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Key Points:

- The field of view of digital rock models can be split to various classes by a hybrid of soft computing methods
- Super-resolution methods can help to compute more accurate k , p_c , and k_r models
- The presented workflow accounts for heterogeneities at the pore and core scale

Supporting Information:

Supporting Information may be found in the online version of this article.

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Predictive Soft Computing Methods for Building Digital Rock Models Verified by Positron Emission Tomography Experiments

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Abstract The influence of core-scale heterogeneity on continuum-scale flow and laboratory measurements are not well understood. To address this issue, we propose a fully automated workflow based on soft computing to characterize the heterogeneous flow properties of cores for predictive continuum-scale models. While the proposed AI-based workflow inherently has no trained knowledge of rock petrophysical properties, our results demonstrate that image features and morphological properties provide sufficient measures for petrophysical classification. Micro X-ray computed tomography (μ xCT) image features were extracted from full core plug images by using a Convolutional Neural Network and Minkowski functional measurements. The features were then classified into specific classes using Principal Component Analysis followed by K -means clustering. Next, the petrophysical properties of each class were evaluated using pore-scale simulations to substantiate that unique classes were identified. The μ xCT image was then up-scaled to a continuum-scale grid based on the defined classes. Last, simulation results were evaluated against real-time flooding data monitored by Positron Emission Tomography. Both homogeneous sandstone and heterogeneous carbonate were tested. Simulation and experimental saturation profiles compared well, demonstrating that the workflow provided high-fidelity characterization. Overall, we provided a novel workflow to build digital rock models in a fully automated way to better understand the impacts of heterogeneity on flow.

Plain Language Summary We demonstrate that soft computing methods can be used to classify rock images into specific classes that have unique flow properties. Without *any prior* knowledge of rock flow properties, a computer is able to interpret rock images in terms of image features that inherently delineate them into classes with unique physical properties. The method is unsupervised, and thus provides a fully automated approach for classification. The characterization approach provides a means to build predictive continuum-scale digital rock models. The predictive nature of the models were tested by conducting flow experiments using Positron Emission Tomography, which provides full 3D real-time images of fluid flow. The strong agreement between simulation and experimental results validated the proposed workflow.

1. Introduction

Problems concerning multiphase flow in porous media are central to a wide range of industrial and natural processes. Accurate and predictive modeling of flow processes requires proper knowledge of pore geometries (Bakhshian et al., 2019) and structural heterogeneity at the relevant length scales. Advanced imaging methods, such as Micro X-ray computed tomography (μ xCT), can provide significant insight into pore structure at the micrometer length scale; however, the field of view (FOV) is limited (Guan et al., 2018; Saxena et al., 2018). Therefore, at high enough resolution to capture the pore geometry to sufficient detail, the heterogeneity within a rock core is not captured sufficiently well. To circumvent this issue, we propose a fully predictive soft computing workflow that captures both pore-structure and core-scale heterogeneity to sufficient details for predictive simulations. We propose that the underlying flow properties governed by specific pore geometry can be captured in low-resolution images by using computer vision techniques followed by subsequent unsupervised clustering of rock types to provide a fully characterized sample at the core length scale. The novelty of the technique is that

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rock petrophysical properties are naturally encoded within image feature extractors (Fan et al., 2020) for unsupervised classification and characterization, such that the proposed method is fully automated and predictive.

The characterization of fluid transport at the pore-scale using image-based methods provides the opportunity of exploring unprecedented micro-scale physical phenomena (Hasan et al., 2020; Y. D. Wang et al., 2021). As a result, Digital Rock Physics (DRP) has been proposed as an innovative method to image rock samples at micrometer resolution to obtain the pore structures followed by modeling techniques to predict and observe the rock behavior under various conditions (Schepp et al., 2020; Verri et al., 2017). Accordingly, the standard workflow of DRP is divided into two main steps: (a) Digital Image Processing (DIP) and (b) Pore Scale Simulation (PSS) (Mehmani et al., 2020; J. Zhao & Wen, 2017). The preparation of a realistic pore-scale model is a significant target of DIP (Al-Marzouqi, 2018). According to the literature, computed tomography is the most common imaging modality employed in earth sciences (Bultreys et al., 2016). Computed microtomography is a non-destructive method that provides 3D and accurate structural knowledge of geomaterials with spatial resolution of micrometers (Chung et al., 2019). Once images are collected they must be processed to identify the various phases and pore space geometry. Typical DIP steps include noise suppression and segmentation, then the generated binary images are stacked and aligned to form a digital 3D representation of the rock core (Blunt et al., 2013). Last, PSS is applied on the segmented images to compute required parameters, such as capillary pressure or permeability (k) (Mostaghimi et al., 2012; Taud et al., 2005). Various PSS tools are available and a comprehensive review of these methods are covered in previous research (Golparvar et al., 2018; B. Zhao et al., 2019).

The generated results of PSS can be questionable due to the trade-off between the spatial resolution and FOV of μ xCT images (Najafi et al., 2021; Yue et al., 2016). The addressed trade-off can result in failure to capture pore sizes less than the spatial resolution and consequently gives rise to uncertainty of pore geometry (Blykers et al., 2021; Saxena, Hofmann, Alpak, Berg, et al., 2017). For instance, prior research has suggested that the calculated porosity of a digital rock sample can be 50% less than the expected values if the effects of sub-resolved pores are not taken into account (Saxena, Hofmann, Alpak, Dietderich, et al., 2017). Other recent research has concluded that poor knowledge of pore geometries might adversely affect PSS results and generate permeabilities up to 10 times greater than experimental values (Orlov et al., 2021; Saxena et al., 2019). Various studies have concluded that the main source of inaccuracies in DRP analyses is the lack of sufficient pore geometry characterization when the FOV is large (Saxena et al., 2018; Sharma et al., 2021). Despite successes made by various studies to create more representative petrophysical parameters based on μ xCT images (Botha & Sheppard, 2016; Ebadi et al., 2020, 2021), the results remain immature in obtaining realistic pore geometries in which the negative consequences of a large FOV are effectively removed (Dong et al., 2018; Soullaine et al., 2016). Another recent emerging approach is the usage of super-resolution (SR) methods that can provide a better resolved μ xCT image in which more details of pore geometries are shown (Chen et al., 2020; Janssens et al., 2020; Y. D. Wang et al., 2021). It has been demonstrated that SR methods generate results for petrophysical analysis that are stable and consistent with low sensitivity to user selected parameters (Niu et al., 2020, 2021). However, the implementation of SR techniques on an entire core image would generate an enormous image with unrealistic computational costs for most fluid flow analyses (Rabbani et al., 2020; Siavashi et al., 2022).

A solution that obtains accurate pore geometry dependent parameters from low-resolution images and still keeps the computational cost low is needed. This generates a clear incentive for using a well-designed scenario of various machine learning approaches commonly known as unsupervised classifiers. In unsupervised classification, an algorithm segregates the unlabeled data into a user-defined number of classes based on similar characteristics inherent in the data (Chauhan et al., 2013; Jouini & Keskes, 2017). In other words, analyzing the unlabeled data by means of unsupervised classifications provides insights that are not likely visible otherwise (Chauhan et al., 2020). The performance and accuracy of various unsupervised algorithms in segmenting μ xCT images of four different rock samples have shown that K -means outperforms other methods (Chauhan, Rühaak, Anbergen, et al., 2016). Moreover, unsupervised algorithms have been used to estimate the pore sizes in μ xCT images of various rock samples (Chauhan, Rühaak, Khan, et al., 2016). They have also shown that the K -means algorithm results in the fastest processing time compared to similar methods.

Furthermore, the DRP technique can be employed to simulate multiphase flow in core samples (Ruspini et al., 2021; S. Wang et al., 2022). Tuning the numerical modeling of multiphase flow in porous media with sub-core-scale heterogeneity, obtained by DRP analysis, to generate results consistent with experimental observations have always been met as a serious and considerably difficult challenge (Wenck et al., 2021). Typically, it has

been observed that the estimation of sub-core-scale permeability based on porosity distribution leads to the saturation distributions not matching with experimental measurements. In studies conducted by (Krause et al., 2011, 2013), the permeability assignment to simulation grids was done not only based on porosity distribution but also with the help of capillary pressure measurements. The results showed substantial improvements. The proposed technique provides the opportunity to carry out greatly refined simulations of core flooding experiments without the usual assumptions regarding the core as homogeneous. In some other studies, the effects of local heterogeneity on capillary pressure data was considered. For example, the X-ray imaging was applied to precisely visualize multiphase flow at the sub-core-scale. The spatial variability in the capillary pressure data was then represented in terms of scaling factors (Pini & Benson, 2013). Similarly, the characterization of drainage multiphase flow properties were made on heterogeneous rocks using 3D numerical simulations and core flood experiments. By scaling of the average capillary pressure curve in the rock core with a simple scaling factor, and calibrating the numerical model versus the observed sub-core-scale saturation heterogeneity, they could correctly predict average pressure drop at the core scale (Jackson et al., 2018). Technically, it is known that capillary pressure varies spatially causing the developments of a spatially heterogeneous saturation distribution. The difficulty of simulating such a condition has been resolved by introducing a workflow including a dynamic measurement of sub-core-scale drainage in heterogeneous porous media. The technique works based on fitting the parameters of capillary pressure curves while describing both pressure and steady-state saturation profiles with a 1D model that considers the variation of sub-core-scale properties in the displacement direction (Hejazi et al., 2019). Effects of sub-core scale heterogeneity on relative permeability has drawn significant attention as well. Analysis of synthetic steady-state core flooding data recorded based on two samples, which their sub-core scale heterogeneity had accurately been characterized, resulted in determination of the characteristic relative permeability at any typical flow rate (M. H. Krause & Benson, 2015). In another case, 3D observations of the fluid saturation distribution in the core sample and studying the effects of heterogeneity on the relative permeability, the capillary pressure heterogeneity was quantitatively inferred (Reynolds et al., 2018).

