

Inverse modelling of core flood experiments for predictive models of sandstone and carbonate rocks

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Key Points:

- This paper demonstrates a workflow for creating predictive models of heterogeneous sandstone and carbonate rocks
- Multi parameter fitting of capillary pressure functions and permeability-capillary pressure correlations are introduced into the iterative modelling approach
- The new parameters are fit in a sequential iterative approach constrained against over fitting
- The developments lead to major improvements in the history matching and predictive capability of models for three carbonate and two sandstone rock samples samples with wide ranging heterogeneities

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Abstract

Evidence from field-scale simulations and on-site observations suggests that multi-scale rock heterogeneities control subsurface fluid flow, and these must be characterised for accurate predictions of fluid migration, such as during CO₂ sequestration. Recent efforts have focused on continuum simulation-based inversion of laboratory observations with X-ray imaging, but models produced in this way have been limited in their predictive ability for highly heterogeneous rocks. We address the main challenges in this approach through the development of an algorithm that combines a number of significant advancements: the use of a 3-parameter capillary pressure model fitting, the implementation of spatial heterogeneity in absolute permeability, the constraint of history match iterations based on marginal error improvement, and more sophisticated image processing incorporating more of the experimental data in the calibration. We demonstrate the major improvement resulting from this workflow on five rocks (two sandstones and three carbonates), representing a range of heterogeneous properties, some of which could not be previously modeled. The algorithm results in physically representative 3D models of all the rock cores, reducing non-systematic error in both calibration and prediction of flow properties to a level comparable to the experimental uncertainty.

Plain Summary

Porous materials, both natural and man-made, exhibit spatial heterogeneity ranging from rock pores to the scales of geological units. Accurately characterising the impact of rock heterogeneity on hydrodynamic properties has been extensively studied but remains an open scientific question, particularly at the core scale of a few decimeters. This study demonstrates a new approach to effectively characterising the flow properties of highly heterogeneous rocks, including sandstone and carbonate rocks. This approach overcomes major barriers that previously prevented the successful modelling of highly heterogeneous rocks. As a result, it is now possible to characterise multiphase flow property heterogeneity in a wide range of rock types.

1 Introduction

Accurately characterising subsurface multiphase flow in permeable rocks is critical for analysing a wide range of natural and engineering phenomena, such as environmental contaminant remediation, subsurface energy resource development, and carbon geosequestration for climate change mitigation. Difficulties in modeling the physical processes governing fluid flow can lead to inaccurate field-scale flow simulations. This issue is prominent at CO₂ storage sites, where scientific pilot and industrial demonstration projects have demonstrated unexpectedly rapid CO₂ migration in directions that are difficult to forecast and history match [Halladay *et al.*, 2018]. Heterogeneity in the multiphase flow properties, relative permeability and capillary pressure, has been identified as one cause of the unexpected flow phenomena observed at field sites [Jackson and Krevor, 2020; Benham *et al.*, 2021]. However, there are no established workflows to characterise these heterogeneities.

Core analysis techniques have been developed to characterise the flow properties of subsurface rocks, including porosity, absolute permeability, capillary pressure, and relative permeability [Calhoun *et al.*, 1949; Jones and Roszelle, 1978; Ali, 1997; McPhee *et al.*, 2015]. Since the 1970s, medical X-ray computed tomography has been used to image multiphase flow experiments, providing direct observations of the 3D distribution of porosity and fluid saturation at controlled flow conditions [Withjack, 1988]. Computer-based inverse modelling is standard practice to account for the effects of boundary conditions on the interpretation of relative permeability from core-flooding tests [Archer and Wong, 1973; Nordtvedt *et al.*, 1999; Berg *et al.*, 2021].

Inverse modeling using X-ray imagery of fluid saturation distributions in core floods has also been used to parameterise heterogeneous capillary pressure characteristics in one-dimensional and three-dimensional models [Huang *et al.*, 1995; Egermann and Lenormand, 2005; Krause *et al.*, 2011, 2013; Kong *et al.*, 2015; Oh *et al.*, 2015; Jackson *et al.*, 2018; Hejazi *et al.*, 2019; Anto-Darkwah *et al.*, 2023]. In these approaches, a model is calibrated by scaling spatially varying capillary pressure characteristic curves until observed and simulated saturations are matched within experimental uncertainty. These models were initially used for the interpretation of core flood tests [Huang *et al.*, 1995; Egermann and Lenormand, 2005]. A number of developments have improved the history match of models to observed saturation distributions, including multi-parameter fitting of capillary pressure curves [Kurotori and Pini, 2021; Anto-Darkwah *et al.*, 2023], the inclusion of variation in absolute permeability [Krause *et al.*, 2011], and the extension of the approach to hysteretic drainage and imbibition cycles [Anto-Darkwah and Rabinovich, 2022]. Expanding the focus beyond history matching observations, Krause *et al.* [2011, 2013] introduced an iterative history match

73 procedure that resulted in models with predictive capability for estimating upscaled flow properties.
74 This was further developed and confirmed to result in physically representative models of sandstone
75 rocks with modest heterogeneities [*Krause and Benson, 2015; Jackson et al., 2018; Wenck et al.,*
76 *2021*]. These predictions can be important for identifying flow properties of heterogeneous rocks in
77 the capillary-dominated flow regimes typical of subsurface reservoirs [*Jackson and Krevor, 2020*].

