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Improved geophysical monitoring of carbon sequestration through parameter linkage to reservoir modeling

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Peer reviewed

- 1 Improved geophysical monitoring of carbon sequestration through parameter linkage to reservoir
- 2 <u>modeling</u>.
- 3
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- 7

8 ABSTRACT

- 9 Predictive reservoir modeling, even if present in the form of only basic hydrogeological model
- 10 assumptions, is expected to accompany the majority of carbon capture and sequestration
- 11 monitoring activities. It thus represents a source of prior information about the migration of
- 12 injected fluids that can benefit geophysical survey planning and ensuing monitoring.
- 13 Constraining the imaging of geophysical monitoring data with reservoir modeling is preferable
- 14 over standalone geophysical imaging because of additional complementary hydrogeological
- 15 information. However, fully coupled hydrogeophysical data inversion for flow-modeling
- 16 parameters that control saturation predictions is an involved process. Within the context of three-
- 17 dimensional electromagnetic (EM) inversion of data from borehole-to-surface layouts, we
- 18 employ a "poor people's" alternative. The approach constrains geophysical inversion parameters
- 19 through saturation predictions. The coupling is realized through spatially variable lower and
- 20 upper parameter bounds that scale with gas saturation magnitudes, the latter provided by
- 21 reservoir modeling. Enhancement of three-dimensional time-lapse plume EM imaging is
- 22 demonstrated for simulated sequestration into a depleted gas reservoir.
- 23

24 **1. Introduction**

- 25 Regional-scale deployment of geologic carbon sequestration (GCS) requires reliable stewardship
- 26 in form of failsafe monitoring in order to reach industrial maturity (e.g., Arts et al., 2008; Shi et
- al., 2008; Ringrose, 2020). Geophysical remote-sensing methods offer the volume coverage
- 28 needed for long-term monitoring of regional-scale GCS activities (Gasperikova and Hoversten,
- 29 2006; Michael et al., 2010; Jenkins et al., 2015; Davis et al., 2019; Gasperikova et al., 2022;
- 30 Tveit and Mannseth, 2022). Among geophysical rock properties, electrical properties have
- 31 shown to correlate with saturation levels of stored carbon dioxide (CO₂) in a porous system (Kim
- 32 et al., 2010; Alemu et al., 2011). Owing to their sensitivity to fluid-induced electrical property
- 33 changes and large exploration depths, geophysical controlled-source electromagnetic (CSEM)
- 34 methods (e.g., Streich et al., 2010; Wirianto et al., 2010; Vilamajó et al., 2013) and concomitant
- 35 CSEM-data inversion methods (e.g., Ayani et al., 2020; Grana et al., 2021; Tveit et al., 2015;
- 36 Tveit et al., 2020) have become viable techniques for GCS monitoring.
- 37 Typical reservoir depths exceed 800 m in order to meet the pressure and temperature
- requirements needed to store CO₂ as a supercritical fluid (van der Meer, 1993). Large reservoir
- 39 depths render borehole-to-surface electromagnetic (BSEM) surveying as suitable because the
- 40 proximity of transmitters to target zones retains its sensitivities (He et al., 2005; Marsala et al.,
- 41 2011; Gasperikova et al., 2022). BSEM is defined by a borehole-deployed transmitter and a
- 42 receiver spread on the surface. Despite its advantage of strategically placing instruments near

