \dots, k_4$). Rewriting Bayes theorem for this case gives

$$f_{\sigma^2}(x|k_0, \dots, k_4) \propto f_{BBF}(k_0, \dots, k_4; x, H, \mu)f_{\sigma^2}(x).$$

The two prior distributions for σ^2 that were employed were both gamma distributions whose probability density function is

$$f_{\sigma^2}(x) \equiv f_{gamma}(x; k, \theta) = \frac{x^{k-1} e^{-\frac{x}{\theta}}}{\Gamma(k)\theta^k}.$$

The shape and scale parameters (k and θ , respectively) were $k = 2$ and $\theta = 1.077$ for the "ignorant" prior, and $k = 25$ and $\theta = 0.1$ for the "incorrect" prior. The square root of σ^2 differs from the sample standard deviation parameter that is discussed in the main text. The sample standard deviation for a fractional Brownian field is scale-dependent, and increases with increasing scale. The fractional Brownian field parameter σ^2 was transformed into the sample standard deviation parameter via

$$\sigma_s = \sqrt{\sigma^2/C}.$$

The constant C is fixed by the scale of the problem, and was empirically determined to be approximately 0.62 for this problem.

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