78 However, *Wenck et al. [2021]* showed that the iterative approach may fail to predict upscaled flow
79 properties when applied to highly heterogeneous rocks. More heterogeneous rocks may exhibit strong
80 variation in the form of local capillary pressure curves, and competing control of viscous and capillary
81 forces on the fluid saturation distribution. Thus the iterative approach for more heterogeneous rocks
82 may benefit from the inclusion of multi-parameter capillary pressure fitting, e.g., *Kurotori and Pini*
83 [*2021*] and spatial variation in absolute permeability, e.g., *Krause et al. [2013]*. At the same time,
84 the introduction of more model parameters brings with it an increased risk of overfitting that must
85 be balanced against the systematic errors arising from underparameterisation.

86 In this work, we demonstrate that addressing these issues collectively results in a model con-
87 struction workflow that can predict upscaled flow properties for sandstone and carbonate rocks with
88 a broad range of heterogeneities. We build on the iterative approaches described in *Jackson et al.*
89 [*2018*] and *Wenck et al. [2021]*, while introducing flexibility in the capillary pressure characteristic
90 curve, incorporating a third parameter to control the model curvature following the work of *Kurotori*
91 *and Pini [2021]*. We reintroduce spatial variation in absolute permeability by utilizing a correlation
92 with the capillary pressure. To mitigate potential model overfitting, we introduce a constraint on
93 iterations, controlled by the marginal error reduction in the calibration. The resulting algorithm
94 minimizes systematic errors to the extent that they are comparable to experimental uncertainty, both
95 in model calibration (history match) and predictive capability of upscaled relative permeability.
96 Analysis of the fit parameter distribution provides insights into the nature of the model calibrations
97 concerning non-uniqueness and over-determination issues.

98 **2 Methodology**

99 **2.1 Experimental datasets**

100 Five experimental datasets were studied in this work. They were derived from two sandstone
101 and three carbonate rock cores representing a range of heterogeneous properties. The datasets
102 comprise observations from steady state core-flooding experiments that were previously performed
103 and reported in *Reynolds and Krevor [2015]; Reynolds et al. [2018]; Manoorkar et al. [2021]; Wenck*

104 *et al.* [2021]. The experiments co-injected nitrogen and water or CO₂ and brine at high (HR) and
 105 low (LR) flow rates to obtain flow parameters in the viscous-limit (VL) and capillary-limit (CL) flow
 106 regimes, with capillary number in Table S6 of *Wenck et al.* [2021]. A medical X-ray CT scanner was
 107 used to take 3D X-ray images of the cores. Permeability and porosity of the rock cores were measured
 108 either or with both a permeameter and the core-flooding rig. Mercury intrusion porosimetry (MICP)
 109 experiments were conducted to obtain the capillary pressure characteristic curves.

110 The X-ray imagery obtained from each sample includes dry, water and gas saturated scans, as
 111 well as scans taken during the co-injection of fluids at ratios, or fractional flows. Each X-ray scan
 112 was repeated several (5-10) times to enable averaging and reduction of image noise. Both porosity
 113 (ϕ^i) and saturation (S_f^i) in each image voxel in the experiments were calculated in the standard way
 114 for medical X-ray CT imagery. The average grey values of the X-ray scans of the dry rock (\mathcal{P}_d),
 115 single phase saturated scans (\mathcal{P}_w and \mathcal{P}_{nw} for wetting and non-wetting phases, respectively), as well
 116 as partially saturated scans (\mathcal{P}_f , with subscript f for fractional flow) were recorded. The greyscale
 117 values of the CT scans were used to estimate the saturation of each phase at each grid block (i) using
 118 Equations 1,

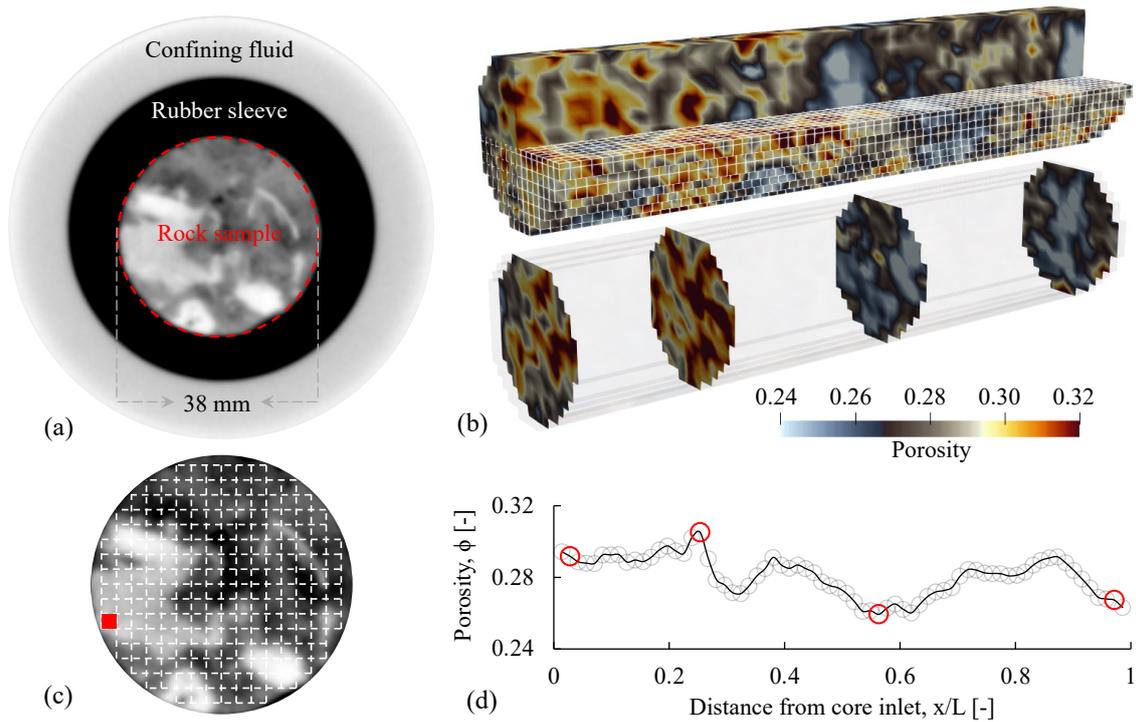
$$\phi^i = (\mathcal{P}_w - \mathcal{P}_d)/\mathcal{P}_0, \quad S_f^i = (\mathcal{P}_f - \mathcal{P}_{nw})/(\mathcal{P}_w - \mathcal{P}_{nw}), \quad (1)$$