- 43 zones of interest, a major challenge to deep reservoir monitoring is a typically thin nature of
- 44 fluid-confining formations (Marsala et al., 2014). There is growing consensus that vertical
- 45 electric dipole (VED) antennas deployed as sources can alleviate this issue because their
- 46 dominating EM-wave mode maximizes sensitivities to thin target structures (Wirianto et al.,
- 47 2010; Girard et al., 2011; Vilamajó et al., 2013; Grayver et al., 2014; Schaller et al., 2014).
- 48 While technical feasibility can be regarded as established, we believe that economic feasibility is
- 49 an equally important but more overlooked aspect. This contribution simulates a low-cost
- 50 scenario by making the BSEM survey design deliberately sparse in terms of the total
- 51 instrumentation. While we exploit the resolution advantages of VED sources, the BSEM setup of
- 52 our imaging demonstrations implies a volume coverage that is relatively small compared to the
- regional target scale. To offset the deficiencies due to a limited instrumentation, we propose the
- 54 incorporation of model constraints provided by reservoir modeling.
- 55 Reservoir modeling (e.g., Hosseini et al., 2012) can be regarded as some subsurface equivalent to
- 56 weather prediction because fluid flow and transport forecasting improves as more monitoring
- 57 data becomes available over time. Reservoir models are expected to be a standard part of GCS
- 58 site management. Doughty and Oldenburg (2020) use the term *operational* reservoir model for a
- 59 hydrogeologic model that is expected to be initially crude at the pre-injection stage due to a
- 60 limited data base. Operational reservoir modeling then involves the assimilation of the
- 61 monitoring data stream for an ongoing model improvement. A model that is deemed sufficiently
- 62 mature thus provides a free source of prior complementary information to help optimize
- 63 geophysical plume-mapping. To offset weak model resolution due to limited instrumentation, we
- 64 hence propose to employ flow predictions in order to construct inversion constraints in the form
- 65 of target-adapted model parameter bounds.
- 66 Spatially variable (lower and upper) model parameter bounds facilitate the incorporation of prior
- 67 information as inversion constraints (e.g., Abubakar et al., 2008; Sosa et al., 2013; Aghamiry et
- al., 2019; Ogarko et al., 2021), because parameter ranges can be scaled with uncertainties.
- Recent studies (Commer et al., 2022) in a crosswell EM context have employed spatially
- variable scaling of bound widths under a different premise. For poorly resolved interwell
- 71 regions, it was shown that bound intervals that are enlarged with respect to a global default can 72 benefit the solution-finding process. Principally, this is achieved through diminishing the chance
- 72 benefit the solution-infining process. Frincipally, this is achieved through diminishing the char 73 for a premature convergence towards local solution minima. The approach is related to the
- 74 concept of inversion constraints with a spatially varying degree of enforcement in order to
- balance out varying sensitivities inherent in a given survey geometry (Yi et al., 2003). In a
- 76 similar manner, to locally enhance model fidelity, we augment lower and upper parameter
- bounds in zones where operational reservoir modeling predicts significant gas saturation
- 78 changes.
- 79 For brevity, we will use the abbreviation ORM for operational reservoir model in the following.
- 80 Section 2 outlines the hydrogeophysical aspects underlying the construction of spatially variable
- 81 parameter bounds from an ORM. These bounds are the input to the constrained inversion of
- 82 synthetic BSEM data simulated for a large-scale reservoir model. The inversion approach
- 83 presented in Section 3 and results in Section 4 demonstrate that expanded parameter bounds have
- 84 the potential to offset weak model resolution in thin target zones that undergo CO₂-induced
- 85 changes in electrical conductivity.
- 86

87 2. Hydrogeophysical reservoir modeling

- 88 Our EM-imaging experiments are based on a reservoir model that is representative of typical
- 89 large-scale depleted natural gas reservoirs in the Sacramento River Delta region of California.
- 90 Reservoirs of this kind are prospective candidates for long-term storage. Extensive CO₂ plume
- 91 evolution simulations by Doughty and Oldenburg (2020) assessed long-term forecasting
- 92 uncertainties associated with pressure and saturation evolution. Their simulated scenario
- 93 involves 8 Mt/year of CO₂ injection over 20 years.
- 94 Doughty and Oldenburg (2020) used two types of reservoir flow models: actual and operational
- 95 (Fig. 1). The actual model (Fig. 1a) features a complex heterogeneous 3D permeability
- 96 representation of a regional-scale geologic model of a depleted gas field. Stochastic modeling
- 97 added small-scale spatial model heterogeneity to ensure a more realistic geological complexity.
- A high-permeability sandstone layer located between depths of 1.4 and 1.8 km forms the actual
- storage reservoir, its thickness averaging roughly 400 m. The storage reservoir is overlain by a
- 100 very low permeability shale (not shown in Fig. 1) that serves as cap rock for the reservoir.
- 101 Starting from an initially crude vertically-layered representation, a series of progressively more
- 102 complex reservoir models was derived. Their complexity reflected incorporation of the gradually
- 103 increasing informational content due to the accumulation and history-matching of periodically
- 104 sampled pressure, saturation, and gas composition data, simulated for a set of 14 observation
- 105 wells. These wells are distributed over approximately 7×13 km² as indicated by black circles in
- 106 the horizontal sections of Fig. 1. Fig. 1b shows the estimated permeability model that would be
- realistically available to the site operator after 5 years of injection and history-matching of the
- 108 corresponding monitoring data.
- 109 The actual model represents the (unknown) true state. Synthetic-data generation is based on this
- 110 model. The ORM represents the best available approximation to the true state at the time 5 years
- 111 after start of injection (at time zero). Geophysical inversion constraints will be constructed from
- 112 this model.
- 113
- 114 2.1. Geophysical monitoring objective: time-lapse gas saturation changes
- 115 Our monitoring objective employs the 5-year ORM (Fig. 1b) for making gas-saturation
- 116 predictions for up to 12 years. Note that the 5-year timeframe refers to model maturity. In a real-
- 117 world case, this maturity would be attained by history-matching the monitoring data collected up
- 118 to 5 years. Predicting the reservoir state up to 12 years hence translates to matching the 5-year
- 119 monitoring history and forecasting the 7 following years. Fig. 2 (left column) compares the 12-
- 120 year forecast of gas saturations between the actual model (a) and (b) the ORM. Striking is the
- 121 more heterogeneous distribution of zones of altered gas saturations at 12 years in the actual
- 122 model (compare subplots of left plot column). While the match is poor on a fine-scale, the ORM
- 123 appears to reproduce regions of heightened saturations on a gross scale.
- 124 Gas saturation includes CH₄ (methane) and CO₂. Isolated pockets of gas as visible in Fig. 2a
- 125 (left) have different origins. First, residual free-phase CH₄ is initially trapped in some attic
- regions forming static accumulations. Second, over the course of injection, degassed CH₄ can
- 127 form due to addition of CO₂. Third, injection-induced changes in pressure and composition can
- 128 create isolated free-phase CO₂ out of dissolved CO₂ as the latter is present more widely.

