Anchoring Multi-Scale Models to Micron-Scale Imaging of Multiphase Flow in Rocks

Shan Wang[1,2], Leonardo C. Ruspini[3], Pål-Eric Øren[3], Stefanie Van Offenwert[1,2] and Tom Bultreys[1,2]

[1]Department of Geology, Pore-Scale Processes in Geomaterials Research (PProGRess), Ghent University, Krijgslaan 281/S8, B-9000, Ghent, Belgium

[2]Centre for X-ray Tomography (UGCT), Ghent University, Proeftuinstraat 86, B-9000, Ghent, Belgium

[3]Petricore Norway A.S., Trondheim, Norway

Corresponding author: Shan Wang (Shan.Wang@UGent.be)

Key Points:

- Improved differential imaging technique is used to quantify porosity and saturation distribution of a heterogeneous rock sample
- A new sub-rock typing method based on the drainage experiment is presented
- The breakthrough pressure plays an important role in multiphase distribution within heterogeneous rocks during capillary drainage

Abstract

Image-based pore-scale modeling is an important method to study multiphase flow in permeable rocks. However, in many rocks, the pore size distribution is so wide that it cannot be resolved in a single pore-space image, typically acquired using micro-computed tomography (micro-CT). Recent multi-scale models therefore incorporate sub-voxel porosity maps, created by differential micro-CT imaging of a contrast fluid in the pores. These maps delineate different microporous flow zones in the model, which must be assigned petrophysical properties as input. The uncertainty on the pore scale physics in these models is therefore heightened by uncertainties on the representation of unresolved pores, also called sub-rock typing. Here, we address this by validating a multi-scale pore network model using a drainage experiment imaged with differential micro-CT on an Estaillades limestone sample. We find that porosity map-based sub-rock typing was unable to match the micrometer-scale experimental fluid distributions. To investigate why, we introduce a novel baseline sub-rock typing method, based on a 3D map of the experimental capillary pressure function. By incorporating this data, we successfully remove most of the sub-rock typing uncertainty from the model, obtaining a close fit to the experimental fluid distributions. Comparison between the two methods shows that in this sample, the porosity map is poorly correlated to the multiphase flow behavior of the microporosity. The validation method introduced in this paper serves to separate and address the uncertainties in multi-scale models, facilitating simulations in complex geological reservoir rocks important for e.g. geological storage of CO_2 and renewable energy.

Plain Language Summary

Understanding multiphase flow within heterogeneous reservoir rocks is crucial for geological reservoir management. These rocks usually have intricate microstructures (unresolved or sub-resolution pores) which are difficult to quantify and have a strong impact on fluid flow. Pore-scale modelling combined with imaged-based experiments can be a useful tool to describe complex pore structures, which is of key importance in the subsequent simulation and prediction of multiphase flow behavior. In this study, we focus on improving the representation of unresolved porous regions of a heterogeneous rock sample (also called sub-rock typing). A drainage experiment was performed and imaged by micro-computed tomography (micro-CT) to characterize the multiphase distribution at increasing capillary pressures. The predictions of two multi-scale models, which were generated according to distinct sub-rock typing methods on the same sample, were compared with the drainage experimental data. We found that the model obtained by the “classical” sub-rock typing method was unable to simulate the correct arrangement of fluids in this sample, while the new method performed better, which illustrates the importance of rock type identification to pore-scale modelling. The validation workflow presented in this paper can be extended and served as a reliable reference to improve simulations in other complex geological materials.

1 Introduction

Multiphase flow through rocks plays an important role in numerous earth science applications, such as hydrocarbon recovery (Olayiwola & Dejam, 2019; Wang et al., 2020), carbon dioxide storage (Arif et al., 2017), remediation of polluted aquifers (Bortone et al., 2013) and subsurface energy storage in the form of hydrogen or compressed air (Amid et al., 2016, Mouli-Castillo et al., 2019). Many reservoir rocks, notably carbonates and clay-bearing sandstones, exhibit complex pore geometries with very wide pore size distributions. The petrophysical properties of such rocks often do not obey classical correlations (Prodanović et al., 2015; Shanley et al., 2004), spurring pore-scale studies of their fluid flow behavior (Mehmani et al., 2020). This can be done based on images of the pore space, obtained with for example micro-computed tomography (micro-CT) and (FIB-)SEM imaging (Bultreys et al., 2016b; Bera et al., 2011; Ciobanu et al., 2011; Cnudde & Boone, 2013; Wirth, 2009).