Classic multiphase flow experiments do not directly visualize or monitor the internal saturation profiles during flow (Kim et al., 2018). This is where the technology of Positron Emission Tomography (PET) emerges to provide a full 3D image of the saturation within a rock core during multiphase flow (Carpenter, 2016). PET technology is recently used in a broad range of geological studies although its advantages were first found in medical imaging (Lippmann-Pipke et al., 2017). The temporal resolution of PET images can be accompanied by a robust reconstruction technique to produce four Dimensional (4D) images of radiotracer transport in a given sample (Fernø et al., 2015). The high sensitivity to small changes in tracer concentration is a key advantage of PET (Zahasky & Benson, 2018). In other words, various materials having very similar densities to each other cannot be differentiated accurately based on μ xCT images. However, the contrast between the non-radioactive fluid and the fluid having the radioisotope is significant with PET (Li et al., 2019). The next major advantage of PET images is that positron annihilation produces gamma rays with high energy of 511 keV (Zahasky et al., 2019), which results in the traveling of photons through geological materials without significant loss (Brattekkås & Haugen, 2020). Accordingly, one of the most prominent usages of PET images is to obtain full 3D maps of fluid saturation at the second time scale that can then be coupled to μ xCT images that resolve the underlying pore geometry (Hu et al., 2020). Using PET images as a references for evaluating numerical simulations of core flooding experiments and characterization studies has the potential to significantly help in evaluating the importance of characterizing both pore-scale geometry and core-scale heterogeneity.

Herein, we put forth a hybrid workflow based on computer vision techniques and unsupervised learning that can characterize the pore geometry and the relevant heterogeneity of core-scale samples from a single FOV image. The workflow is a fully automated characterization method that provides a realistic 3D domain with rock properties assigned, such that continuum-scale modeling can be conducted. Simulations are conducted on sandstone and carbonate rock images and validate by experimental flooding studies of the same rocks imaged by PET.

2. Methodology

The key objective of the presented research is to employ a fully automated characterization workflow that captures the effects of pore-scale geometry and core-scale heterogeneity at sufficient detail to allow for accurate continuum-scale flow models. A multidisciplinary workflow based on statistical operators, machine learning

methods, classical petrophysics, and numerical simulation is proposed. As shown in Figure 1, the developed workflow can be explained in eight steps:

1. The workflow begins with the μ xCT image acquisition of a full core plug.
2. The collected images are filtered to remove noise followed by image segmentation of the solid and pore regions.
3. To split the μ xCT domain into a certain number of classes, sets of features from sub-volume pairs of binary images and the corresponding gray-scale images are extracted. Terminologically, each *pair* implies a sub-volume from the stack of gray-scale images and its twin from the binary equivalent.
4. Using unsupervised classification, each sub-volume pair is automatically labeled with a specific class based on its dimensionality-reduced features.
5. To obtain a better understanding of the pore morphology, a SR technique is applied to randomly selected sub-volumes of each class.
6. The super-resolved sub-volumes of each class are used for PSS. The results are used to assign the required petrophysical parameters to all members of that class.
7. Each binary sub-volume can be considered as a computational grid, which provides the opportunity to use a continuum-scale simulator to predict flow. The simulation results are analyzed to generate the corresponding water saturation (S_w) profiles at various pore volumes injected.
8. For a well characterized core sample, the simulated S_w should be in strong agreement with experimentally measured values using PET. In the case of a noticeable mismatch, the offered workflow provides the opportunity to adjust the number of classes that the unsupervised classifier uses.

The proposed workflow was tested using flow experiments and acquired images from two water-wet porous rocks—sandstone and limestone. The Bentheimer sample (sandstone) has the porosity (ϕ) of 23.81%, the permeability (k) of 1.3 Darcy (D), the length of 5.05 cm and the diameter of 2.48 cm. Also, for the Indiana sample (limestone), ϕ is 16.47%, k is 0.25 D, and it has the length and diameter of 4.75 and 2.55 cm, respectively. The details for each step of the workflow are explained in the following subsections.

2.1. Imaging

2.1.1. PET Experiments

The Bentheimer sandstone and the Indiana limestone have the average pore sizes of 37.4 and 25.1 μ m. The samples were cleaned with 95% ethanol, dried in a vacuum oven for 24 hr at 60°C, and encased within epoxy which limits reaching high spatial resolutions with μ xCT. A core holder of araldite epoxy and PVC plastic was fabricated to mount the sample on the PET stage (Hu et al., 2020). The employed experimental setup has been shown in the Figure S1 in Supporting Information S1. The core flooding was conducted at ambient conditions using a standard syringe pump. The samples were initially saturated with water followed by the injection of oil (decane, 10 ml) at 3 ml/hr. Water flooding was then initiated at 3 ml/hr while the sample was imaged.

Experimental data was acquired using a Siemens Inveon preclinical PET/CT scanner (Visser et al., 2009). This scanner had been used in the past to visualize underlying physical phenomena in core samples using 2-deoxy-2-[fluorine-18]fluoro-D-glucose ([18F]-FDG) (Hu et al., 2020). The scanner consists of four rings of 16 lutetium oxyorthosilicate (LSO) crystal blocks with an inner diameter of 16.1 cm and an axial extent of 12.7 cm. Each detector module was composed of a 20×20 array of LSO crystals coupled to a position-sensitive photomultiplier tube via a light guide and was placed in time coincidence with opposite modules. The scanner offers an effective trans-axial FOV of approximately 10 cm and an axial FOV of 12.7 cm. A 90-min PET scan was collected while water doped with [18F]-FDG was injected into the sample at 3 ml/hr. It should be mentioned that the concentration of the FDG is extremely low so that it has a negligible effect on the viscosity and surface properties, and therefore the doped water has the same properties as pure water. The syringe pump held 10 ml of fluid with an activity reading of 40–60 MBqs during the reported experiments. The PET data was acquired as “raw list” mode enabling retrospective histogramming into the required time frames. Data was histogrammed and reconstructed using Inveon Acquisition Workplace version 2.0 into 3D frames every 2 min. The 3D attenuation map generated from the associated CT data was used to correct the reconstructed PET data for scatter and attenuation. Finally, the generated PET images have the resolution of 194 μ m/voxel in x - and y -directions, and 796 μ m/voxel in the z -direction.

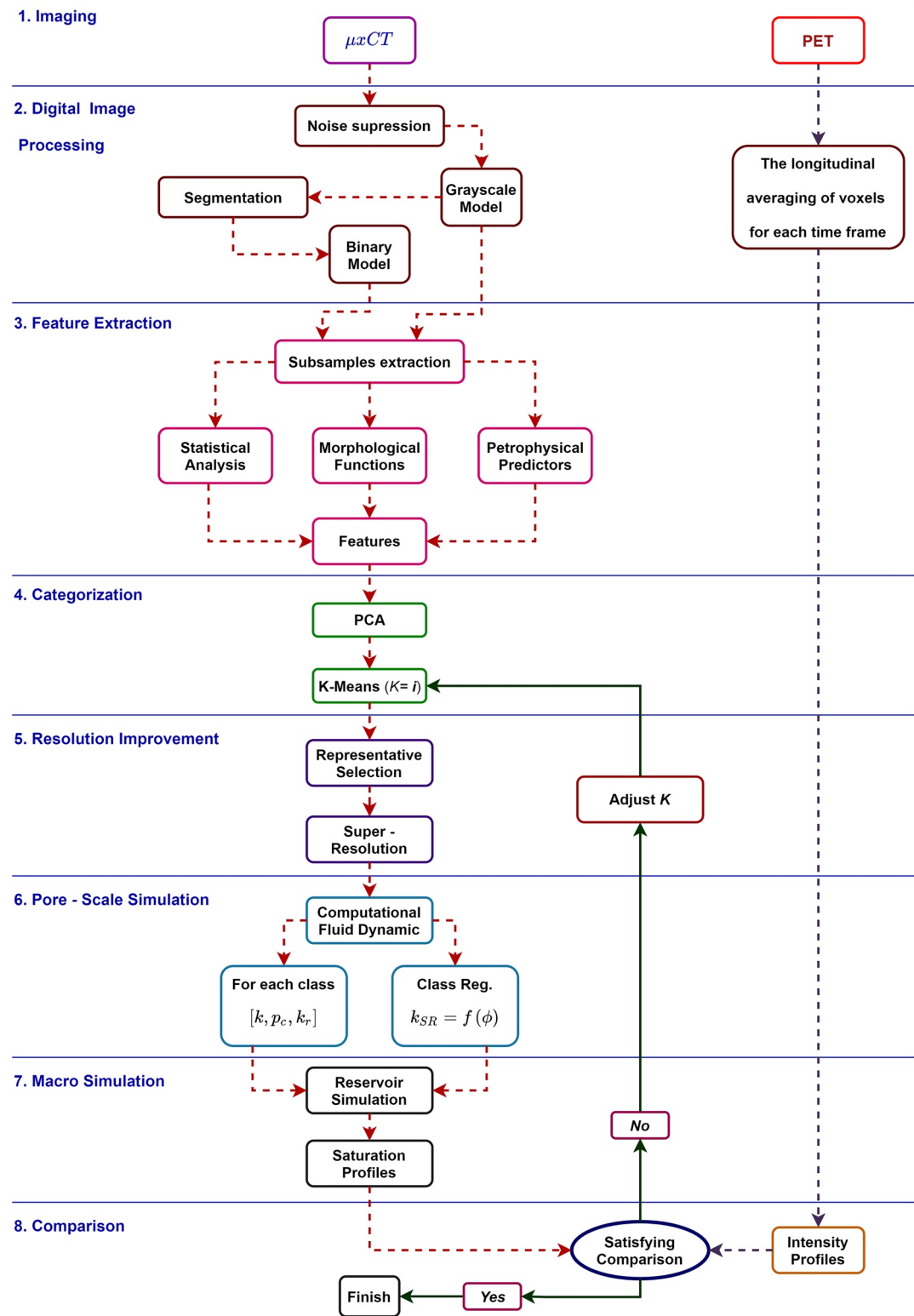


Figure 1. The proposed workflow to validate the pore-scale simulation based on μxCT images with the use of Positron Emission Tomography images.