119 where \mathcal{P}_0 is the difference in grey value between a fluid phase and air.

120 2.2 Model calibration

121 The first stage in the generation of the numerical model of the rock cores from X-ray imagery
 122 involves pre-processing the images. The images of the rock core are made of stacks of image slices.
 123 In each slice, we extracted the section comprising the rock core with a circle pattern by detecting
 124 the boundary of the core and rubber sleeve, as shown in Figure 1(a). The structural similarity index
 125 from *Wang et al.* [2003] was also calculated for different scans to further adjust the core extraction
 126 locations before averaging the images yielded from repeated scans to reduce the noise.

130 Next, numerical continuum models of the rock cores were created from the images. The grid of
 131 the models was created by meshing the raw X-ray CT imagery to element-based models by applying
 132 a 3D convolution matrix with a specified element size, Figure 1(b). The size of the element volume,
 133 Figure 1(c), chosen for the models was guided by combined consideration of the apparent length
 134 scales of rock heterogeneity, the experimental saturation precision, and the computational cost. The
 135 element volume must be large enough such that the assumption of a continuum property such as
 136 permeability is valid, while sufficiently small so that heterogeneities in these properties are captured



127 **Figure 1.** The upscaled core-scale structure. (a) Raw image from CT scanning with effective domain in the
 128 red circle. (b) 3D porosity field and the cross-sectional map. (c) The upscaled element volume concept (red
 129 square) and the meshed grey image. (d) The cross-sectional average porosity profile from inlet to outlet.

137 (See *Jackson et al. [2018]*). The size of the element volume for this work was chosen to be 2 mm
 138 [*Manoorkar et al., 2021; Wenck et al., 2021*].

139 The initial setup, depicted in Algorithm 1 and Figure S1 of Supplementary Information (S1),
 140 is followed by the image processing and upscaling of experimental parameters. The porosity field
 141 obtained from the X-ray imagery (Equation 1) was used to parameterise the model. The inlet
 142 flux and outlet pressure conditions of the simulation were intended to represent the experiments
 143 by using two buffer layers with high permeability and zero capillary pressure. To initialise the
 144 model, the hydrodynamic properties (e.g., permeability, capillary pressure) of local grid blocks were
 145 approximated based on the parameters of host and neighbouring grids, which we refer to as a cell
 146 unit in this work. As an alteration, the cell unit can also be implicitly assumed to be a slice of the rock
 147 core (especially layers perpendicular to the flow direction) through the assumption that the capillary
 148 pressure in each slice was constant. In the initial model setup, a prior measured capillary pressure
 149 curve (usually from MICP measurements) was assumed to represent the core-average parameter. The

150 experimental saturation (S_f^i) of the cell unit (rock core slice) is an observed parameter. Therefore,
 151 in each cell unit, the capillary pressures at distinct fractional flows can be estimated using the whole
 152 core capillary pressure curve and the phase saturation of the cell unit. Then, experimentally observed
 153 saturation fields within a cell unit at distinct fractional flows were used to estimate an initial capillary
 154 pressure - saturation relationship for each grid block. In summary, the initial parameterisation of
 155 heterogeneous capillary pressure characteristics is based on three observations: an *a priori* measured
 156 capillary pressure characteristic curve assumed to represent the rock core as a whole, the average
 157 saturation within each cell unit to constrain the capillary pressure in that cell unit, and the saturation
 158 distribution within the cell units to generate the various $P_c - S_w$ pairings comprising the capillary
 159 pressure characteristic curves. Subsequently, the capillary pressure characteristic curves were used
 160 as matching parameters in a sequential algorithm, described in detail below. We minimise the
 161 mismatch in observed and simulated local saturation using a capillary pressure function as the tuning
 162 parameter.

163 One of the main advancements highlighted in this work is the introduction of a multi-parameter
 164 fitting approach for local capillary pressure relationships. The model used in this work was proposed
 165 by Li [2004] based on the classic Brooks and Corey capillary pressure model [Brooks and Corey,
 166 1966],

$$P_c = P_{\max} \left(1 - \left(1 - \alpha^{-\lambda} \right) S^* \right)^{-\frac{1}{\lambda}}, \quad (2)$$

167 where $\alpha = P_e/P_{\max}$ is the ratio of entry capillary pressure to the maximum capillary pressure, λ is a
 168 parameter related to the pore throat size distribution, and the wetting phase saturation normalised to
 169 an irreducible saturation, S_{wi} , is $S^* = (S_w - S_{wi})/(1 - S_{wi}) \in [0, 1]$.