Despite the wide interest in simulating fluid flow in complex, multi-scale pore spaces, the trade-off between image size and resolution in most imaging techniques complicates the development of suitable image-based approaches (Blunt et al., 2013). Typical imaging workflows identify resolved pores and zones with unresolved porosity (below the µm scale) in micro-CT images of mm-scale samples, which usually capture the largest pore features. Unresolved porosity is visible in these images as zones with grey values that are intermediate between solid and void, due to their intermediate density (Cnudde & Boone, 2013). These regions can then be imaged by higher-resolution techniques, that are then correlated back to the lower-resolution micro-CT scan (De Boever et al., 2015; Devarapalli et al., 2017; Lin et al., 2019). The unresolved pores, which we will by definition refer to as the microporosity, can play a crucial role in the sample's multiphase flow behavior (Bultreys et al., 2016c; Mehmani et al., 2020). Therefore, specialized multi-scale models are required that fuse the resolved pores with information on the microporosity features, typically obtained using higher-resolution images on small sub-sections of the sample (Menke et al., 2019).

Multi-scale models are an extension of pore-scale, image-based modelling techniques, consisting of either direct numerical simulations (Alhashmi et al., 2015; Pan et al., 2004; Raeini et al., 2012) or pore network models (PNMs) (Blunt et al., 2013; Dong & Blunt, 2009). Direct numerical simulations of multiphase flow usually require large computational resources and therefore struggle to capture capillary-dominated flow on large images (Blunt et al., 2013). PNMs feature higher computational efficiencies due to simplifications on the geometry and the fluid displacement physics, which makes them well-suited for multi-scale simulations. Networks obtained at different resolutions or scales can be extrapolated in space and fused to reconstruct a multi-scale pore network (Jiang et al., 2013; Mehmani & Prodanovic, 2014), resulting in detailed but very large networks. Alternatively, the micropores can be treated as a continuous porous medium with specific petrophysical properties to reduce the size of the network while still representing the connectivity caused by microporosity (Bultreys et al., 2015; Bauer et al., 2012; Youssef et al., 2008).

Despite the progress in representing multi-scale pore networks, it remains difficult to assess the model uncertainties. Multi-scale pore network models depend on a significant amount of uncertain input information to describe the microporosity behavior, which complicates the validation of the physical assumptions in the model itself (e.g. quasi-static fluid displacement). An important aspect of the input uncertainty is that only a limited volume of microporosity is typically imaged at the highest resolutions, while there is often significant heterogeneity in its properties. Recent approaches have addressed this information gap by incorporating sub-voxel porosity maps (Ruspini et al., 2016, 2021). The porosity map can be generated based on differential imaging: measuring the calibrated grey value change when the pore space is filled with a high-contrast fluid such as high-concentration potassium iodide or cesium chloride (Boone et al., 2014; Ghous et al., 2007, Lin et al., 2016). The resulting map is then used for “sub-rock typing”: identifying and characterizing zones with different microporosity properties in the model. The common approach is to perform a segmentation on dry images or differential images directly to separate distinct phases, sometimes followed by a series of image processing operations to alleviate artifacts at phase boundaries (Bauer et al., 2012; Bultreys et al., 2015). However, there is still a lack of validation to reveal whether these approaches can provide a reasonable representation for unresolved pores and how much uncertainty they introduce into the multi-scale PNM simulations. Recent work on single-scale pore network models has illustrated how pore-by-pore validation of the fluid distributions during drainage or imbibition can serve to study model uncertainties (Bultreys et al., 2018, 2020, Øren et al., 2019). A similar principle used to generate porosity maps can be used to track the fluid saturation in microporous regions during multiphase flow experiments (Lin et al., 2016, Gao et al., 2017). In this paper, we propose a pore-by-pore validation workflow for multi-scale PNM by comparing fluid distributions in the model to a differential micro-computed tomography (micro-CT) based drainage experiment on a heterogeneous Estaillades limestone (as shown in Figure 1). Using this data, we validate the porosity-map based workflow, and explain its uncertainties by comparing to a novel data-based model, which takes its microporosity information from the micro-CT drainage experiment. The experiment and the image processing workflows are introduced in Section 2.1. Then, the multiscale PNM workflow including the two sub-rock typing methodologies (porosity-based and drainage-based methods) are explained in Section 2.2. In Section 3, we compare the predictions from the two models with experimental data and discuss the reasons that may lead to simulation uncertainties. Section 4 discusses the conclusion and the outlook for our future research.