2.1.2. μ xCT

The μ xCT imaging was performed at the University of New South Wales Tyree X-ray imaging facility using a HeliScan μ xCT system (Sheppard et al., 2014). The system has a GE Phoenix Nanofocus tube and a high-quality flatbed detector of $3,072 \times 3,072$ pixels. Both dried cores were imaged from top to bottom using a helical trajectory. The resulting images had a spatial resolution of $18.7 \mu\text{m}/\text{voxel}$, and consistent grayscale values.

2.2. Digital Image Processing

A Non-Local Means (NLM) filter is applied to all images to reduce the image noise (Buades et al., 2005, 2011). For NLM filtering, OpenCV cv2.fastNlMeansDenoising was used with the default values. Then Otsu's method was used to segment the images into pore and matrix phases (Otsu, 1979). Otsu's method was used since it has no user input, and thus can be applied within the workflow as an automated procedure despite its inherent drawbacks (Leu et al., 2014). Furthermore, the digital processing of PET images was performed by calculating the intensity-average of each image slice for a given *Time frame* to observe the advancement of the water phase, which is doped with a radioisotope.

2.3. Feature Extraction

A gray-scale image and its binary pair are used for feature extraction. The PET images have lower spatial resolution than the μ xCT images. Therefore, cubic sub-volumes with the same size as a single PET voxel were taken regularly from the μ xCT data. Each voxel of the PET image had the resolution of $(x, y, z) = (194, 194, 796) \mu\text{m}/\text{voxel}$, and each voxel of the μ xCT image had the resolution of $(x, y, z) = (18.7, 18.7, 18.7) \mu\text{m}/\text{voxel}$. Therefore, each taken sub-volume pair of binary and gray-scale images have the size of $(x, y, z) = \left(\frac{194}{18.7} \approx 10, \frac{194}{18.7} \approx 10, \frac{796}{18.7} \approx 42\right)$ voxels. These sub-volume pairs were then analyzed for feature extraction. An overview of the feature extraction process is provided in Figure S2 in Supporting Information S1.

First, the statistical operators of minimum (min), maximum (max), mean (*mean*), median (*med*), mode (*mod*), standard deviation (*Std*), and variance (*Var*) were applied to the gray-scale sub-volumes to generate features (F. J. Brooks & Grigsby, 2013). For morphological features, the binary sub-volumes were characterized by the Minkowski Functionals (MF). It is well-known that physical processes depend on the geometry and topology of bodies or multiple bodies in 3D space as characterized by the MF (Armstrong et al., 2018). By considering a solid body (X) embedded in Euclidean space (Ω) with boundary surface of (δX) , the size of X in various dimensions is measured based on volume, surface area, integral of mean curvature, and a topological invariant called the Euler characteristics (Slotte et al., 2019). In other words, the intrinsic values of volume, surface area, integral mean curvature, and Euler characteristic or total curvature for X are collectively the MF (Ivonin et al., 2020).

Last, an applied petrophysical analysis was conducted by running a pre-trained Convolutional Neural Network (CNN). The employed deep learning method takes a series of binary images in the form of a cube, and generates an estimate of the permeability in the x , y , and z directions (Alqahtani et al., 2021). To expand on this point, a 3D variant of a deep residual network was pre-trained in previous works to estimate the permeability of μ xCT images. The architecture includes Convolutional layers, Batch Normalization, and Rectified Linear Unit (ReLU) activation functions, the full network structure and further details are provided in (Alqahtani et al., 2021).

2.4. Categorization

Based on the features extracted from the sub-volume pairs, the FOV was partitioned into a number of classes or "rock types." Having a certain number of classes in the domain provides a means to assign a unique set of petrophysical models to each class. These classes are not necessarily of the sample size used to define a representative elementary volume in the traditional sense (Bear, 1988). The sub-samples within each class are, however, representative of their class based on the extracted features. The categorization is done based on the implementation of the unsupervised classifier K -means. To avoid over-fitting and to reduce the computational cost, Principal Component Analysis (PCA) was used to reduce the extracted features to only those important for categorization (Jolliffe & Cadima, 2016). PCA converts a comprehensive set of variables into a smaller one that still contains

the most important information from the initial set (Webb et al., 2011). Decreasing the number of variables often comes at the expense of accuracy, but dimensionality reduction is often advised to trade off accuracy for simplicity (Lever et al., 2017).

The main approach of PCA and K -means is illustrated in Figure S3 in Supporting Information S1. In Figure S3a in Supporting Information S1, each regularly extracted sub-volume has a set of various features. First, the PCA is applied to reduce the n -dimensionality of gathered features into a 2D space of principal components ($C1$ and $C2$). Next, the K -means algorithm was implemented to $C1$ and $C2$ for all sub-volumes, which segregates them into K (user-defined) classes, Figure S3b in Supporting Information S1.

2.5. Resolution Improvement

Having K classes in the domain provides a means to assign a unique set of petrophysical models to each class. The sub-volumes within each class were representative of their class but were not necessarily an REV in the traditional sense, and thus in Section 3 we will demonstrate that each class provided a unique set of petrophysical properties.

To capture the geometrical structure of each class at sufficient detail for pore-scale modeling, the selected sub-volumes from each class were up-sampled using a SR algorithm (Sidorenko et al., 2021; Y. D. Wang et al., 2019). However, it is not necessarily practical to apply the SR technique to the entire core image. Therefore, a fixed number of sub-volumes from each class were randomly selected. Then, the SR algorithm was implemented to each randomly chosen sub-volume. A few recent studies have employed CNNs as SR algorithms (Wang, Armstrong, & Mostaghimi, 2020; Wang, Chen, & Hoi, 2020). Prior research suggests that the generated super-resolved images have not only higher resolution but also reduced noise. Taking the inherent simplicity and quality of the generated results into consideration, improving the resolution of μ xCT images can be obtained by the implementation of the trained Enhanced Deep Super Resolution (EDSR) (Y. D. Wang et al., 2019). Finally, the SR images of each sub-volume were binarized using Otsu's method.

2.6. Pore-Scale Simulation

Regarding an incompressible, Newtonian fluid at steady-state laminar flow, the Navier-Stokes equations can be employed to compute the velocity field, which can be up-scaled using Darcy's law to determine permeability (k). The simulations were performed using the FlowDict module of the GeoDict software (Jacob et al., 2019). Assuming the existence of a two-phase system in a porous medium where other forces are negligible compared to capillary ones, the saturation-dependent parameters such as p_c and k_r were computed using the GeoDict software module called SatuDict. The randomly selected super-resolved sub-volumes from each class (as explained in the previous step) were used for simulation. Next, the computed permeabilities of each class were averaged, and the average result is assigned to other members of the same class.

The p_c data for the super-resolved subsamples of each class were represented as a global correlation for the same class based on the model presented by Brooks and Corey (R. H. Brooks & Corey, 1966) as

$$p_c = p_{th} \left(\frac{S_w - S_{wr}}{1 - S_{wr}} \right)^{-1/\lambda}, \quad (1)$$

where threshold pressure is p_{th} and S_{wr} is residual water saturation. Also, λ is introduced as the pore size distribution index. The final capillary pressure model of each class was then assigned to all other sub-volumes of that class. It must be underlined that the required models for different classes have been estimated based on the `optimize.curve_fit` function of `scipy` (Python library).

Following the same logic, a curve of k_r versus S_w based on the simulations of each class can be inferred by the relative permeability model put forward by (Behrenbruch et al., 2020) as

$$k_{ro} = k_{ro,max} \left(\frac{S_o - S_{or}}{1 - S_{or} - S_{wr}} \right)^{n_o}, \quad (2)$$

$$k_{rw} = k_{rw,max} \left(\frac{S_w - S_{wr}}{1 - S_{or} - S_{wr}} \right)^{n_w}, \quad (3)$$

where n_o and n_w are the Corey exponents, and S_o and S_{or} are the oil saturation and residual oil saturation, respectively. The maximum value of computed relative permeability for each phase is shown by $k_{r,max}$.

2.7. Macro-Scale Simulation

A macro-scale simulation domain was built after assigning the required petrophysical properties to each class, as shown in Figure S3 in Supporting Information S1. Each grid cell in the simulation domain was constructed to represent a set of $(x, y, z) = (10, 10, 42)$ voxels from the μ xCT images. Therefore, each grid cell was assigned a given class and subsequent petrophysical properties. Then, a two-phase flow simulation of water displacing oil was conducted on the constructed grid model to extract the S_w profiles. The simulations were conducted using tNavigator (Jaoua & Rafiee, 2019). The first and last grid cells are completed with open-hole injector and producer wells. The injection was performed based on constant flow rate, and the production was conducted with constant bottom hole pressure. Also, the other four sides of the domain were no-flow boundaries. For each time frame, if the extracted saturation profiles are in strong agreement with the concluded intensity profiles from PET images, it indicates that the proposed algorithm was successful in developing a digital rock model as a valid representative of the core sample.

3. Results and Discussions

By assuming that the radiotracer remains in the liquid phase, and adsorption to the pore surface was negligible, the radiation intensity of the PET-images can be used to calculate the tracer-labeled fluid saturation. Figure 2 shows the average of detected radiation for each slice of the PET image in both samples under water flooding. A time frame is collected every 2 min. Regarding the Bentheimer sample, the smooth movement of the injected water with the radiotracer can clearly be observed in the volume-rendered images of time frames 5 (Figure 2a), 7 (Figure 2b), and 9 (Figure 2c). The indicated smooth advancement of the injected phase (Figure 2d) was mainly due to the inherent homogeneity of Bentheimer sandstone (de Argandoña et al., 2009). The observations are in strong agreements with previous literature focusing on multiphase flow and front movements in homogeneous domains, like Bentheimer sandstone.

In contrast, Figure 2h does not indicate the same smooth moving trend of frontal advancement for Indiana limestone. The PET images suggest the existence of local heterogeneity and zones with dissimilar petrophysical properties. In particular, there appears to be a high conductivity zone within the top half of the sample where the detected radioactivity was high. While Figure 2e indicates the minimal movement of the front, Figure 2f had a concentrated zone of radiotracer within the top half of the core sample. Interestingly, in Figure 2g, where the radiotracer spans the entire sample, significant regions of the core have no radiotracer present. These flow observations are aligned with observations in other heterogeneous limestone samples presented in the literature (Dernaika et al., 2015; Saenger et al., 2016).