170 The parameters used in the fitting are the entry pressure, P_e , the maximum capillary pressure,
 171 P_{\max} , which is the capillary pressure at the residual non-wetting phase saturation, and the model
 172 curvature λ which is related to the pore throat size distribution. We use a sequential approach
 173 in varying these parameters to fit the data to avoid non-uniqueness arising from the simultaneous
 174 coupling of multiple parameters. We first fit the entry capillary pressure while limiting any variation
 175 of the other parameters as an initial estimation. Then the maximum capillary pressure and curvature
 176 are subsequently varied by gradually increasing the range constraint. To mitigate the risk of over-
 177 fitting, a range limit is implemented when expanding the boundary conditions of fitting parameters
 178 does not improve the fitting accuracy. The first loop of Algorithm 1 in the SI iterates until the tuning
 179 results in a saturation distribution achieving the preset tolerance.

180 Subsequently, a second loop is carried out which is the same as the first loop, except that the
 181 absolute permeability is also varied for each grid block. Permeability is estimated for each grid block
 182 using a correlation with the porosity and capillary pressure curve developed by *Li et al.* [2021]. The
 183 correlation was based on a bundle of tubes and the classic Purcell-Burdine model [*Purcell*, 1949;
 184 *Burdine*, 1953; *Nakornthap and Evans*, 1986], Equation 3.

$$k = 10.66 \frac{\beta}{2n} (\sigma \cos \theta)^2 \phi^3 (1 - S_{wi})^3 \int_0^1 \frac{1}{P_c^2} dS^*. \quad (3)$$

185 Combining Equations 2 and 3, results in the basic form of the correlation for absolute perme-
 186 ability,

$$k = 10.66 \frac{\beta}{2n} (\sigma \cos \theta)^2 \phi^3 (1 - S_{wi})^3 \frac{1}{P_{max}^2} \frac{\lambda}{\lambda + 2} \frac{1 - \alpha^{-(\lambda+2)}}{1 - \alpha^{-\lambda}}. \quad (4)$$

187 A more general form of the function was then given by,

$$k = a_1 \phi^{a_2} (1 - S_{wi})^{a_3} \frac{1}{P_{max}^{a_4}} \left(\frac{\lambda}{\lambda + 2} \frac{1 - \alpha^{-(\lambda+2)}}{1 - \alpha^{-\lambda}} \right)^{a_5}. \quad (5)$$

188 *Li et al.* [2021] empirically fit the coefficients in Equation 5 using measurements made on 151
 189 rock samples across a range of lithologies. In this work, the coefficients $a_2 \dots a_5$ were adopted from
 190 *Li et al.* [2021]. The value of a_1 for all grid blocks is shifted such that the absolute permeability of
 191 the whole core remains equal to the measured value. The updated absolute permeability is utilized
 192 in subsequent simulations and further affects the sequential capillary pressure fitting.

193 While considering relative permeability heterogeneity is a possibility, doing so would necessitate
 194 the imposition of more experimental constraints. Although models have been developed to correlate
 195 relative permeability to other properties, particularly the capillary pressure characteristics [*Li*, 2004],
 196 these models are less well validated relative to the capillary pressure - permeability relationships. In
 197 this work, the input relative permeability is the same for all grid blocks throughout the model.

198 **3 Results and discussions**

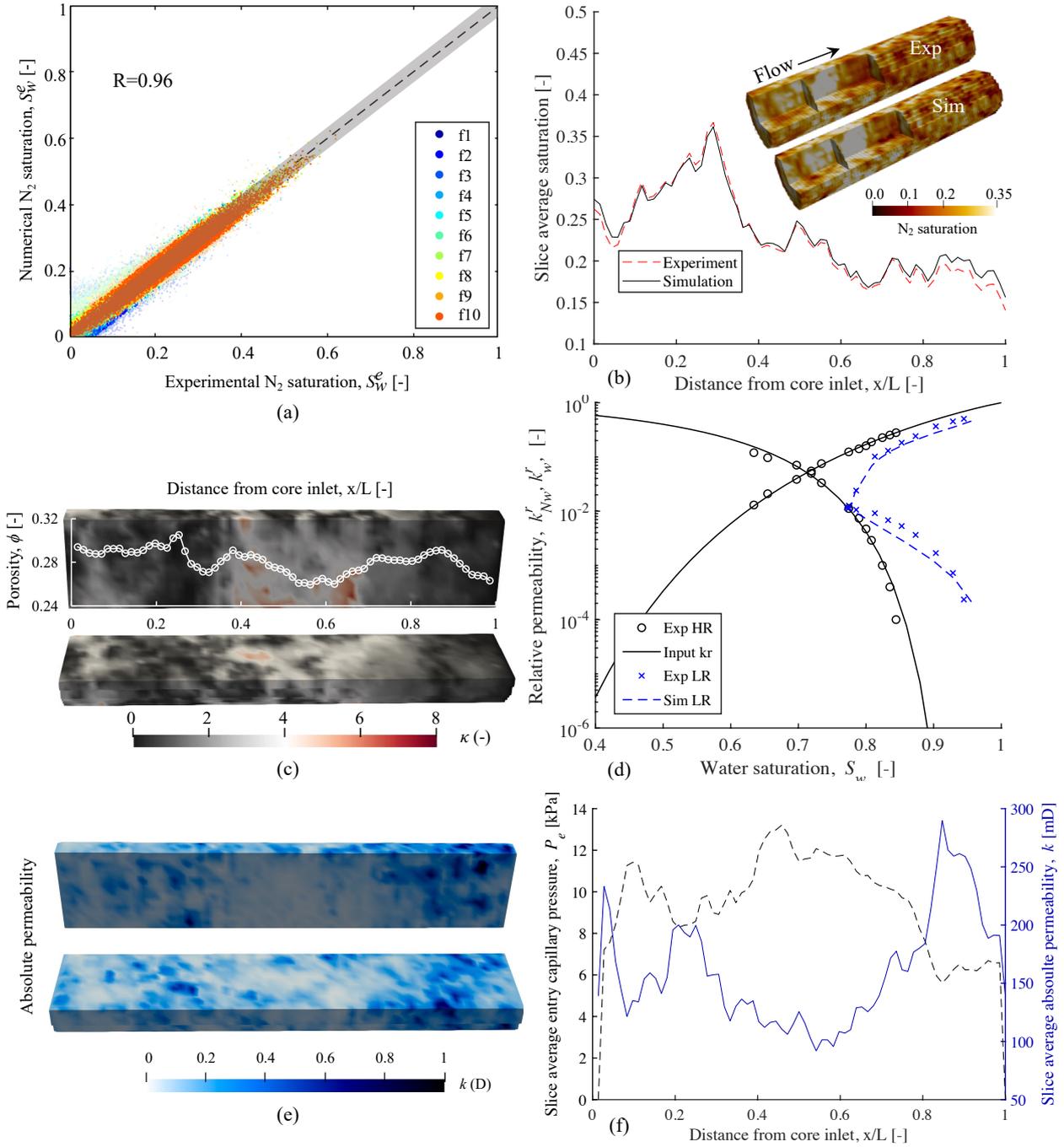
199 The results for the Estailades Limestone sample are described in detail, followed by a discussion
 200 of the results for the other rocks. The properties of the sample (absolute permeability, open-source
 201 image data, MICP data, relative permeability, etc.) can be found in *Manoorkar et al.* [2021]; *Wenck*
 202 *et al.* [2021]. Using the modified X-ray image processing algorithm, about 82% of the sample
 203 volume is included in the numerical model, Figure 1. The experimental MICP data was fitted using
 204 Equation 2 to obtain the whole core representative capillary pressure curve. The viscous limit

