Supplementary Information: Characterisation of multiphase flow in heterogeneous rocks

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1 The flow chart of model calibration algorithm

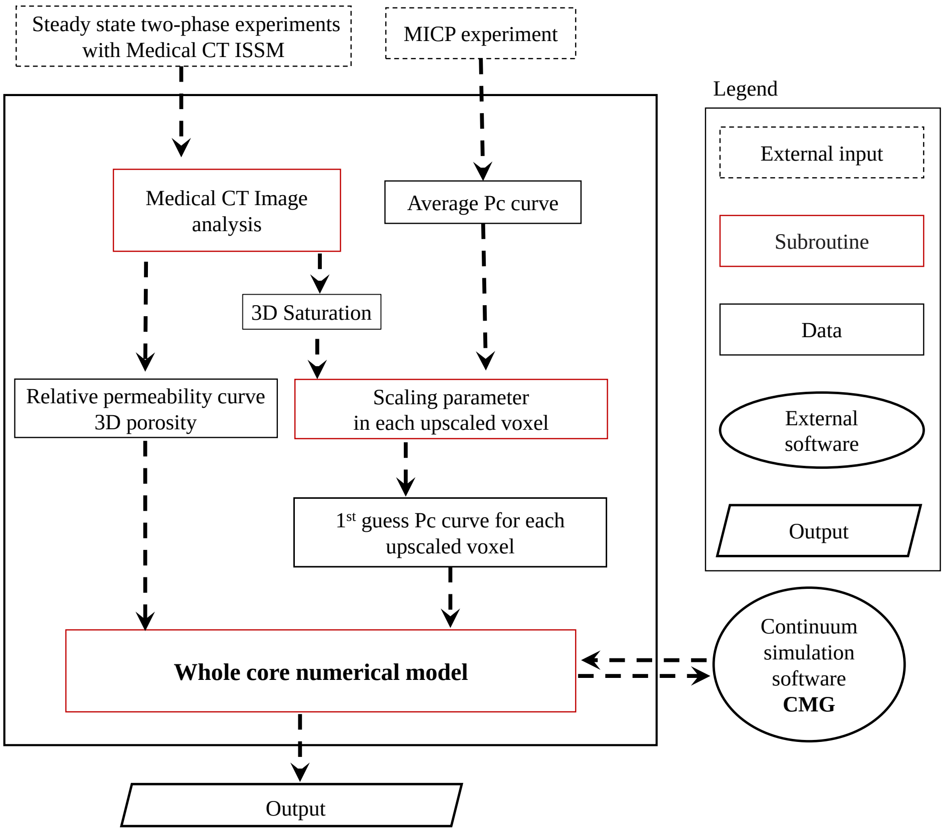

Figure S1. The flow chart of calibration algorithm.

The data utilized in this study includes steady state corefloodiing experiments that were conducted with medical X-ray CT imaging, as well as mercury injection capillary pressure (MICP) experiments to obtain capillary pressure characteristic curves. As illustrated in Figure S1, the processed data, such as porosity distribution, saturation field at different fractional flows, and capillary pressure, are inputted into the fitting iteration algorithm (Algorithm 1 in the main text). In each iteration step, the CMG solver is utilized to simulate the continuum two-phase flow.

Algorithm 1: Pore to Core Upscaling

Input : Experimental data from steady-state two-phase X-ray CT scans and MICP

Output : A constructed core-scale numerical model, sample characterization, and observations of multiphase flow

Image processing, and upscaling of parameters to obtain the porosity distribution and the dynamic saturation in each elementary volume under various fractional flows

Fitting relations for experimental relative permeability and capillary pressure data

Continuum model construction, and inlet and outlet boundary conditions setting to mimic the steady state two-phase experiments, as well as the initial parameters calculation

for $k = 1, \cdots, K_i$ **do**

  Continuum scale flow simulation with uniform absolute perm and relative perm

  PC curve fitting in each element based on numerical P_c and experimental S_w

  The comparison of numerical and experimental saturation for tolerance judgement

end

for $k = 1, \cdots, K_j$ **do**

  Continuum-scale flow simulation in whole core

  PC curves updating in each element

  Absolute updating in each element

  The comparison of numerical and experimental saturation

end

2 Capillary pressure fitting

An important advancement introduced in this study is the adoption of a multi-parameter fitting approach for capillary pressure relationships in each local element. The fitting process employs the entry pressure, P_e, the maximum capillary pressure, $P_{\max}$ (which corresponds to the capillary pressure at the residual non-wetting phase saturation), and the model curvature λ (which is linked to the pore throat size distribution) as parameters. To demonstrate the effectiveness of the combined fitting parameters, a single cell in the Estaillades Limestone sample is selected to showcase the fitting results, as shown in Figure S2.