- 129 Our inversion objective is based on earlier assessments about the storage potential of the
- 130Sacramento River Delta region (Oldenburg et al., 2001). The region hosts many geological
- 131 structures with gas storage capacity. Reinjecting gas into a depleted reservoir associates the
- question of permanence with properly forecasting where buoyant rise would make the gas
- accumulate over time. Therefore, we choose the attic region underneath the caprock (indicated as
- Northern attic in Fig. 1 and Fig. 2) as focus area as it is representative for locally closed highpermeability structures that are crucial as long-term repositories. To predict saturation changes
- due to fluid transfer and substitution processes, we choose the time span between 8 and 12 years.
- Fig. 2a (right column) exhibits that the particular permeability makeup of the actual model leads
- 138 to significant saturation changes within this time interval. Properly forecasting these changes in
- 139 the reservoir cap region can aid the reduction of reservoir performance uncertainty.
- 140 The ORM's prediction of the time-lapse saturation change between 8 and 12 years (Fig. 2b, right
- 141 column) appears similar to the absolute saturations: there exists agreement on a gross scale;
- 142 however, saturation changes in the Northern attic region appear with an error in the predicted
- 143 elevation. Our objective thus also involves the question to what degree deviations from the true
- 144 case would corrupt geophysical-data inversions that use prior information derived from the
- 145 ORM.
- 146

147 2.2. Petrophysical transformation of the reservoir model

- 148 Petrophysical transformation functions are the key linking elements between two physical
- 149 systems: the reservoir flow model and the geophysical model for EM data simulation. The
- 150 petrophysical relationship derived in the following establishes a connection between rock
- 151 properties that control fluid transport and electrical properties.
- 152 Synthetic geophysical EM data creation is based on the actual permeability model (Fig. 1a) and
- 153 its corresponding hydrogeological flow state during CO₂ injection. In a first step, the function

$$\rho_f = \frac{\rho_{18C}}{1 + \alpha(T - 18)} \tag{1}$$

- 154 calculates pore fluid electrical resistivity ρ_f (with unit Ω m) from temperature *T* and content *c* of
- total dissolved solids (TDS), the latter affecting the reference resistivity at 18 degrees Celsius,

$$\rho_{18C} = \frac{3549}{c^{0.924}}.\tag{2}$$

- 156 Eq. (1) uses the constant $\alpha = 0.025$ which together with the constants in Eq. (2) reflects the
- 157 temperature dependence of electrical resistivity as detailed by Hayashi (2004). These constants
- 158 are chosen here as representative for the bulk resistivity ρ_b of the Sacramento River Delta region
- 159 expressed by means of Archie's law,

$$\rho_b = a\phi^{-m}\rho_f,\tag{3}$$

- 160 where a = 1, ϕ is porosity, and the cementation exponent *m* varies between 1.1 for clay layers
- and 2 for sand layers. The bulk resistivity value of each model grid cell results from Eq. (3) and
- 162 the cell's gas saturation value S_g ,

$$\rho = \frac{1}{\sigma} = \frac{\rho_b}{(1 - S_g)^n},\tag{4}$$

- 163 using a constant exponent of n = 2. Our imaging method operates on the electrical conductivity 164 $\sigma = \frac{1}{\rho}$ (with unit S/m). Eq. (4) represents the final petrophysical transformation function linking
- 165 the (geophysical) σ -model to the reservoir flow model.
- 166