Following the proposed workflow represented in Figure 1, and for the ease of next computational steps, two cuboids were extracted from the μ xCT images of both samples. Based on the cropping shown in Figure S4 in Supporting Information S1. The resultant cuboids of μ xCT for the Bentheimer and Indiana images have the sizes of (900, 900, 2700) and (900, 900, 2550), respectively.

After imaging, the generated μ xCT images were applied with the described DIP in Section 2.2. Accordingly, the NLM filter followed by Otsu's method was implemented, and the results are depicted in Figure S5 in Supporting Information S1. For the sandstone sample, a very uniform distribution of pores can be observed. Conversely, for the limestone sample, the images display a complex pore structure involving a multiple porosity system with various degrees of interconnectivity.

According to the concept described in part 2.3, and visualized in Figure S3a in Supporting Information S1, the paired μ xCT images (filtered and binary) were split into sub-volumes. Each sub-volume had the size of a single PET voxel. Table S1 in Supporting Information S1 provides the required details of how the regular sub-volumes were performed. The Bentheimer cuboid had $900 \times 900 \times 2,700$ voxels resulting in 518,400 sub-volumes. The Indiana data had $900 \times 900 \times 2,550$ voxels, resulting in 486,000 sub-volumes. These sub-volumes were then categorized into classes based on their extracted binary and gray-scale features.

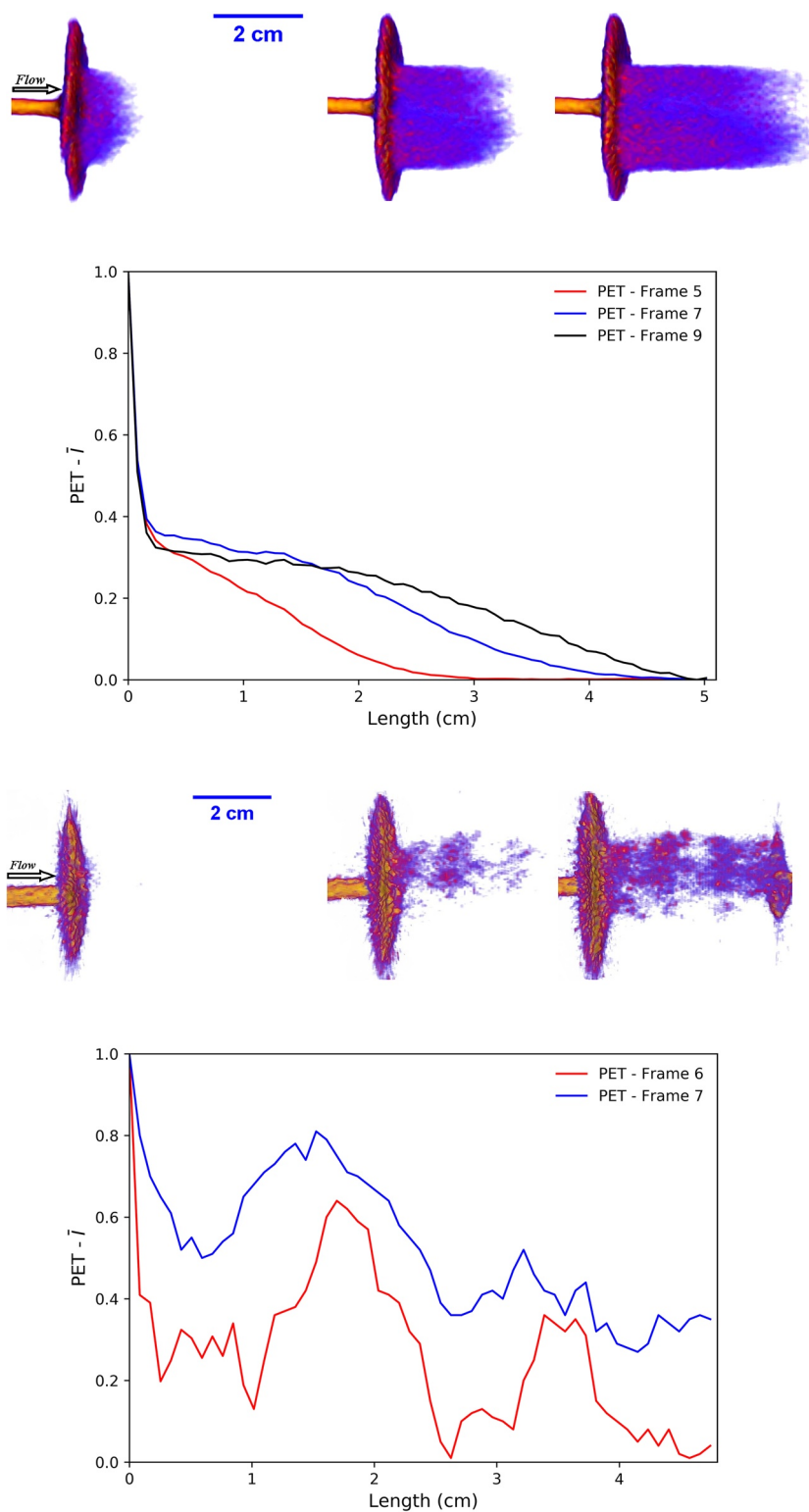


Figure 2. The progress of radiotracer dilution in both samples based on forced imbibition (*The higher and lower radioactivity have been shown by the color spectrum ranging from orange to purple, respectively*). The averaged distribution of radiotracer in each slice for different Time frames along the core sample: (d) Bentheimer (h) Indiana.

As shown in Figure S2 in Supporting Information S1, each sub-volume was characterized based on various features. The results from a sub-volume of Indiana limestone are provided in Table S2 in Supporting Information S1. It is essential to remark that while the statistical analysis was implemented on the gray-scale sub-volume, the morphological and petrophysical analyses were measured on the paired binary sub-volume. The advantage of using the CNN-based petrophysical analysis was that permeability on all sub-volumes was rapidly estimated in all three-directions. This was facilitated by using a Graphics Processing Unit (GPU) for accelerating the inference of the permeability where batches of sub-volumes were fed to the CNN model. The inference of permeability in each direction averages 100 milli-second per batch of four sub-volumes using a single RTX 2080 Nvidia GPU.

According to Figure 1, the K -means algorithm was applied to classify all sub-volumes into K classes (Figure S3b in Supporting Information S1). However, the data set had a relatively large number of features (13 features for each sub-volume). Hence, PCA was applied, and the first two generated components were used to capture the greatest amount of variance. Figures 3a and 3b indicated that the variance drop-off points for both samples occurred after passing the second component. Following the PCA analysis and considering the homogeneity of Bentheimer sandstone, all sub-volumes were categorized into a single class, Figure 3c. The sub-volumes of Indiana limestone, however, can have high or low ϕ and at the same time high or low k . Consequently, four pairs of (low ϕ , low k), (low ϕ , high k), (high ϕ , low k), and (high ϕ , high k) were taken as the main reason for K -means to classify sub-volumes into four different groups, Figure 3d. The number of sub-volumes assigned to each class for both samples has been provided in Table S3 in Supporting Information S1.

The petrophysical relationships for permeability were developed using pore-scale simulations of randomly selected sub-volumes from each class. In detail, the introduced CNN in **part 2.5** was applied to grayscale images of 11 randomly-selected sub-volumes from each class. The chosen sub-volumes having a size of (10, 10, 42) voxels were up-sampled to (40, 40, 168) voxels using the proposed EDSR model. Next, each set of 11 samples was split into two subsets having 6 and 5 members. The first set were binarized based on Otsu's method and then given to the FlowDict module of GeoDict for permeability computations. Afterward, the estimated permeability was plotted versus the corresponding porosity, as presented in Figure 4a. As observed, each rock class provide a unique cluster in the permeability versus porosity cross plot. Therefore, the primary outcome was that an average value of permeability, ($\bar{k}$), could be assigned to each class. The other 5 randomly selected sub-volumes were used to evaluate the uniqueness of $\bar{k}$ for each class. Using the GeoDict, the 5 computed k_{SR} of each class were compared versus the representative $\bar{k}$ of the same class computed based on the first set of 6 sub-volumes. The described procedure shows how much the computed $\bar{k}$ for one class is unique to only that class. The uniqueness test was performed based on the R^2 index. For the single Bentheimer class, the $R^2 = 0.76$ has been calculated as the similarity between the $\bar{k}$ of the first 6 sub-volumes and the second 5 sub-volumes. For the Indiana sample, the average of 5 computed k_{SR} of each class were not only compared to the $\bar{k}$ for that class but also to the other three $\bar{k}$ of the other classes, Figure 4b. The results show that the largest value of R^2 for each class corresponds to the $\bar{k}$ developed for that class, however, there remained some cross-over between classes as expected for a highly heterogeneous sample.

After the permeability analysis, the SatuDict module of GeoDict was used to compute the p_c and k_r relationships for the 11 random sub-volumes of each class. Similar to the permeability analysis, the computed p_c results of the 6 sub-volumes were correlated based on the p_c model explained in **part 2.6**. Before using the `optimize.curve_fit` function of `scipy` to find the p_c model for each class, the *pth* of the model was assigned as the mean value of all 6 samples at $S_w = 1$. Moreover, the S_{wr} was assigned based on the minimum value of S_w reported by SatuDict among all 6 samples of each class. The corresponding simulation results and corresponding models are provided in Figure 5.