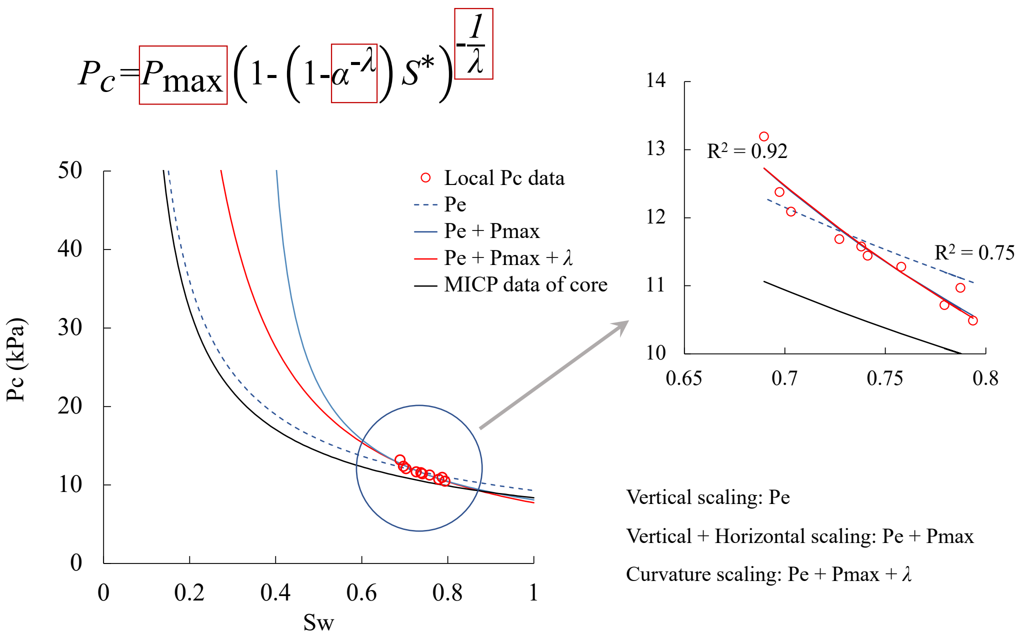

Figure S2. Results and evaluations of the multi-parameter fitting process are obtained using the adopted capillary pressure equation in a cell of the Estaillades sample.

3 Fitting accuracy of distinct algorithms

The accuracy of various fitting algorithms was evaluated, as shown in Table S3. Results showed that the accuracy of the fitting algorithms varied depending on the heterogeneous complexity of rocks. The multi-parameter capillary pressure fitting approach was found to be more accurate than former work. When both the multi-parameter capillary pressure fitting approach and the absolute permeability fitting approach were used together, the accuracy of the parameter estimates may improve a little bit further.

In summary, *Wenck et al.* [2021] evaluated the accuracy of fitting algorithms using a simulation-based approach and found that the accuracy varied depending on the complexity of the samples. We found that using both a multi-parameter capillary pressure fitting approach and an absolute permeability fitting approach together improved the accuracy of the parameter estimates, and generate one more characterized property (absolute permeability).

Table 1. Fitting accuracy of distinct algorithms, the previous work from *Wenck et al.* [2021], the results from multi-parameter capillary pressure fitting approach, and the results with both capillary pressure and absolute permeability fitting.

Rock type	Estaillades	Bentheimer	Bunte	Edwards	Indiana
Previous work	0.86	0.83	0.86	0.65	0.63
Multi Pc fitting	0.94	0.95	0.93	0.92	0.94
Current work	0.96	0.96	0.95	0.93	0.94

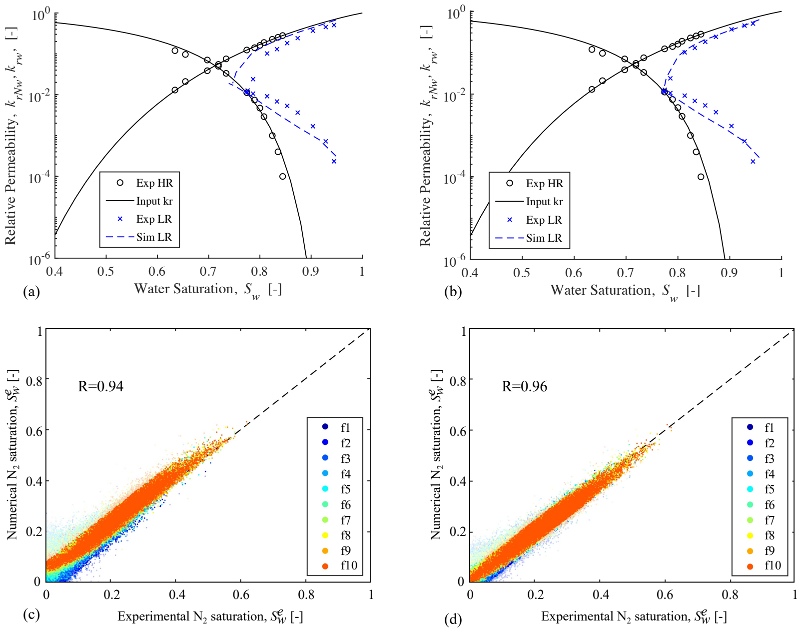

Figure S3. Multi parameter fitting results of saturation field and predicted relative permeability. (a) and (c) are fitting results with constant absolute permeability, while (b) and (d) with updated absolute permeability.

References

Wenck, N., S. J. Jackson, S. Manoorkar, A. Muggeridge, and S. Krevor (2021), Simulating core floods in heterogeneous sandstone and carbonate rocks, *Water Resources Research*, *57*(9), e2021WR030,581.