167 2.3. BSEM survey layout

- 168 Eqs. (1)-(4) represent the hydrogeophysical linkage between the modeling of the reservoir states
- 169 of interest (between 8 and 12 years) and the corresponding geophysical property evolution. The
- 170 outcome of Eq. (4) produces the model of electrical rock resistivity used to calculate synthetic
- 171 data of a BSEM layout shown in Fig. 2. Recall that these data calculations are based on the ρ -172 distribution originating from the actual reservoir model. Synthetic data are given as electric fields
- 172 that would be excited by borehole source antennas and measured via the surface electrode array.
- The employed controlled-source EM forward-modeling algorithm approximates Maxwell's
- 175 equations on a finite-difference grid representing the geophysical modeling domain.
- 176 Computational and algorithmic details can be found in the work of Commer and Newman
- 177 (2008).
- 178 CSEM sources are deployed in monitoring wells U1 and U2 (indicated in Fig. 1 and Fig. 2). The
- sources are vertical electric dipole antennas with a length of 50 m, centered at a depth of 1850 m.
- 180 We simulate data for both sources at four frequencies, 0.25, 0.5, 1, and 2 Hz. There are 13 north-
- 181 south oriented receiver profiles spaced 250 m apart (along the Easting direction), with a receiver
- 182 separation of 125 m (along the Northing direction). Two perpendicular electric-field
- 183 components, E_x (parallel to Easting) and E_y (parallel to Northing) are recorded at 45 receiver
- stations per profile, thus amounting to a total of 585 stations and 1170 complex electric field data
- 185 points per source frequency.
- 186 Magnitudes of artificial noise imposed on the synthetic data are based upon 0.5 % of the data
- 187 amplitude and an additional noise floor of 10^{-12} V/m (normalized to unit dipole moment).
- 188 Theoretical estimates for sensor noise-floor limits were reported between 10^{-14} V/m (Streich *et*
- 189 *al.*, 2010) to 10⁻¹³ V/m (Wirianto *et al.*, 2010).
- 190

191 2.4. Simulating operational model uncertainty

- 192 Uncertainty in the understanding of reservoir processes is prevalent owing to monitoring data
- that is always insufficient in view of the reservoir system's size and complexity. Uncertainties
- associated with the history-matching process and the ensuing incompleteness of a given state-of-
- the-art reservoir model have been discussed at length (e.g., Subbey et al., 2004; Ma, 2011). Our
- scope touches on synthetic uncertainty, namely, does the ORM's incompleteness with respect to
- 197 the actual model properly reflect the degree of incompleteness one would face in a corresponding
- 198 real-world case?
- 199 Table 1 of Doughty and Oldenburg (2020) details reservoir properties of the actual model and
- 200 the initial (at 0 years) ORM. Without going too much into detail, we reiterate here that the
- 201 difference in permeability distribution, three-dimensionally heterogeneous versus layered (Fig.
- 202 1), already precludes the ORM from achieving a perfect data fit. Moreover, the ORM uses
- simpler relative permeability and capillary pressure functions. While both are based on the van
- 204 Genuchten (1980) formulation, the actual model includes hysteresis and all function parameters

depend on permeability. In contrast, the ORM is non-hysteretic and only the parameter capillary

- 206 pressure strength depends on permeability via Leverett scaling.
- 207 The following initial reservoir conditions match their actuals by the 5-year stage of the ORM:
- 208 Initial (hydrostatic) pressure, temperature (using a geothermal gradient), initial CH₄ (methane)
- distribution, and vertical salinity profile as derived from regional estimates by Kang and Jackson (2016). Note that CIL is initially changed and a labor of the second se
- (2016). Note that CH₄ is initially absent and only becomes an added feature in the 5-year ORM.
 One could argue that a more realistic simulation of an incomplete ORM would involve more
- 211 One could argue that a more realistic simulation of an incomplete OKW would involve more 212 deviating initial conditions. However, assuming the existence of prior knowledge due to the
- site's depletion history, realistic deviations would not significantly affect the degree of error that
- is already present in the saturation predictions (Fig. 2). In other words, fine-scale improvements
- in the saturation prediction will not affect the geophysical plume imaging as the latter only
- 216 requires a gross-scale saturation profile. More of these aspects are also discussed further below.
- 217

218 **3. Constrained inversion of BSEM data**

219 The total number of estimated parameters that make up the geophysical inversion domain

- amounts to 1,538,974 active finite-difference grid cells, where each cell hosts an electrical-
- 221 conductivity parameter. The large discrepancy between the sizes of the parameter and data
- spaces causes solution ambiguity rendering the inverse problem ill-posed. Bound constraints aim
- at reducing the ambiguity by narrowing the solution space in zones where physical property
- ranges are known prior to inversion. The common approach reduces bound intervals according to
- the prior information's certainty (e.g., Kim and Kim, 2011). Our approach differs by widening bound intervals in zones where the ORM suggests significant time-lapse property changes. In the
- following, we describe the method of mapping the degree of gas saturation changes to its
- function parameters controlling spatially variable bound widths. The general concept of bound
- 229 constraints was introduced earlier together with our employed inversion algorithm (Commer and
- Newman, 2008). The algorithm employs a non-linear conjugate gradient (NLCG) scheme which
- 231 uses a line-search based upon quadratic interpolation, safeguarded with backtracking.
- Logarithmically transformed model parameters define the search space, which facilitates boundconstraints as logarithmic functions are amenable to inequality constraints.
- 255 constraints as logarithmic functions are amenable to inequality constraints.
- 234 *3.1. Spatially variable lower and upper parameter bounds for enhanced model resolution*
- 235 Lower and upper parameter bounds are also known as inequality constraints (e.g., Kim et al.,
- 1999) and are abbreviated by a and b in the following. Inequality refers to the evolution of a
- 237 model parameter *m* during an inversion process, so that *m* is bounded by a < m < b. In order to
- 238 impose a positivity constraint on electrical conductivity, the bounds usually occur in conjunction
- 239 with logarithmic or hyperbolic types of parameter transformation functions. Generalized
- 240 functions were formulated by Kim and Kim (2011),

$$x = \frac{1}{n} \log\left(\frac{m-a}{b-m}\right) = \frac{2}{n} \tanh^{-1}\left(\frac{2m-b-a}{b-a}\right); \quad a < m < b,$$
(5)