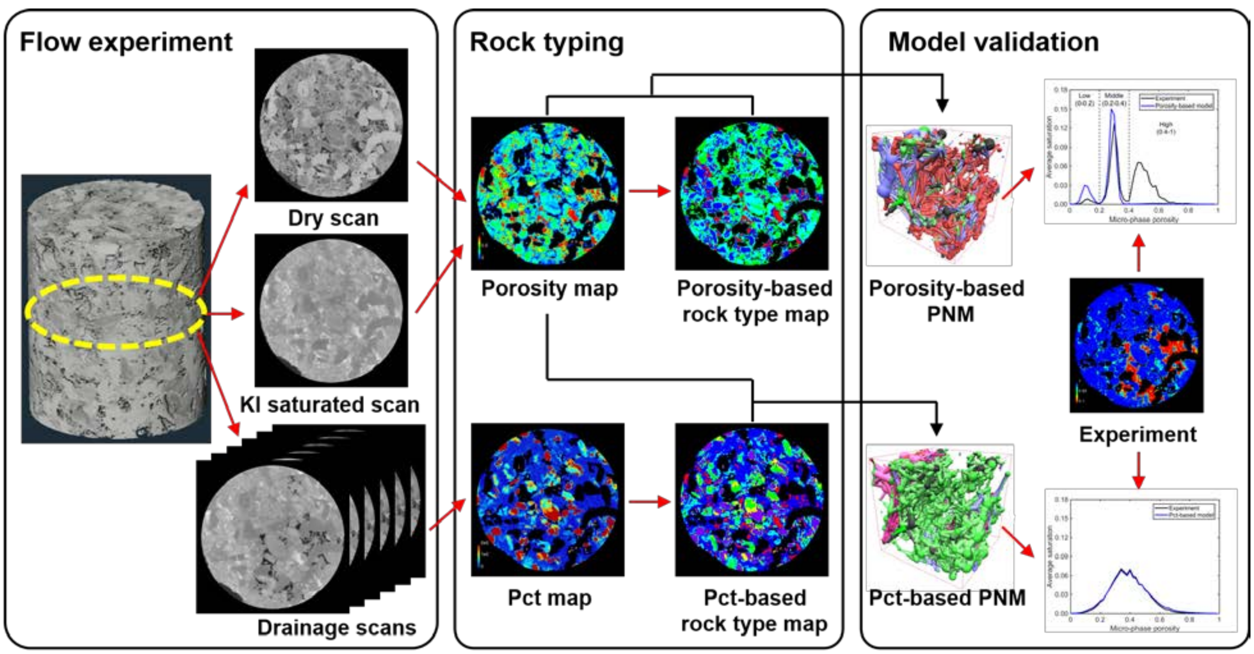


Figure 1. The validation workflow for multi-scale pore network model.

2 Materials and Methods

2.1 Experiment

The main goal of the experiment presented here is to measure the brine and decane distribution within both macropores and microporous regions of the sample during capillary drainage. In the following, the sample and fluid preparation, the set-up, the experimental procedure and data processing workflow will be discussed in detail.