The other 5 random sub-volumes of each class were employed to investigate the uniqueness of the developed p_c models. First, SatuDict was implemented to calculate the p_c data of each sub-volume. Then, `scipy.optimize.curve_fit` was used to find the optimal fit to the data of all 5 sub-volumes of a given class. Afterward, the given lambda by the `scipy.optimize.curve_fit` (λ_{scipy}) was compared with the lambda of the model (λ_{model}) already obtained for the other 6 sub-volumes belonging to the same class. The best case is when $\lambda_{scipy} = \lambda_{model}$ which results in $\frac{\lambda_{model} - \lambda_{scipy}}{\lambda_{scipy}} = 0$. Applying the described procedure to the single class of the Bentheimer sample generated, $\frac{\lambda_{model} - \lambda_{scipy}}{\lambda_{scipy}} = 0.009$. For the Indiana sample, the computed λ_{scipy} of each class was compared with the λ_{model} of

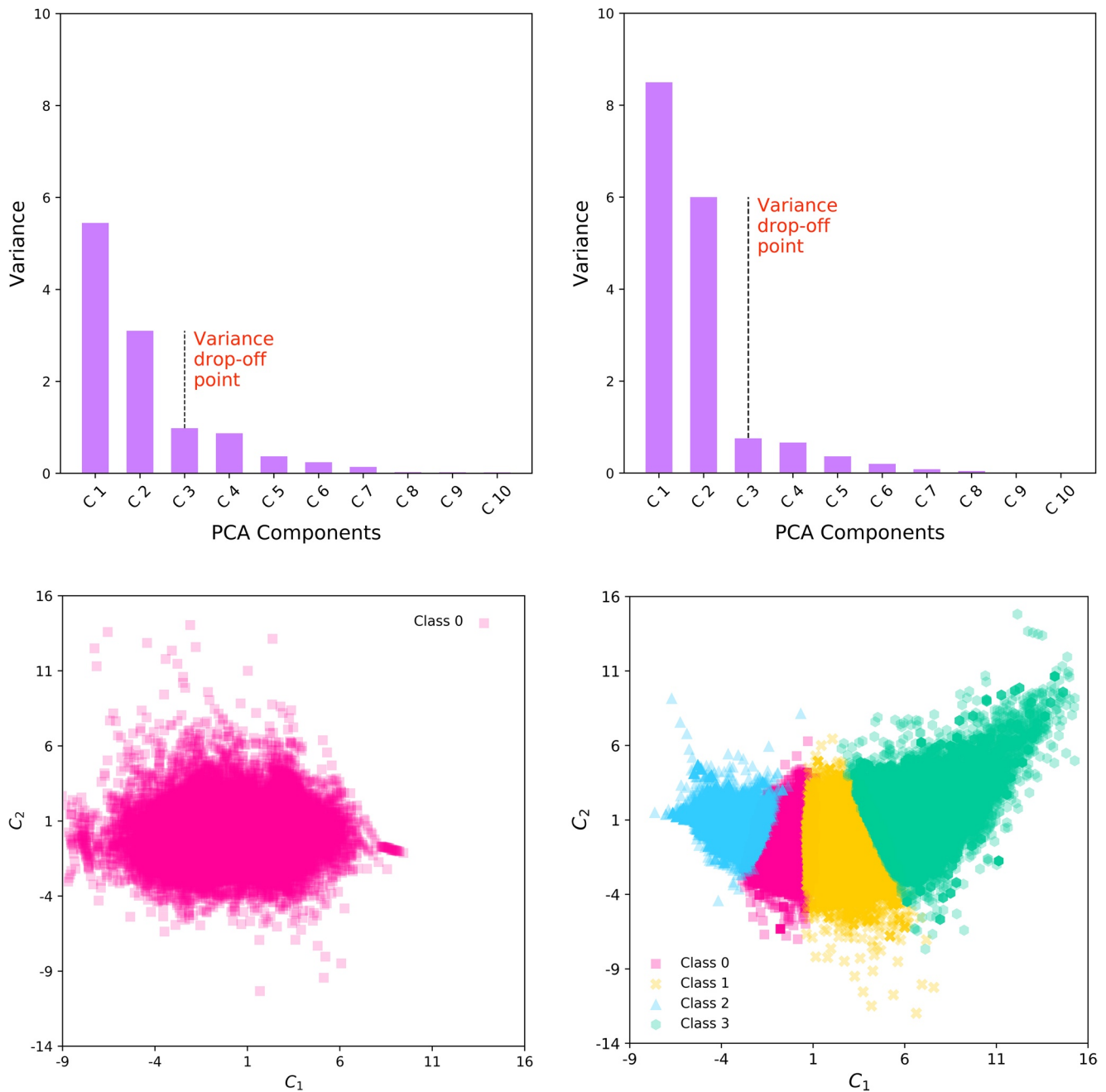


Figure 3. The Principal Component Analysis analysis and *K*-means application.

all other classes. The results are illustrated in Figure 6. The values closest to zero lie on the main diagonal, which demonstrated the high similarity of capillary pressure behavior within a single class. The comparison between λ_{scipy} of a class and λ_{model} of all other classes indicates large deviations. Overall, the results suggested that the developed p_c model of each class was unique to that class.

In addition to the p_c data, the SatuDict module was also used to compute the k_r relationship. The `scipy.optimize.curve_fit` function was implemented to find the most appropriate parameters for the k_r model (Behrenbruch et al., 2020) based on the simulation results. The importance of pore geometry and its effects on multiphase flow can be noticed by analyzing the generated k_r models for the various classes of the Indiana sample. Figures 7b and 7e shows that the cross points of the k_r curves belonging to classes 0 and 3 of the Indiana sample occur before $S_w = 0.5$. On the contrary, k_r models for classes 1 and 2 have different behavior. Figures 7c and 7d indicate that

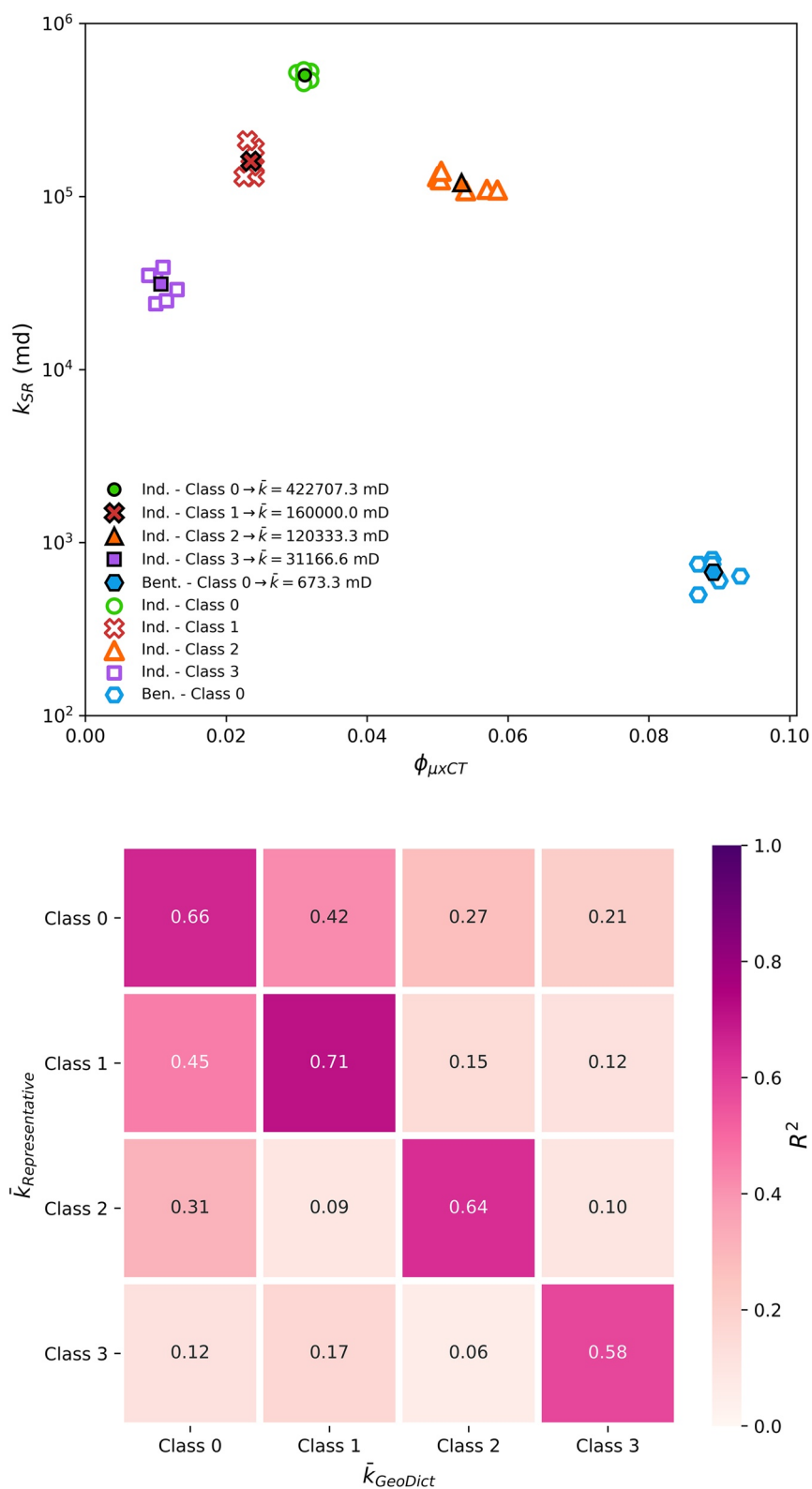


Figure 4. The developed petrophysical models (a) The cross-plot of k_{SR} versus $\phi_{\mu xCT}$ (b) The uniqueness of a developed petrophysical model based on the index of R^2 .