205 relative permeability curve was obtained by fitting a Chierici function [Chierici, 1984] to the high
206 flow rate (20 mL/min) experimental data and used as input to the simulation.

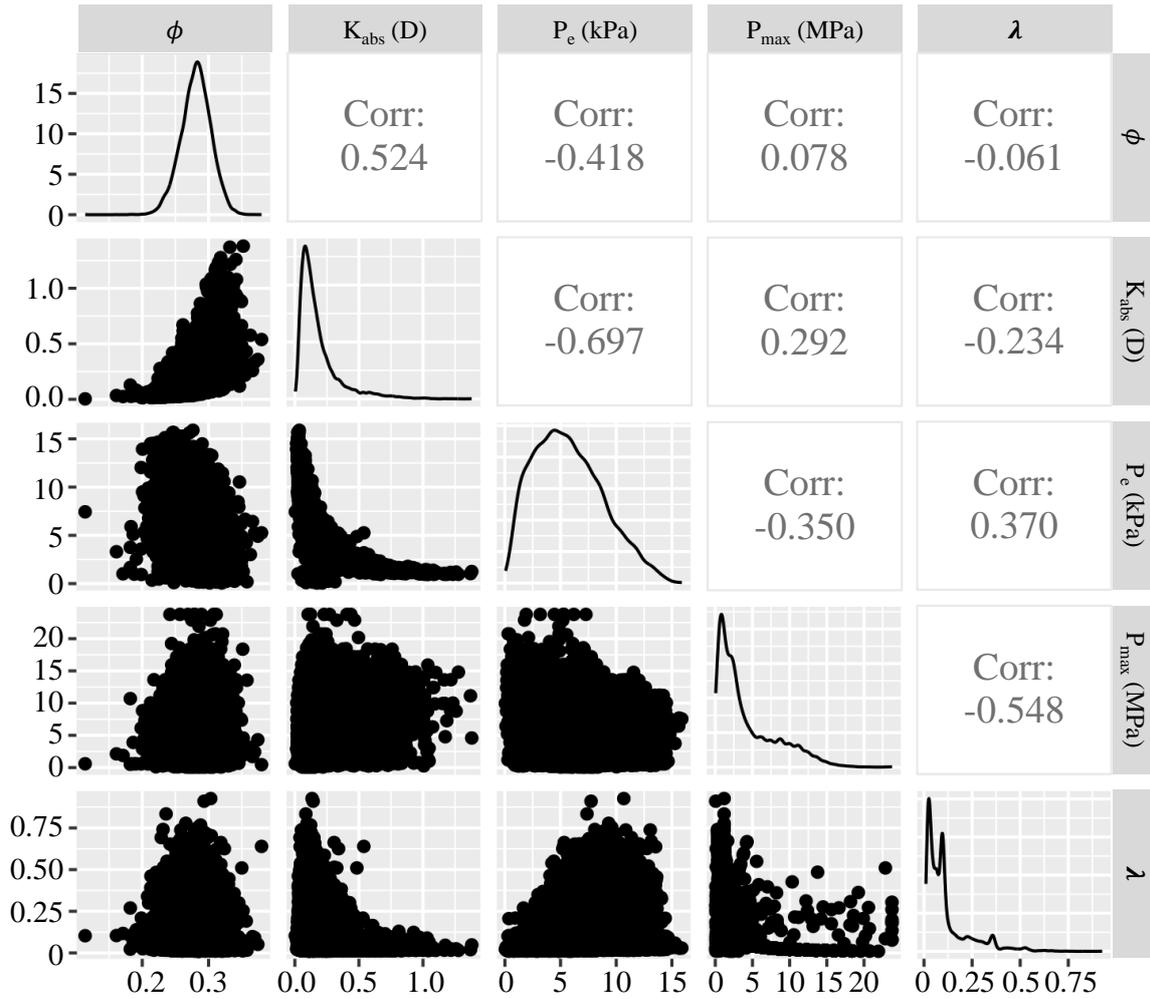
207 After initialising the numerical model, iterations were carried out to match the saturation field
208 from low flow rate experiments (0.5 mL/min). The matching results are shown in Figure 2 by visual
209 comparison of saturation distributions in 1D and 3D, and by plot of simulated and observed saturation
210 values for corresponding locations in the rock and model, respectively. The 3D distribution patterns
211 of N₂ saturation are visually similar between the experiment and simulations, particularly the larger
212 scale features. The slice averaged N₂ saturation profile at the final state is shown in Figure 2(b),
213 and further shows that the fitting result is able to accurately capture the saturation distribution. The
214 goodness of fit is quantified in the graph of Figure 2(a), showing the location by location comparison
215 of simulated and observed saturations at all fractional flow stages. The data mostly falls within the
216 experimental uncertainty. Experimental N₂ saturation and numerical values have a linear dependence
217 with a Pearson correlation coefficient of 0.95.