2.1.1. Rock samples and fluid preparation

The rock sample used in the experiment is Estaillades limestone, which has a complex pore structure featuring a bi-modal pore size distribution. The broad pore size distribution has two peaks with modes of respectively 390 nm and 19 μm (Han et al., 2007). Estaillades limestone is composed of 99% calcite (Alyafei & Blunt, 2016). A sample with a diameter of 6 mm and a length of 20 mm was cored and vacuum-saturated with deionized water to ensure that all the air was removed from the pores before the experiment.

As fluid phases in the drainage experiment, we used KI-brine and decane. The former acted as wetting phase, while the latter was the non-wetting phase. The brine was made from deionized water doped with 25 wt% potassium iodine (KI) as a contrast agent due to its high X-ray attenuation coefficient. This solution provided a strong contrast to identify the fluid phases in the micro-CT images.

2.1.2. Drainage experiment

The experimental apparatus and flow lines are shown in Figure 2. The rock sample was placed on top of a water-wet ceramic porous plate (Cobra Technologies B.V., NL) and then wrapped in a Viton sleeve. The hydrophilic porous plate had a breakthrough pressure of 1300 kPa to prevent early breakthrough of the non-wetting phase. This assembly was placed in an X-ray transparent flow cell made out of PEEK (RS Systems, Norway), connected to high-precision syringe pumps supplying the experimental fluids. A differential pressure transducer (Keller PD-33X) was connected to the inlet and outlet of the sample. The flow cell was then placed on the Environmental Micro-CT (EMCT) scanner at Ghent University's Centre for X-ray Tomography (UGCT) (Dierick et al., 2014; Bultreys et al., 2016a). This scanner consists of a rotating source-and-detector gantry, meaning the flow cell remained static during the full experiment. Throughout the experiment, the X-ray beam was filtered with 1 mm aluminium to reduce the beam hardening effect. The experiment was performed by executing the following steps:

1. A confining pressure of 3500 kPa was set to compress the Viton sleeve, to avoid fluid bypassing along the wall of sample.
2. The water-saturated sample was scanned by micro-CT at room temperature and pressure. The imaging settings were: 6.5 μm voxel size, 2400 projections, 1150 ms integration time per radiograph; 110 kV and 8 W X-ray tube settings. Since water has a low grey value similar to air in the images, we will refer to this as the “dry scan” or “dry image” in following sections for convenience.
3. The water was flushed out by brine, which was injected through the sample with a maximum flow rate of 0.075 ml/min for 4 hours and left overnight. A high-quality micro-CT scan was conducted to capture the sample’s 100% brine saturated state (same imaging settings as step 2).
4. The drainage was started by injecting decane from the top of the flow cell at a low flow rate (0.001 ml/min). To set a constant pressure drop over the sample, which at vanishing flow rates yields a set capillary pressure in the sample, the flow rate was subsequently gradually lowered based on manual inspection of the pressure transducer reading. This proved to be more reliable than using automated constant-pressure settings on the syringe pump, particularly at low set pressures. The experiment remained capillary dominated at all times during this equilibration procedure, as the maximum capillary number was 6.2×10^{-8}.
5. Radiographs of the sample were collected and subtracted from each other to track the saturation change in the sample during the equilibration (supporting information Figure S1). In addition, a short micro-CT scan (6.5 μm voxel size, 2400 projections, 115 ms exposure time) was performed every hour to further compare flow distribution changes. When no more changes were found from both the differential radiographs and the subsequent micro-CT images at the target pressure, a high-quality scan (imaging settings see step 2) was taken.
6. Steps 4 and 5 were repeated with gradually increasing pressure. We performed 6 capillary pressure steps during the experiment, at 8, 14, 80, 180, 220 and 400 kPa. Equilibration took between 4 and 7 hours for the different pressure steps, in all cases having reached very low final flow rates (below 0.0003 ml/min).