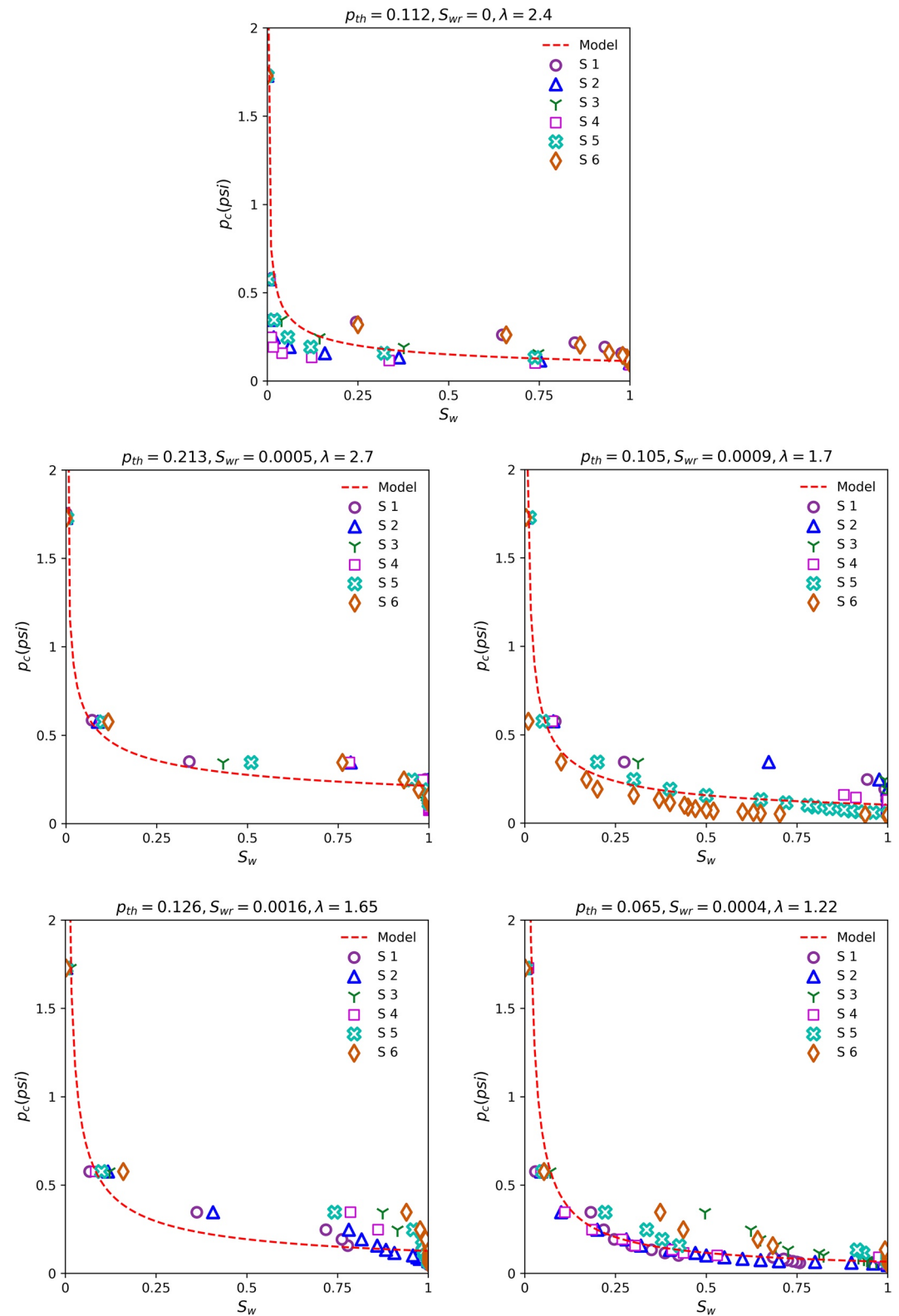


Figure 5. Development of the capillary pressure models.

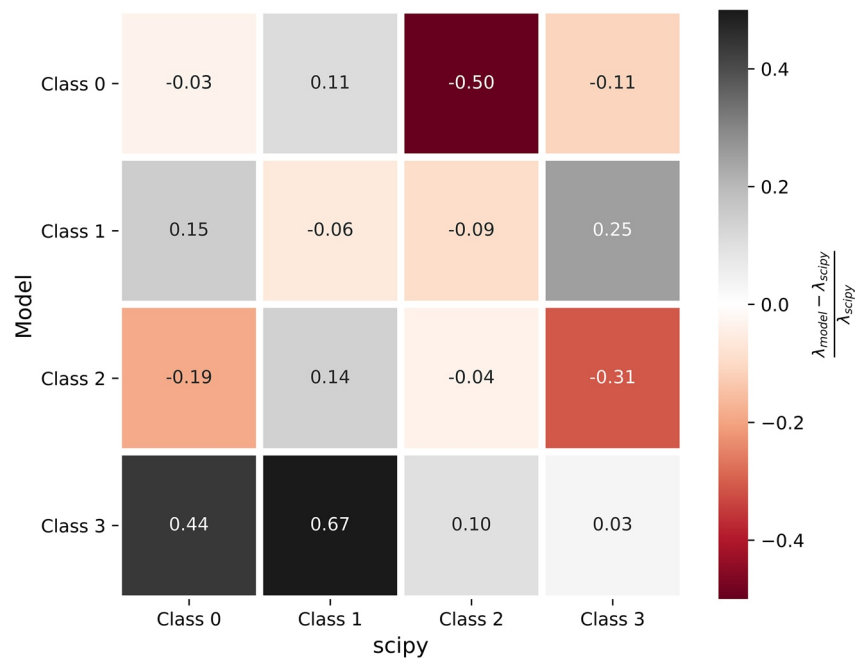


Figure 6. The similarity of λ_{scipy} to λ_{model} for the various classes of Indiana sample. The subscript of “model” refers to the λ computed based on the first 6 sub-volumes, and the subscript of “scipy” is relevant to the next 5 sub-volumes.

their cross points occurred at S_w greater than 0.5. It should also be noted that the generated data of SatuDict for all classes have S_{wr} , S_{or} , and $k_{r,max}$ of zero, zero, and one, respectively; based on the assumptions used in the SatuDict model.

The uniqueness of developed relative permeability models for each class were checked based on the same logic applied to the p_c models. Therefore, 5 randomly selected sub-volumes from each class were processed with SatuDict and then analyzed with `scipy.optimize.curve_fit`. The resultant models for each class have two exponents determined with `scipy` ($n_{o_{scipy}}$ and $n_{w_{scipy}}$). Next, the difference between the exponents obtained from the first 6 sub-volumes ($n_{o/w_{model}}$) and the next 5 sub-volumes ($n_{o/w_{scipy}}$) were compared based on $\frac{n_{o/w_{model}} - n_{o/w_{scipy}}}{n_{o/w_{scipy}}}$. Accordingly, the introduced ratio should be equal to zero when there is no differences between `scipy` and model results. For the single class Bentheimer sample, the introduced ratio resulted in 0.085 and 0.063 for n_o and n_w , respectively. The outputs for Indiana limestone are presented in Figure 8. Figure 8a, which shows that results near zero occurred along the diagonal meaning that the model was unique to a given class. Similarly, the same trend was observed for n_w (Figure 8b) as well. It is also observed that comparing the exponents ($n_{o_{scipy}}$ and $n_{w_{scipy}}$) of a class with the exponents of any other class results in the introduced ratio being one order of magnitude greater than the values located along the main diagonal, see Figure 8. For more details, the semi-logarithmic plots of Figure 7 have been shown in Figure S6 in Supporting Information S1.

After finalizing all the petrophysical analyses, the members of each class were assigned with a corresponding value of $\bar{k}$ and the relevant models of p_c and k_r . Then, a continuum-scale simulator (tNavigator) was used to run the required multiphase flow simulations. However, the accessible computational resources to consider almost half a million grids for each sample (Table S1 in Supporting Information S1) were limited. Therefore implementing upscaling to reduce the computational cost for run the required simulations was inevitable.

Accordingly, the simulation domain of the Indiana sample before the upscaling, which included $90 \times 90 \times 60$ grids, was divided into five overlying sectors in the z -direction. Each sector consisted of $90 \times 90 \times 12$ grids. Then, distributions of the highest and lowest permeable classes (Class 0 and 3) in each sector were analyzed. Figure S7 in Supporting Information S1 shows that the main flow path in the top sector of the limestone sample was mostly composed of the high permeable class, while the low permeable class dominated the bottom sector.