218 The saturation distribution is the fitting target to construct the numerical model. The validation
219 of the calibrated model comes from its use in predicting the observed relative permeability data for
220 the experiment data at the low flow rate, and this is shown in Figure 2 (d). The experimentally derived
221 datapoints are direct observations of the average saturation and relative permeability calculated from
222 the observed pressure differential using Darcy's law, and do not use any correction for capillary
223 end effects. We are, in essence, predicting the observables of the experiment with the simulation
224 to validate our model. The deviation of the data and curves at low fluid flow rates from the data
225 and corresponding simulation input obtained at high flow rate (black points and curve in Figure 2
226 (d) reflects the combined impact of heterogeneities in the rock, and capillary end effects. From the
227 comparison, we can conclude that the low flow rate relative permeability is successfully predicted
228 with a correlation coefficient of 0.98.

229 The proposed algorithm provides a way to characterise the absolute permeability and capillary
230 pressure distribution in the decimeter-scale rock sample, and these results are shown in Figures 2(c),
231 (e), and (f). Comparing Figures 2(c) and 1(b), we can observe the entry capillary pressure field
232 has a positive relation with porosity distribution in this instance, although this is not imposed by
233 the models. There is an imposed correlation between absolute permeability, capillary pressure, and
234 porosity from Equation 5, and this can be seen in Figures 2(e) and (f).



235 **Figure 2.** The results of the history matching, characterisation, and prediction for Estailades Limestone
 236 sample. (a) The voxel saturation correlation plot comparing the experiment and the simulation based saturations.
 237 The grey bar shows the experimental uncertainty in the estimate of saturation from the imaging. (b) The cross-
 238 sectional average saturation from inlet to outlet at the final state, with 3D saturation distribution from CT
 239 scanning and simulation. (c) The characterisation of capillary heterogeneity using κ , with slice average porosity
 240 embedded. (d) The fitted relative permeability curves at a high flow rate for simulation input, and the comparison
 241 of simulation results and experimental curves at a low flow rate to estimate the prediction. (e) The 3D absolute
 242 permeability field in the characterisation domain. (g) The slice averaged entry capillary pressure (left y axial)
 243 and absolute permeability (right y axial) from inlet to outlet.