- 241 where x is the transformed parameter and n is a positive integer constant. Our studies employ a
- 242 version realized by n = 1. Other choices for n are discussed by Kim and Kim (2011).
- 243 Transforming *x* back into the original model parameter space then leads to (Commer and
- 244 Newman, 2008)

$$m = \frac{a+b\exp(x)}{1+\exp(x)}; \quad -\infty < x < \infty.$$
(6)

Constant bounds may be most suitable for inversion applications where no prior information is available, that is, the bound interval [a, b] applies to every cell parameter m_i (i = 1, ..., M) of the finite-difference mesh representing the inversion domain. In the presence of location-dependent prior information, [a, b] can become spatially variable so that each cell m_i is subjected to an individual bounding interval $[a_i, b_i]$.

- 250
- 251

252 *3.2. Designing bounds from gas-saturation predictions*

Gas saturation predictions provide the basis for constructing lower and upper conductivity parameter bounds in order to achieve a local resolution-enhancing effect. The general approach

is to widen a preset default bound interval $[a, b] = [10^{-3}, 1.5]$ S/m within regions of interest, so

that [a, b] becomes $[a \cdot f_a, b \cdot f_b]$ with positive factors f_a and f_b . The choice of the default

257 bounds are based on estimates of extremal conductivity values that result from reservoir

258 modeling over the whole 12-year period of interest. The focus regions are linked to injection-

induced gas saturation changes predicted from the ORM (Fig. 2b). With the focus being on

- delineating gas saturation changes between year 8 (quantified by S_g^{08y}) and year 12 (S_g^{12y}), the
- 261 zones of interest are defined by their absolute percentage saturation change

$$\left|\Delta S_{g}^{\%}\right| = \left|\frac{S_{g}^{12y} - S_{g}^{08y}}{S_{g}^{08y}}\right| \cdot 100$$
⁽⁷⁾

exceeding a given threshold $\Delta S_g^{thr\%}$. This threshold is set to $\Delta S_g^{thr\%} = 5$ % which is the minimum gas saturation change in percent that has to occur in order to augment the default interval [a, b]. In practice, the widening is achieved through two factors, $f_a = \frac{1}{f_{lb}(x,y,z)}$ and $f_b =$ $f_{ub}(x, y, z)$, applied to [a, b] so that the interval becomes spatially variable, $[a, b] \rightarrow$ $\left[\frac{a}{f_{ub}}, b \cdot f_{ub}\right]$.

267 Dividing by the lower-bound factor
$$f_{lb} = f_{lb}(\Delta S_g^{\%})$$
 decreases the lower bound *a*. In our

- 268 particular case, f_{lb} varies linearly between 1 and 100, i.e. $f_{lb}(\Delta S_g^{\%} = 0) = 1$ and
- 269 $f_{lb}(\Delta S_g^{\%} \ge 100) = 100$. Hence, with higher saturation changes, the lower bound decreases up to
- a minimum of a/100. Enlarging the upper bound is achieved via multiplication of b with the
- 271 factor f_{ub} , which varies linearly between 1 and 10, i.e. $f_{ub}(\Delta S_g^{\%} = 0) = 1$ and $f_{ub}(\Delta S_g^{\%} \ge 1)$
- 272 100 = 10. The default bound interval thus increases to an extremum of $[a_{min}, b_{max}] =$
- 273 $[10^{-5}, 15]$ S/m.
- 274 Setting the expansion factor for the lower bounds an order of magnitude larger than for the upper
- bounds reflects the fact that positive gas saturation changes and corresponding conductivity
- 276 decreases dominate over the 12-year simulation period. Undocumented trial inversions with
- 277 larger expansion factors, for example $f_{lb}(\Delta S_g^{\%} \ge 100) = 1000$ and $f_{ub}(\Delta S_g^{\%} \ge 100) = 100$,
- 278 revealed no significant differences in the inversion outcome. Fig. 3 illustrates both bound
- extremes, the lower-bound (left) range $[a_{min}, a_{max}]$ and the upper-bound (right) range