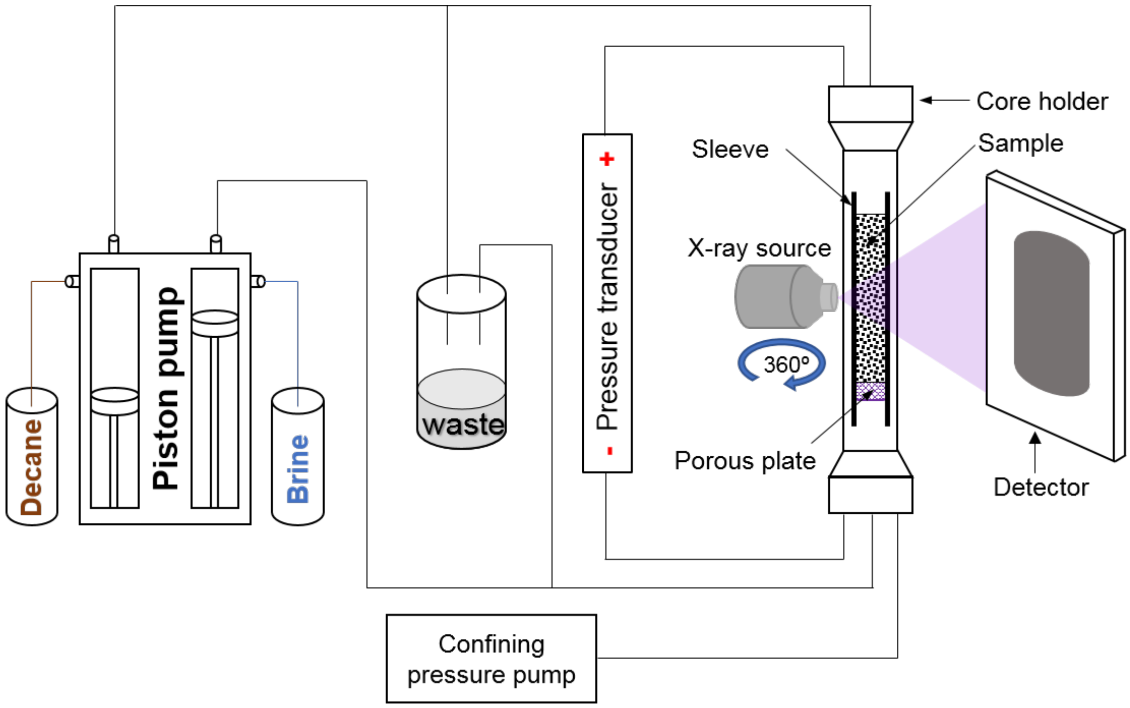
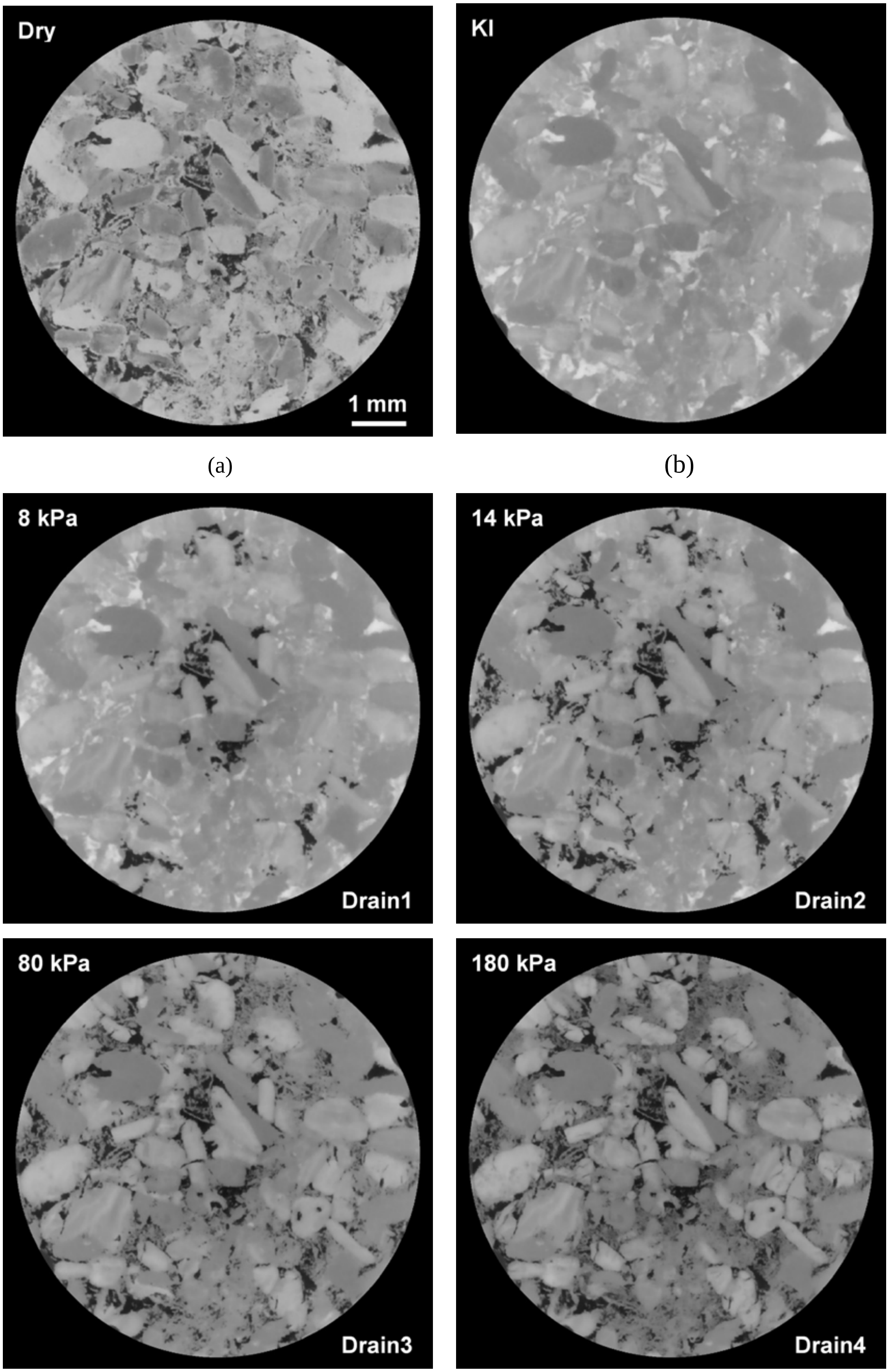