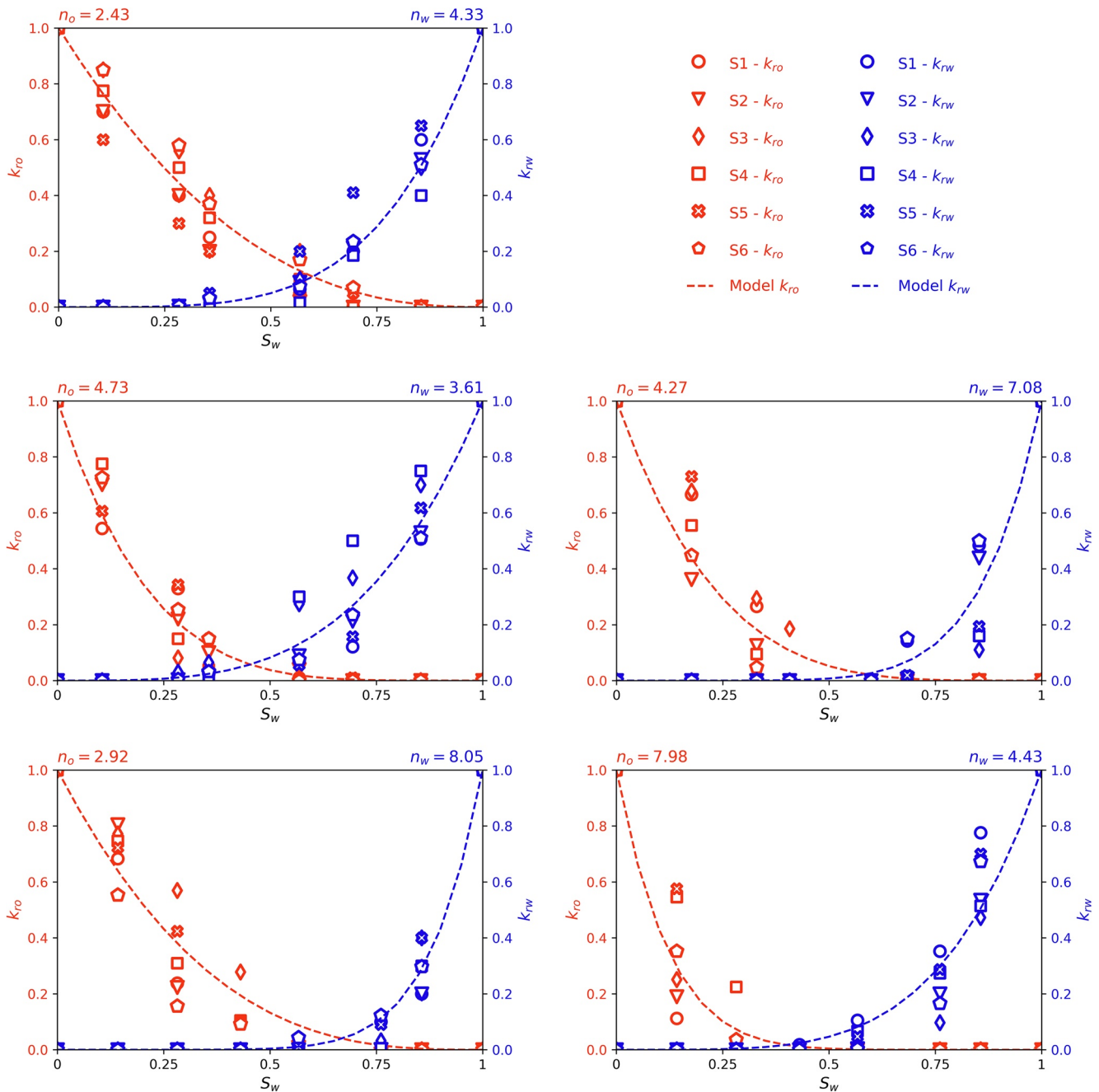


Figure 7. Development of the relative permeability models.

Figure S7 in Supporting Information S1 also indicates that within the up-scaled sectors, either the lowest permeability or highest permeability class dominated. These results suggested that using the *majority vote* upscaling method (Zhang, Pickup, & Christie, 2008; Zhang, Pickup, Monfared, & Christie, 2008) was reasonable. Consequently, it was decided to turn every 5^3 grids into a single block to reduce the computational cost for further simulations. In terms of upscaling, the resultant block was assigned with the volume-weighted average porosity of the former 125 grids. It must be underlined that for the Bentheimer domain, each up-sampled block has the same k , p_c , and k_r models as before, due to only one class. The geometric mean technique was used for the Indiana sample to find the representative value of permeability for each up-scaled block. Also, the p_c and k_r models were taken based on the quantitatively dominant class in the former 5^3 grids.

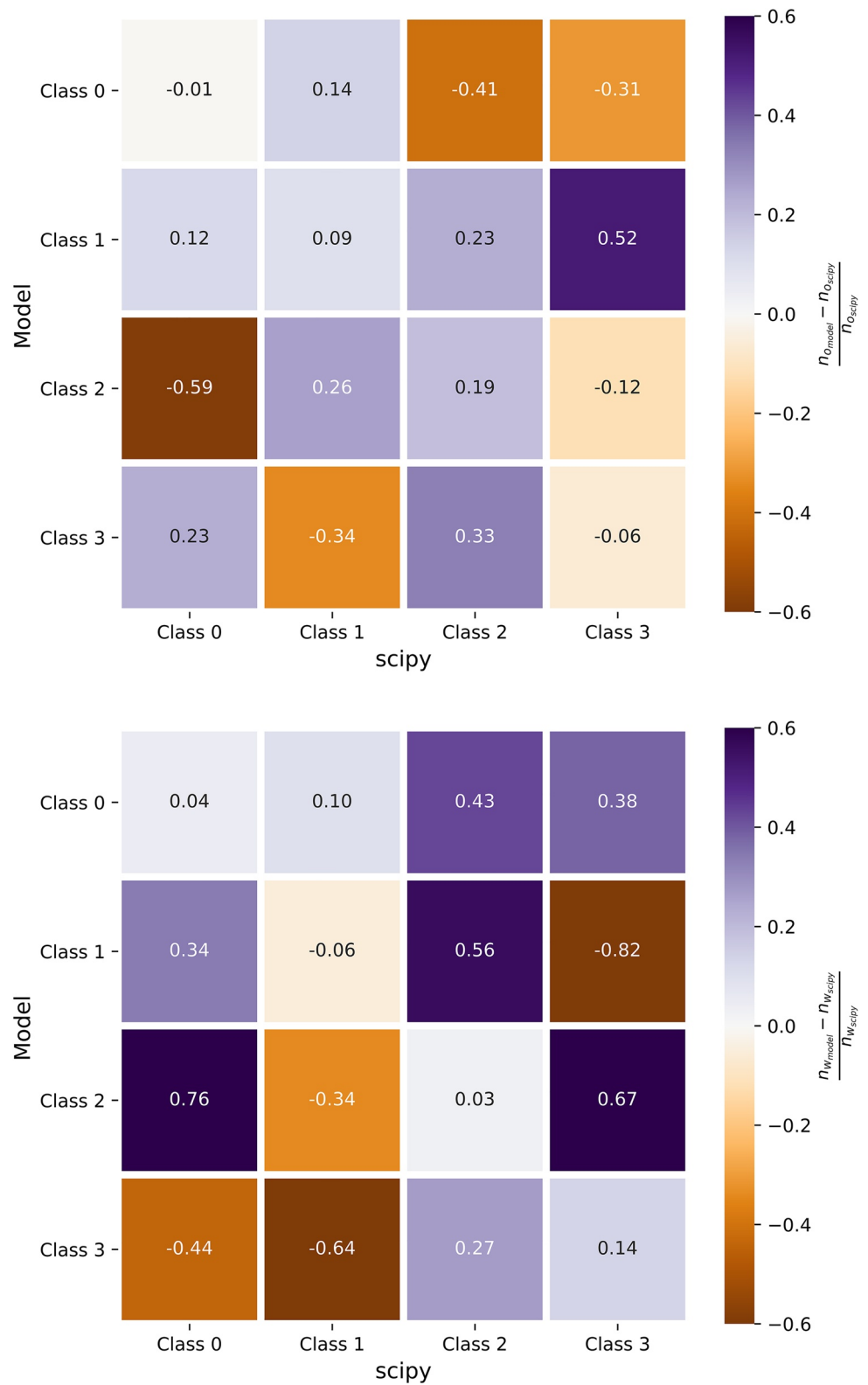


Figure 8. The obtained exponents of k_r models for the second set (5 super-resolved sub-volumes) of each class versus the first set of that class and other classes. The subscript of “model” refers to the first 6 sub-volumes, and the subscript of “scipy” is relevant to the next 5 sub-volumes.

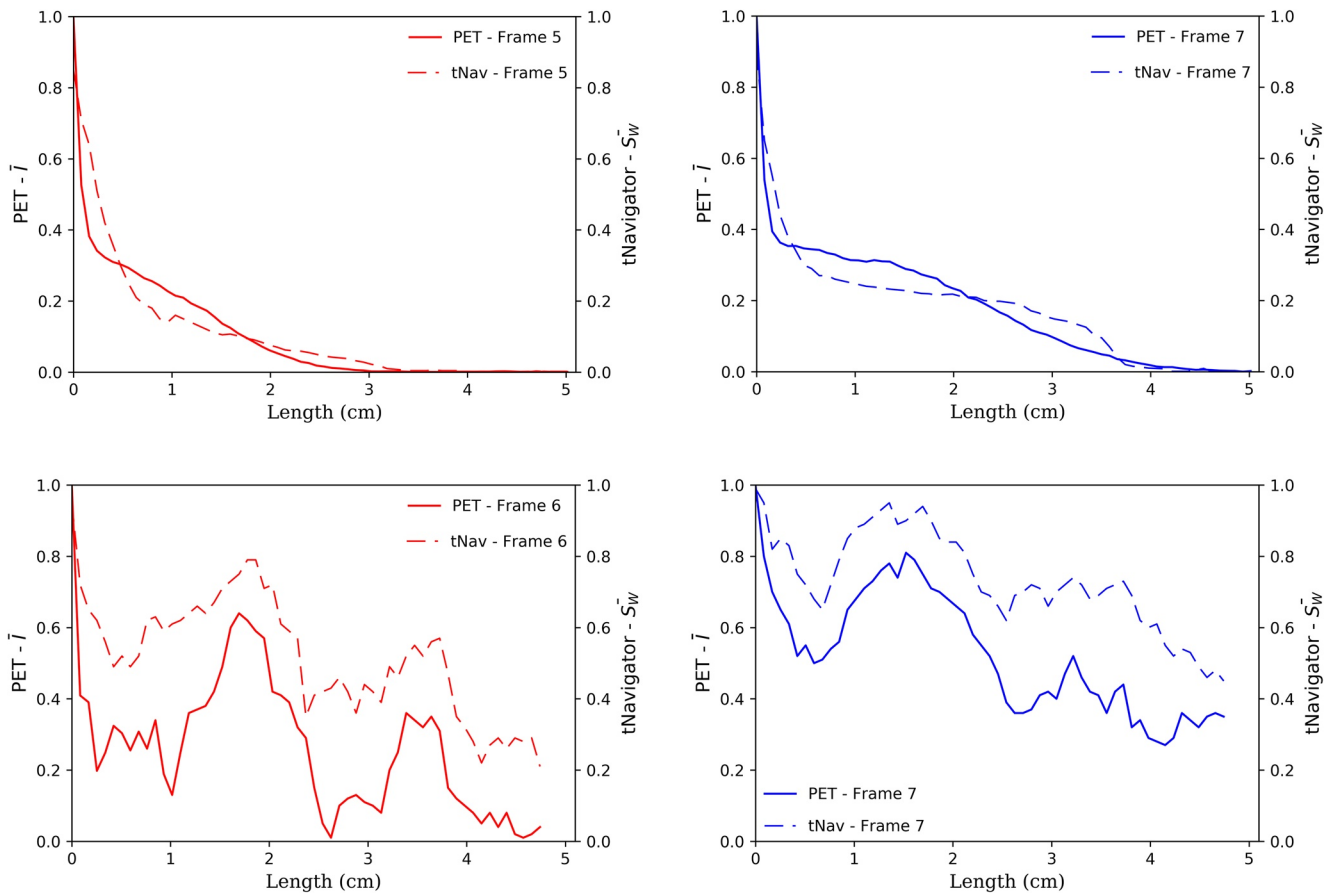


Figure 9. The comparison of generated profiles by tNavigator based on the proposed algorithm against the Positron Emission Tomography (PET) measurements. PET- $\bar{I}$ shows the average of detected radiation for each slice of the PET image.