- $[b_{min}, b_{max}]$, for one vertical cross section. The selected plane is parallel to the Northing axes 280
- 281 and cuts through the Easting coordinate at E=240 m.
- Bounds construction starts by feeding the saturation S_g^{08y} and S_g^{12y} , calculated from the ORM, to 282
- Eq. (7). The output are sets of lower and upper bounds with augmented intervals for zones where 283
- 284 the 5-%-threshold criterion is met. Upon input of the inversion's starting model, an individual
- 285 bound pair a_i, b_i is then assigned to each cell parameter m_i of the inversion domain.
- 286

287 3.3. Gradient weighting and parameter masking

- 288 In addition to parameter bounds, we employ two other approaches that essentially impose
- 289 constraints on the NLCG inversion process, namely gradient weighting and parameter masking.
- However, we abstain from a study that would systematically investigate the interplay of all three 290
- 291 constraining methods as this would go beyond our intended scope. More systematic studies of
- 292 combinations of different constraints were carried out by Portniaguine and Zhdanov (1999) and 293
- Boulanger and Chouteau (2001) in the context of gravity data inversion. Here, we use both
- 294 gradient weighting and parameter masking in a rather empirical manner owing to their
- 295 individually demonstrated benefit.
- 296 Gradient weighting as used in this work is a method of assigning weighting factors to each
- 297 component of the gradient vector **g** of the NLCG scheme. The gradient vector **g** contains
- 298 derivative information and is at the base of optimizing the direction of the line-search in model
- 299 space. Methodological details and successful application of gradient weighting within the same
- 300 NLCG scheme were demonstrated earlier (Commer et al., 2016). Principally, high sensitivities of 301 cell parameters m_i pertaining to regions near surface spreads or instrumented wells are damped
- 302 through assigning weighting factors $w_i < 1$. The corresponding weighted gradient component
- 303 $w_i g_i$ then becomes down-weighted with respect to cells in unweighted model regions. Similar to
- the bound constraints, gradient weighting basically boosts the NLCG line-search in areas of low 304
- 305 sensitivity, causing weak resolution, at the expense of high-sensitivity zones. For BSEM, the
- 306 desired effect is to nudge model updates away from the vicinity of transmitters and receivers,
- 307 where sensitivities are high, towards less resolved center regions.
- 308 Parameter masking as employed here is a straightforward way of disabling an arbitrary subset of
- 309 cell parameters of a rectangular inversion domain. Geological horizons derived from seismic
- 310 data usually provide the prior information needed to define parameter masks (e.g., Hoversten et
- 311 al., 2021). We employ the upper horizon shown in Fig. 4 in order to deactivate all mesh cell 312 parameters that are above it. The underlying assumption is a no-leakage scenario, that is, our
- imaging objective does not consider the case of buoyancy-driven gas flow into the caprock. The 313
- 314 present inversion study assumes that the background geology above the delineating seismic
- 315 horizon would be known from preliminary baseline (pre-injection) data inversions and prior
- 316 information.
- 317
- 318 3.3. Sequential inversion scheme
- 319 Delineating property changes between the two observation times (8 years and 12 years after the
- 320 start of injection) involves a three-step inversion procedure. Three inversion runs pertain to the
- 321 refinement of the baseline (pre-injection) model and, with respect to this baseline, the delineation

- 322 of fluid-induced anomalous resistivity alterations after 8 and 12 years. Synthetic time-lapse data
- 323 for these inversions are obtained by using the actual reservoir model and the BSEM
- 324 configuration for three times, referred to as Year00, Year08, and Year12. For these times, Eqs.
- 325 (1)-(4) convert the corresponding flow properties (porosity, saturation, and content of TDS) to
- 326 electrical conductivity (σ).
- 327 The first step of the inversion sequence refines the 3D baseline model. Fig. 4 shows slices along
- 328 the Northing direction for the initial σ -distribution resulting from the transform of the pre-
- 329 injection state calculated for the actual (left) and ORM (right). The latter one is the starting
- 330 model for the first NLCG inversion sweep which refines the pre-injection state (at year 0) below
- the upper seismic horizon (annotated in Fig. 4, cell parameters are fixed above). The output
- 332 σ (Year00) serves as the starting model for the second inversion sweep, estimating the σ -333 distribution after 8 years of injection. In the third sweep, the estimated model σ (Year08) then
- becomes the initial guess for the delineation of the plume after 12 years of injection, the output
- 335 referred to as σ (Year12).
- 336 We perform the three-step inversion sequence twice in a comparative way. The first sequence
- 337 uses constant lower and upper parameter bounds $[a, b] = [10^{-5}, 15]$ S/m; the second uses
- 338 variable bounds (Fig. 3), $[a, b] = \left[\frac{a}{f_{lb}}, b \cdot f_{ub}\right]$, that widen according to the factors f_{lb} and f_{ub} as
- described above. Variable bounds are active only for the estimation of the Year08 and Year12
- 340 states, that is, both inversion sequences employ constant bounds for the Year00-inversion. Note
- that the constant-bound sequence uses the extremal interval $[a_{min}, b_{max}]$ occurring in the
- 342 variable-bound inversion sequence. The initial reasoning for a globally wide interval was to let
- 343 the inversion practically be unbounded in order to avoid any bias due to potentially too tight
- bounds. However, other undocumented trial inversion experiments with the narrower default
- bound interval $[a, b] = [10^{-3}, 1.5]$ S/m yielded no significant difference in the final model
- outcomes.