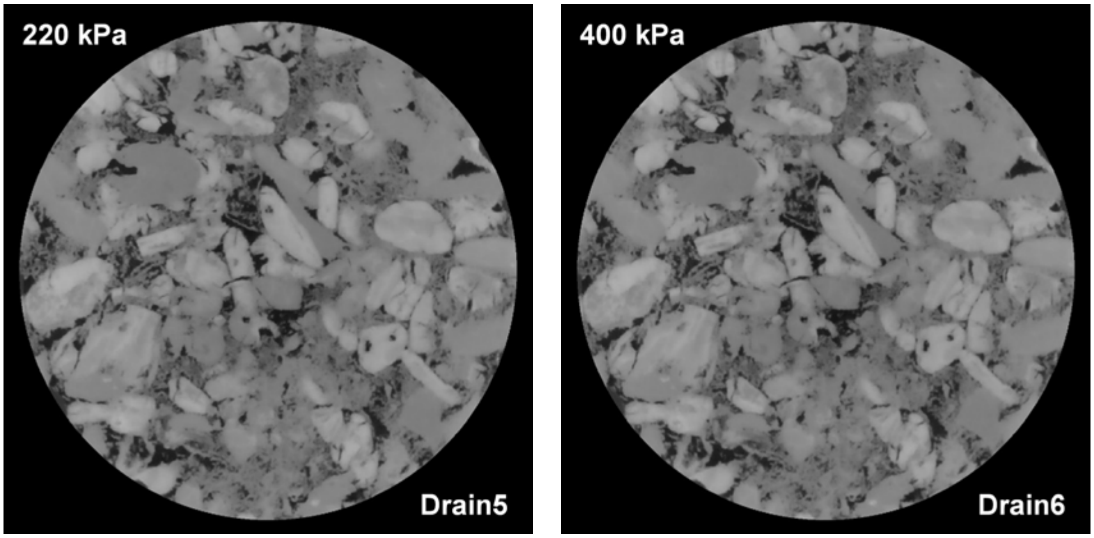