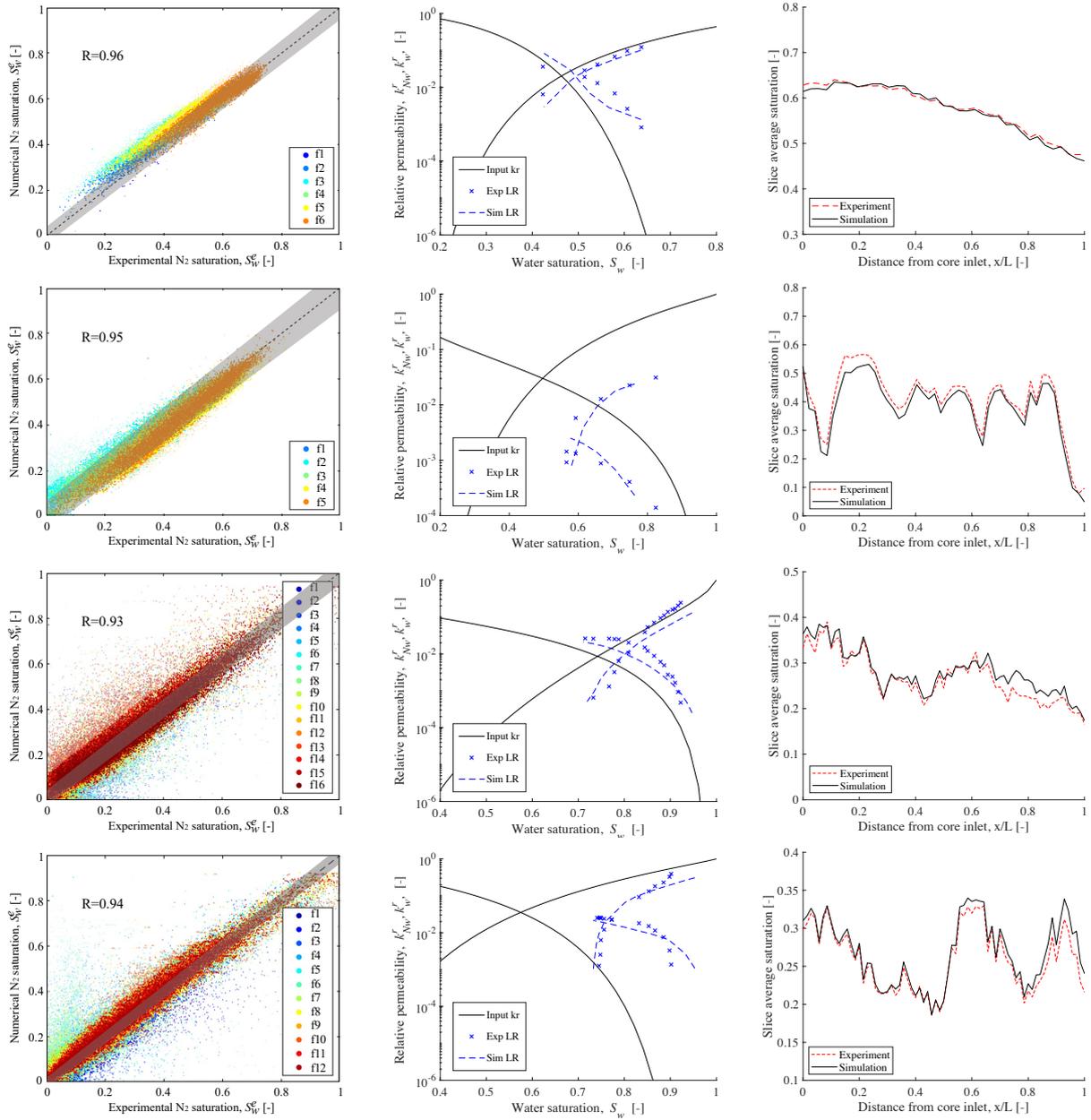
244 **Figure 3.** The correlation of characterised parameters (namely porosity, absolute permeability, entry capillary
 245 pressure, maximum capillary pressure, and the curvature λ) for Estailades Limestone sample.

246 The algorithm in this study is a multi-parameter non-linear fitting process. To diagnose the
 247 potential for over-fitting, the cross correlation between porosity, absolute permeability, and capillary
 248 pressure parameters is calculated using GGally *Schloerke et al.* [2018]. These are shown in Figure 3.
 249 As expected, the entry capillary pressure is negatively correlated with porosity. Additionally, among
 250 all the correlations, the absolute permeability has stronger correlations with porosity, entry capillary,
 251 and even the curvature characterisation parameter (λ), as we derived the values using Equation 5.
 252 The few systematic errors (Figure 2(a)) and low cross correlations between parameters (Figure 3),
 253 other than the ones that are imposed, indicate that the model has high fidelity.

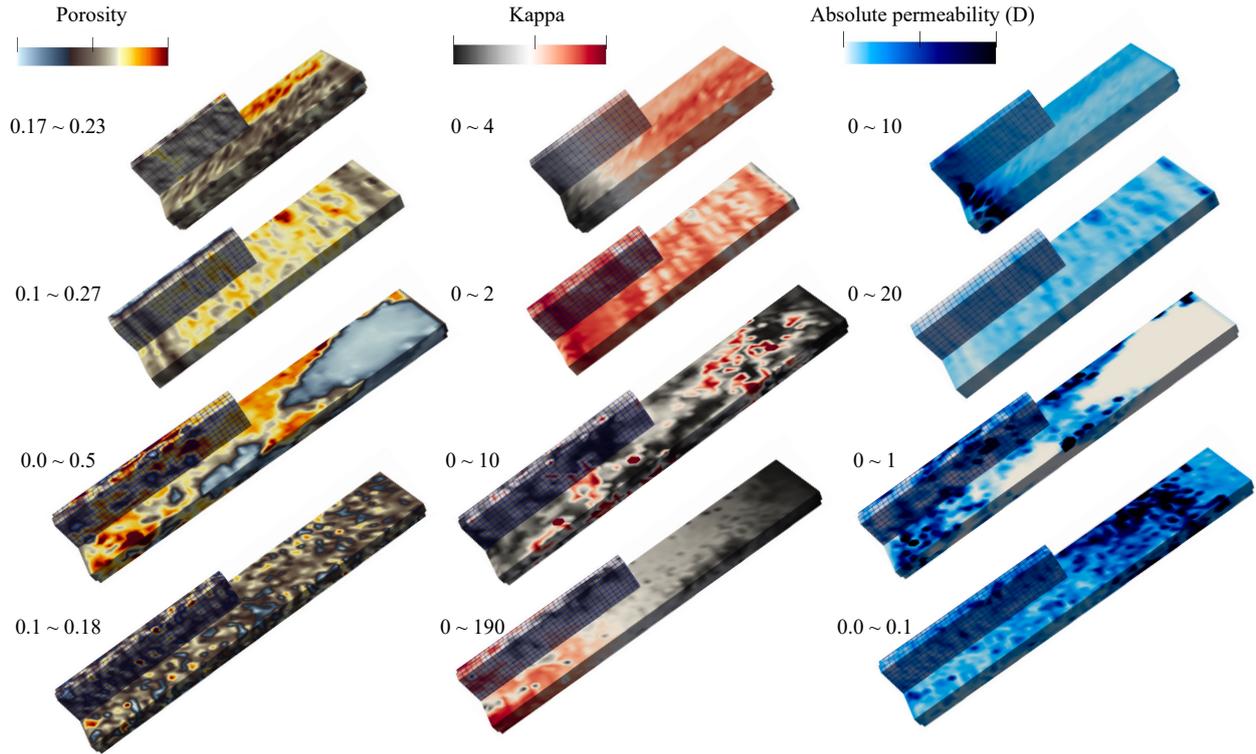
254 The results for the other four rocks, two sandstone (Bentheimer and Bunter) rocks and two
255 carbonate (Edwards and Indiana) cores, are shown in Figure 4. The 3D porosity, capillary pressure
256 and absolute permeability distributions are shown in Figure 5. The calibrated saturation distribution
257 and the validating predictions of relative permeability indicate that the constructed models are able
258 to represent the salient flow properties of the rocks.