347 Computing times amounted to a total of 126 hours for the inversion sequence with constant

bounds versus 147 total hours for the variable-bounds sequence. All inversions employed 250

349 cores of a cluster architecture with Intel Cascade Lake processor compute nodes (40 cores per

- 350 node) connected with a Mellanox EDR infiniband fabric.
- 351
- 352

353 4. Results and Discussion

354 The final plume image output is represented in Fig. 5 as differences in σ between the estimated

- 355 Year08 and Year12 models. We compare the differences $\Delta \sigma = \sigma$ (Year12) σ (Year08) in
- 356 percent for two realizations of the three-step sequential inversion outlined above. The first uses
- 357 constant bounds, the second uses spatially variable bounds. Fig. 5a shows the true distribution
- 358 $\Delta \sigma^{true}$ which is calculated from the petrophysical transform of the actual reservoir model state at
- 359 Year08 and Year12. Fig. 5b and Fig. 5c compare the estimated counterparts, these are,
- 360 respectively, the differences $\Delta \sigma^{con}$ (constant bounds) and $\Delta \sigma^{var}$ (variable bounds). Negative
- 361 changes greatly dominate in the actual outcome $\Delta \sigma^{true}$ and are visualized here since our
- 362 inversion objective focuses on the time-lapse accumulation of CO_2 which causes negative time-
- 363 lapse changes.

- 364 Most notable between the two estimates $\Delta \sigma^{con}$ and $\Delta \sigma^{var}$ is a lack of delineation of any
- 365 property changes in zones of interest away from the injection well for the image $\Delta \sigma^{con}$. In
- 366 contrast, $\Delta \sigma^{var}$ exhibits the fluid-induced property alterations across the regional scale. The
- 367 variable-bound method thus yields indicators for negative time-lapse changes associated with
- 368 CO₂ accumulation and migration. Deviations from the true case manifest in an overestimated
- 369 volume undergoing fluid-induced conductivity alterations in the Northern attic region.
- Concurrently, conductivity decreases in the region around the wells U1 and U2 remain
- 371 underestimated in terms of their magnitudes.
- 372 A certain degree of image blurring can be expected from CSEM inversions of low-frequency
- 373 data, because model resolution is limited due to corresponding large wavelengths of the
- 374 generated EM fields. However, despite the low resolution and the limited coverage using two
- 375 transmitter wells, the final image of $\Delta \sigma^{var}$ is sufficient to support predictions of CO₂-
- 376 breakthrough in the Northern attic region (Fig. 2b) with first-order accuracy. For this zone, Fig. 2
- 377 revealed a discrepancy in the elevation of predicted saturation changes (between Year08 and
- 378 Year12). This discrepancy appears only marginally in the image $\Delta \sigma^{var}$.
- 379 The large image improvement provided by the modified bounds indicates an optimization of the
- 380 model-updating line-search procedure. In essence, the method translates to steering and scaling
- the conjugate search direction of our NLCG inversion scheme such that it more closely
- 382 resembles the Newton direction. The latter is characterized by faster convergence and less
- 383 potential for a premature end of the line-search in a local minimum, yet is computationally very
- expensive. This point of view also hints at a resemblance with the method of regularized
- 385 focusing inversion (Portniaguine and Zhdanov, 1999), where stabilizing functionals convey prior
- information with the goal of image focusing.
- 387

388 5. Conclusions

- 389 Spatially variable lower and upper parameter bounds provide a straightforward way of
- 390 incorporating prior model information in an inversion workflow. Our example inversion studies
- demonstrated that such prior model information can be obtained through rough spatial estimates
- 392 of anticipated fluid-induced property alterations. Regions of property alterations that qualify as
- anomalous with respect to the property range of the underlying baseline geology are target zones
- of interest in time-lapse imaging problems. Prior-model information of such target zones
 translates to enlarged bound intervals. Our inversion study demonstrated that widened bound
- translates to enlarged bound intervals. Our inversion study demonstrated that widened bound intervals can selectively enhance model resolution in target zones. Spatially balanced bounds can
- intervals can selectively enhance model resolution in target zones. Spatially balanced bounds can thus greatly improve the imaging process through their potential of steering the NLCG search
- 397 thus greatly improve the imaging process through their potential of steering the NLCG 398 direction away from local solution minima
- 398 direction away from local solution minima.
- 399 Since reservoir modeling will likely be a minimum required tool for GCS site management, it
- 400 represents an inexpensive source of auxiliary information for constraining geophysical plume 401 imaging problems. One may thus call the presented method a "poor people's approach" to
- 401 imaging problems. One may thus call the presented method a "poor people's approach" to 402 hydrogeophysical data analysis, because inexpensive also holds for the relative simplicity in
- 402 incorporating flow information as parameter bounds. Approximate bound intervals make the
- 403 method somewhat forgiving towards petrophysical uncertainties while still constraining
- 405 geophysical parameter estimation to the physical processes of the flow system. In contrast, more
- 406 rigorous and involved fully-coupled hydrogeophysical joint inversion approaches are generally
- 407 susceptible towards erroneous petrophysical relationships (e.g., Sun and Li, 2017).