Figure 2. Experimental apparatus used in the drainage experiment.

2.1.3. Micro-CT image processing

The acquired tomograms, which represent the 3D distribution of X-ray attenuation coefficients in the sample, were reconstructed using Octopus Reconstruction software (Tescan-XRE, Belgium). After reconstruction, the image processing was performed using Avizo 2020.2 (ThermoFisher, France). The brine-saturated and drainage-step images were all registered to the dry image using normalized mutual information and resampled using the Lanczos algorithm to make sure all the images are aligned in space. The images were then filtered with a non-local means edge-preserving filter to reduce the image noise. As shown in Figure 3, the pores in the dry scan image are dark grey and have significantly lower grey values than solid calcite grains. In the brine-saturated image, the brine-invaded pores are brighter than other phases in the sample. A cross-section of the fluid distribution in the 6 capillary pressure steps is shown in Figure 3(c). With the increase of drainage pressure, the brine is displaced by decane, and brighter pores gradually become “black”.


Dry
1 mm
KI
(a)
(b)
8 kPa
Drain1
14 kPa
Drain2
80 kPa
Drain3
180 kPa
Drain4



(c)

Figure 3. (a) Dry san. (b) KI saturated scan. (c) Drainage scans at 6 capillary pressures.

Although the KI-brine visually already indicates the presence of different fluid phases within macropores, further processing is necessary to quantify the brine saturation in the unresolved porosity. We propose an improved workflow here based on differential imaging with normalized water-filled and brine-filled images to calculate the sub-resolution saturation in voxels that contain microporosity.

The image normalization is based on selecting fixed grey values for two known materials, setting them to the same value in the different images, and doing a linear rescaling of everything in between. To normalize the brine-saturated image to the dry image, we first cropped 3 region-of-interests (ROI) of solid grain to determine the upper normalization value, and an ROI in the sleeve (which has a low grey value) for the lower value. The rescaled image was calculated following equation (1), which is adapted from Lin et al, (2017):

$$I_{new} = (I - p_{s\_bine}) \cdot \frac{p_{g\_dry} - p_{s\_dry}}{p_{g\_brine} - p_{s\_brine}} + p_{s\_dry} \tag{1}$$

Where I_{new} is the rescaled image, I is the image before normalization, p_{g_dry} is the average mode of the 3 solid grain ROIs from the dry image, p_{s_dry} is the mode of the grey value histogram of the sleeve ROI from the dry image, p_{g_brine} is the average mode of the 3 solid grain ROIs from the brine saturated image, and p_{s_brine} is the mode of the sleeve ROI from the brine saturated image.

For the drainage images, we first cropped 3 ROIs in solid grains and 3 ROIs in water-filled resolved pores from the dry and the 6 drainage images, extracted their grey value histograms and calculated their modes. The drainage images were then rescaled according to equation (2):

$$I_{new} = (I - p_{d\_drain}) \cdot \frac{p_{g\_dry} - p_{w\_dry}}{p_{g\_drain} - p_{d\_drain}} + p_{w\_dry} \tag{2}$$

Where p_{g_dry} is the average mode of 3 solid grain ROIs in the dry image, p_{w_dry} is the average mode of 3 water-invaded-pore ROIs from the dry image, p_{g_drain} is the average mode of 3 solid grain ROIs from the drainage images, p_{d_drain} is the average mode of 3 decane-invaded-pore ROIs from drainage images.