259 We now describe the improvements made using this approach relative to past approaches. The
260 sandstone rocks in this study were already successfully modelled using the approach of *Jackson*
261 *et al.* [2018]; *Wenck et al.* [2021], and benefit marginally from the developments in this work. The
262 Bentheimer sandstone is a shallow marine deposit, composed of ~95% fine to medium-grained
263 quartz [*Peksa et al.*, 2015]. The sample is characterised by a layer parallel to the flow direction.
264 The modelling of the Bentheimer benefit mostly from the improved image processing algorithm, i.e.,
265 incorporating a larger fraction of the imaged sample into the modelling. We successfully characterised
266 the laminated structure parallel to the flow direction. The heterogeneity was also reflected in the
267 capillary pressure and absolute permeability distribution. The other utilised sandstone, the Bunter
268 sandstone, is composed mainly of subangular to subrounded quartz grains with a minor component
269 of detrital K-feldspar, clay, as well as carbonate clasts, and exhibits characteristics of early diagenetic
270 processes [*Brook et al.*, 2003]. From the characterisation, the chosen Bunter sample shows lamination
271 perpendicular to the flow direction. Compared with other carbonate rocks, the two sandstone samples
272 have orders of magnitude larger absolute permeability, and smaller variations in the capillary pressure
273 characteristics.

274 In contrast to the sandstone rocks, modelling of the carbonate rocks was significantly improved
275 relative to *Wenck et al.* [2021]. The Edwards Brown - from the Upper Cretaceous in Texas, USA
276 - is mainly composed of ~90% dolomite and calcite, as well as ~10% quartz [*Lai et al.*, 2015].
277 The sample has decimeter-scale correlated porosity, with low-porosity regions near the outlet of the
278 sample, as shown in Figure 5. This is the largest scale correlation among all samples. The capillary
279 pressure and absolute permeability field also exhibit strong heterogeneity. The Estailades rock from
280 the Estailades quarry (SE, France) is a Cretaceous bioclastic limestone with ~98% calcite, as well
281 as ~2% dolomite, silica and other minerals [*Le Guen et al.*, 2007; *Manoorkar et al.*, 2021]. The
282 characterisation (Figures 1 and 2) indicates that the Estailades sample has centimeter-scale spatial
283 correlation lengths in petrophysical parameters. Another carbonate sample (Indiana limestone)
284 contains ~97% calcite, ~1.2% magnesium carbonate, and other minor components [*Churche et al.*,
285 1991]. The porosity of the Indiana limestone rock has a millimeter-scale correlation length and the
286 smallest variation among three carbonate samples.



287 **Figure 4.** Rows from top to bottom represent Bentheimer sandstone, Bunter sandstone, Edwards carbonate,
 288 and Indiana carbonate rocks, respectively. Left column: The voxel saturation correlation plot comparing
 289 the experiment and simulated saturations from the calibration stage. Middle column: The fitted relative
 290 permeability curves at a high flow rate for simulation input, and the comparison of predicted simulation results
 291 and experimental curves at a low flow rate. Right column: the cross-sectional average saturation from inlet to
 292 outlet at the final fractional flow.



293 **Figure 5.** Rows from top to bottom represent Bentheimer sandstone, Bunter sandstone, Edwards carbonate,
 294 and Indiana carbonate rocks, respectively. Columns from left to right represent the 3D porosity, capillary entry
 295 pressure, and absolute permeability fields.

296 The improvements in generating physically representative models arose from all of the modi-
 297 fications introduced in this work. Through changes to the image processing algorithm, the size of
 298 the characterised domain for the rocks used in this study has been increased from ~50% to ~80%,
 299 compared to previously published results [*Jackson et al., 2018; Wenck et al., 2021*]. Although the
 300 expanded domain may lead to more numerical errors, the aligned images more accurately depict the
 301 experimental situation. A more general capillary pressure model with three fitting parameters was
 302 used to fit the capillary pressure curve in each local element. Figure S2 in SI illustrates that the local
 303 capillary pressure property was more reasonably fitted using a combination of entry capillary pres-
 304 sure, curvature, as well as maximum capillary. The correlation coefficient (R^2) increased from 0.75
 305 to 0.92 for the example cell. The heterogeneous absolute permeability field also led to improvements
 306 in the relative permeability prediction. Finally, constraints on the number of iterations mitigated
 307 the potential for over fitting. At this stage, the proposed algorithm represents a versatile approach

308 to creating the physically representative models of a wide range of rock types needed for accurate
 309 modelling of field scale fluid migration processes.

310 **Acknowledgments**

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 312 London.

313 **Data Availability**

314 The readers can find the input data and raw data of figures presented in the manuscript in the
 315 Mendeley repository with the doi: 10.17632/wwt pcsng76.1.

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