- 408 In light of a need for cost-effective monitoring, our synthetic experiments consider limitations
- 409 likely present at future GCS sites. A relatively sparse volume coverage results from employing
- 410 two existing monitoring wells for source deployment. However, fluid-induced conductivity
- 411 alterations could still be mapped, suggesting that the variable-bounds concept can help offset
- 412 model resolution loss due to limited survey coverage.
- 413 While we deem the simulated BSEM survey layout as relatively economic, more involved
- 414 studies similar to the works of Eidsvik et al. (2008) and Trainor-Guitton et al. (2014) could
- 415 figure out an informative cost measure in form of a benefit-cost ratio. Such a measure would
- 416 essentially help the operator decide whether the BSEM data's added value in form of more
- 417 accurate plume predictions outweighs the survey costs. Eidsvik et al. (2008) used the decision-
- 418 theoretic concept of value of information (VOI) with rock physics and spatial statistics in order 419 to compare the value of seismic amplitude-versus-offset data against CSEM. In our case, this
- 419 to compare the value of seising amplitude-versus-offset data against CSEW. In our case, u 420 comparison would be between well-based reservoir monitoring data against BSEM data.
- 421 Trainor-Guitton et al. (2014) presented a VOI methodology that quantifies the impact of
- 421 Tranor-Outton et al. (2014) presented a vor methodology that qualities the impact of422 inaccuracies of multidimensional geophysical inversions on geothermal resource identification.
- 423 Translated to GCS contexts, a VOI assessment of constrained EM data inversions as presented
- here might help analyze aspects of interest to the operator that go beyond cost, for example
- 425 leakage risk and environmental impact.
- 426 A final related comment concerns ORM uncertainty, as discussed in Section 2.4., as a major
- 427 factor influencing VOI of BSEM monitoring. Despite fairly significant deviations from the
- 428 actual model, the 5-year ORM produced a gross-scale match of the actual gas saturation that
- 429 turned out sufficient for the bound construction and ensuing delineation of anticipated target
- 430 zones. A follow-up study similar to Harp et al. (2019) would investigate at what point larger
- 431 deviations, caused by larger ORM parameter errors, would render the BSEM imaging outcome
- too distorted. Harp et al. (2019) developed a metric for quantifying the degree to which ORM
- 433 parameters can deviate from their actuals without violating preset reservoir performance criteria.
- 434 We envision a similar kind of robustness measure for assessing when an ORM may become too
- 435 erroneous for properly constraining geophysical reservoir imaging.
- 436

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592

Fig. 1: Actual (a) and operational (b) permeability model. Vertical slices (lower subplots) are along the diagonal (A-A', dashed) line and show the stratified reservoir heterogeneity with highpermeability attic zones. The actual model features vertical faults as black line segments (one blue line in the simplified model). Vertical exaggeration is two times. Note that the (*x-y*) plan

597 views are not horizontal as they are a projection of the top layer in the reservoir model.

598



600

601 Fig. 2: Gas saturation predictions calculated from the actual (a) and 5-year operational (b) 602 reservoir flow model. The right plot column shows gas saturation differences between predictions made at 8 and 12 years. Each monitoring well U1 and U2 hosts one borehole EM 603 604 transmitter at a depth of 1850 m, sourcing the shown surface receiver grid. Receiver profiles 605 extend from y=-1500 m to y=4000 m, with a station interval of Δy =125 m. 606





608 Fig. 3: Augmented lower and upper parameter bounds. The example cross sections are through 609 the Easting coordinate E=240 m.

- 610
- 611





613 Fig. 4: Petrophysical transform of the actual (left) and operational (right) flow model into the 614 baseline (Year00) electrical conductivity. Conductivities derived from the operational model 615 serve as the initial model guess for the inversion that refines the Year00 (pre-injection) model

- below the upper seismic horizon (indicated by the white lines). The upper horizon delineates the upper boundary of the inversion domain.



- Fig. 5: Electrical conductivity change $\Delta \sigma = \sigma$ (Year12) – σ (Year08) resulting from the
- corresponding gas saturation changes between Year08 and Year12. (a) True difference $\Delta \sigma^{true}$
- calculated from the actual model. (b) Estimated difference $\Delta\sigma^{con}$ resulting from the constant-bound inversion sequence. (c) Estimated difference $\Delta\sigma^{var}$ resulting from the variable-bound
- inversion sequence.