The S_w profiles were generated according to the temporal resolution of the PET images, Figure 9. For example, Figures 9a and 9b illustrates that applying the proposed workflow Figure 1 for the Bentheimer data provided simulated S_w profiles that agree well with the S_w profiles of the PET experiment. Overall, the homogeneous Bentheimer was well characterized by the single class model. The Indiana limestone results are presented in Figures 9c and 9d. The results used no optimization procedures; the assigned properties were completely data-driven based on feature extraction, clustering, and petrophysical measurements using pore-scale simulations. In this way, the results were purely predictive. Although the S_w profiles generated by the proposed workflow do not precisely matched with the PET S_w profiles, it can generally be observed that similar trends as the experimental data were captured. For improvement of the results, we suggest that higher spatial resolution μ CT images are required. This could be achieved by using a region-of-interest scan on the core sample to provide more details about the underlying pore geometry, which would provide more accurate evaluation of the petrophysical properties leading to a better understanding of the various classes. In particular, the classes with high conductivity and low porosity or micro-porosity could required further characterization.

An important question associated with the illustrated results was how much adjusting the K value of the K -means classifier impacts the performance of the proposed workflow. To address this question, we measured the Mean Square Error (MSE) between the saturation profiles generated by tNavigator and those obtained by the PET experiments; the results of which are presented in Figure 10. MSE measures the average squared differences between the generated S_w profile by tNavigator and corresponding PET S_w profile. The reduced-dimensional data of the Bentheimer sample after the implementation of PCA was classified into 2 and 3 classes by the K -means algorithm. Figure 10a demonstrated that increasing K had a minimal effect on the MSE values of each time frame for the Bentheimer sample. The same analysis performed on the Indiana sample demonstrated the importance of K , see Figure 10b. The computed MSE for different time frames increased logarithmically for K less than 4. For

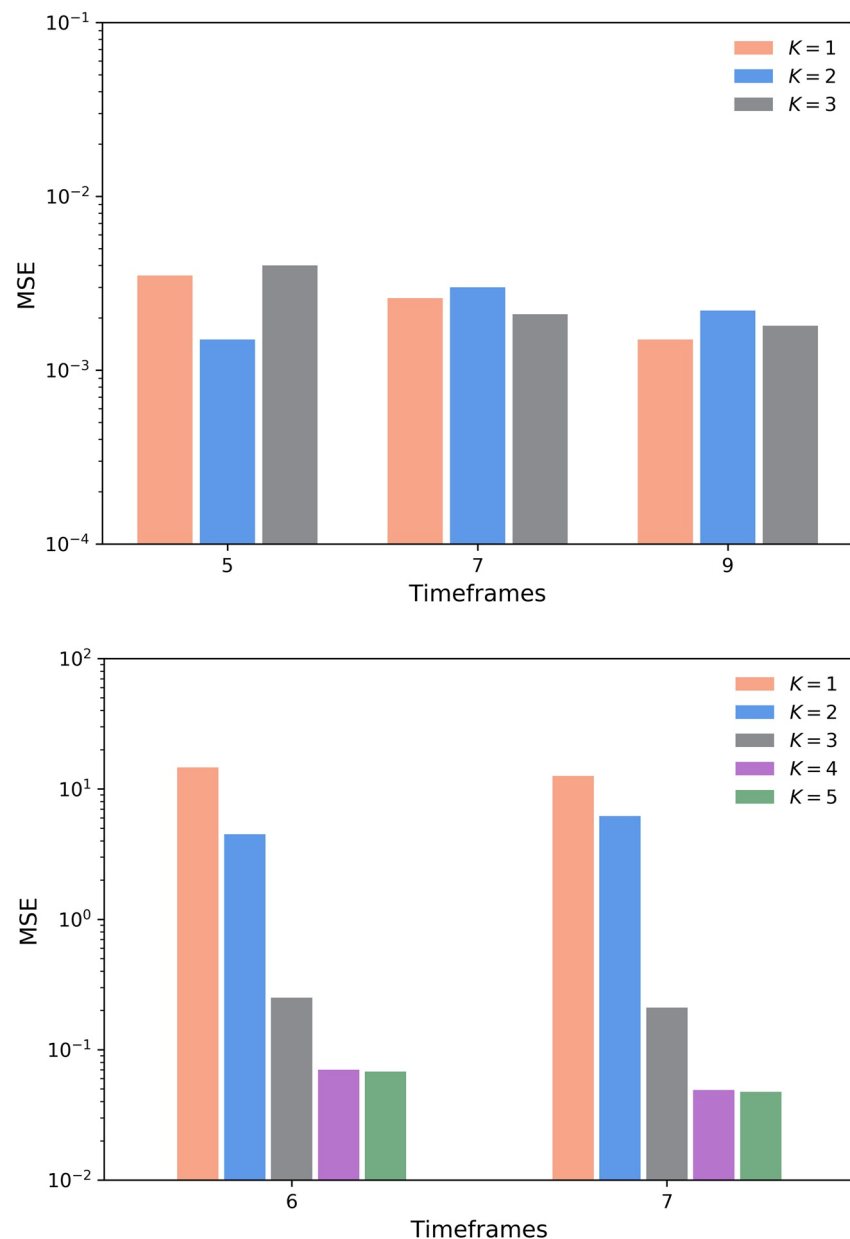


Figure 10. Accuracy of the generated results dependent on the value of K .

$K = 5$, the trend of MSE values remained stable. Overall, the results suggested that $K = 4$ is the optimum point to suitably account for the sample heterogeneity.

4. Conclusions

The proposed workflow combines various imaging techniques, advanced numerical simulations, machine learning, and computer vision techniques to investigate and obtain a deeper understanding of pore-scale and core-scale structures that influence multiphase flow. The implementation of PET imaging displayed the movement of water during immiscible displacement at an unprecedented level of detail. Moreover, μ xCT imaging provided high-resolution 3D representation of the pore structure necessary for direct numerical simulations. However, a lack of knowledge about the core-scale heterogeneity was inherent to high-resolution μ xCT images, which was necessary information for predictive core-scale simulations. Without a well characterized core-scale domain, simulation results for fluid saturation were not comparable to experimental PET observations. To overcome the

addressed difficulty, the current research proposed a workflow to acquire a better understanding of pore-geometry dependent petrophysical properties using low-resolution large FOV μ xCT images with using soft computing methods. By taking advantage of various pore-scale simulation techniques, deep learning methods, morphological characterization, and classical unsupervised machine learning, we were able to fully characterized a heterogeneous rock core using a fully automated workflow. The fully characterized core was validated by comparing numerical simulation results with experimental PET images. Overall, the key advantages of the proposed workflow are the following:

- The proposed algorithm uses a full-automated approach to characterize petrophysical properties based on low-resolution micro-CT images.
- The validation was conducted by comparing PET images collected during core flooding to simulation results using the fully characterized 3D domain from the proposed workflow.
- The proposed workflow is straightforward and provides predictive capabilities for capturing the complex flow patterns that develop in heterogeneous rock cores.

In addition, future works should focus on the following key points:

- It remains unclear to what extent using other similar methods of dimensionality reduction, SR, image segmentation, and unsupervised classification can affect the final results. These specific details would require a full systematic analysis of all available options.
- Regarding the Indiana sample, although the simulation results are similar to the PET analysis, the implemented algorithm was not entirely successful in characterizing the core to sufficient detail to capture exactly the experimentally measured saturation profiles.
- The employed upscaling method can perform well only if there are dominant classes in defined regions. In other words, the success of used upscaling technique would be case-dependent. In terms of having no limitation of computational resources and running the continuum-scale simulation without upscaling, following the presented workflow could provide more satisfying results because of avoiding features loss.
- Further works are required to establish data fusion techniques to provide higher fidelity images for the pore-scale simulations since the current work was based on relatively low resolution images and the implementation of a single SR technique.
- The usage of nanoscale imaging like Scanning Electron Microscope (SEM) in applying the introduced workflow to tight and ultra-tight systems should be taken as the topic of future research. Furthermore, using SEM images to verify and improve the results of applying the SR methods can be considered.
- Generally, the success of applying the introduced workflow is a strong function of the taken samples. The performance of applying the workflow to other samples with a higher level of heterogeneity or even tight and ultra-tight systems is an open-ended question.

While future investigations are necessary to validate the conclusions drawn from this research for other rock types and unconventional resources, other image modalities, fusion techniques, and other machine learning approaches, the novelty of the work is within providing a vision for how recent advancements in soft computing methods can be used for automatic core analysis by taking both pore-scale and mm-cm scale rock heterogeneity into account.

Data Availability Statement

Moreover, the data and codes used in the conducted research are addressed as below:

1. Part 2.1— **μ xCT and PET images**: All the images used in the current research are available at <https://data.mendeley.com/datasets/ysyx6z6x8/1>.
2. Part 2.3—**Morphological Analysis**: The employed codes of Minkowski Functionals are available at <https://www.mathworks.com/matlabcentral/fileexchange/33690-imminkowski>.
3. Part 2.3—**Petrophysical Analysis**: The implemented pre-trained CNN is a standard ResNet50. The instantiating of ResNet50 architecture is described at https://www.tensorflow.org/api_docs/python/tf/keras/applications/resnet50/ResNet50. The training protocols and relevant data are fully discussed on the (Alqahtani et al., 2021).
4. Part 2.5—**EDSR**: The code of the applied SR method is available at
5. <https://github.com/yingDaWang-UNSW/EDSRGAN-3D.git>.

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