Then, the differential image was obtained by calculating the differences between the rescaled drainage- or brine saturated images and the water-filled image:

$$I_{diff\_drain} = I_{new\_drain} - I_{dry} \tag{3}$$

$$I_{diff\_brine} = I_{new\_brine} - I_{dry} \tag{4}$$

The dry-brine differential image was used to quantify sub-resolution porosity in the image, due to the assumed linear dependence of the grey value in the differential image and the volume percentage of brine present in each voxel. We denote the thresholds set for solid (0% porous) and open porosity (100% porous) voxels as CT1 and CT2, respectively. CT1 was determined based on the valley between the grey value distributions of the solid and microporous phase in the histogram. CT2 was found by masking the differential image with the macropores segmented from the dry image, and finding the peak of the associated grey value histogram (supporting information Figure S2). Voxels with grey values equal to or less than CT1 are assigned 0% porosity, those equal to or higher than CT2 are assigned 100% porosity, the microporous region between CT1 and CT2 is assigned 0~100% porosity, using:

$$\varphi_{micro} = \frac{I_{diff\_brine} - CT1}{CT2 - CT1} \tag{5}$$

Where φ_{micro} is the porosity within microporous voxels. The total porosity can be calculated by:

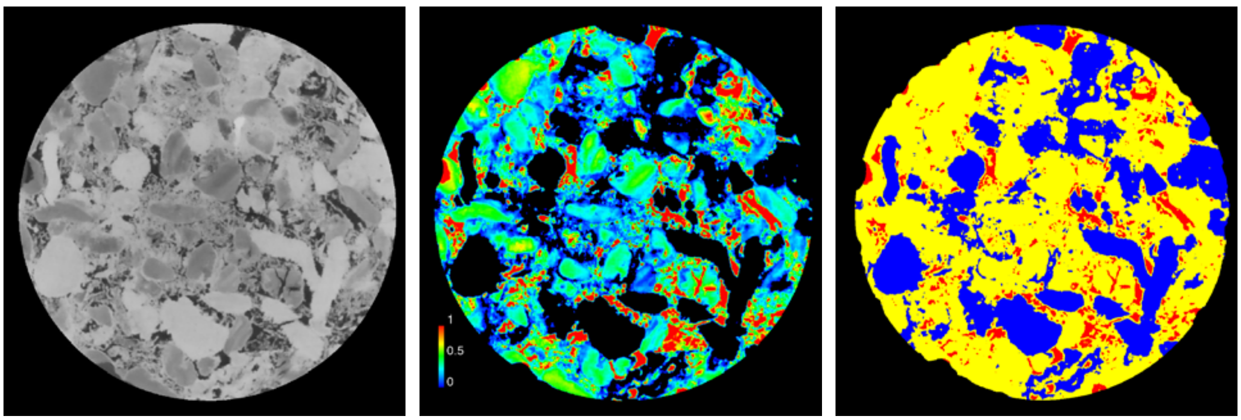
$$\varphi_{total} = \frac{V_{macro} + V_{micro} * \varphi_{micro}}{V_{sample}} \tag{6}$$

Where V_{macro} is the number of macropore voxels, V_{micro} is the number of micro-pore voxels, V_{sample} is the number of voxels in the whole sample.

Simarly to the porosity map, we also calculated the brine saturation map at each capillary pressure step using the equation (7):

$$S_{w\_drain} = \frac{\varphi_{drain}}{\varphi_{micro}} = \frac{I_{diff\_drain} - CT1}{I_{diff\_brine} - CT1} \tag{7}$$

With this method, the porosity distribution map was obtained, shown in Figure 4(b), which provided a 3D distribution of the porosity variation within the microporous phase. Table 1 shows the porosity calculation results. The total porosity of this sample was 25.43%, of which the sub-resolution porous regions contributed 78.53%. The 3 components, macropores, microporous regions and solid grains, were extracted from this porosity map (Figure 4(c) and supporting information Figure S3).



(a) (b) (c)

Figure 4. Porosity distribution map. (a) A slice from the filtered dry image (b) The corresponding porosity distribution map at the same slice (c) Three-phase segmentation of the sample into macropores (red), microporous regions (yellow) and solid (blue).

Table 1. Porosity calculation

Phase	Threshold	Voxel ($\times 10^8$)	Voxel*Porosity ($\times 10^8$)	Average porosity	Volume fraction	Contribution	Total porosity
macro	>1	0.42576		1	0.05463	0.05463	
micro	0-1	5.01773	1.55637	0.31017	0.64381	0.19969	0.2543
grain	<0	2.35033		0	0.30156	0	

2.2 Multi-scale model

2.2.1 Sub-rock typing

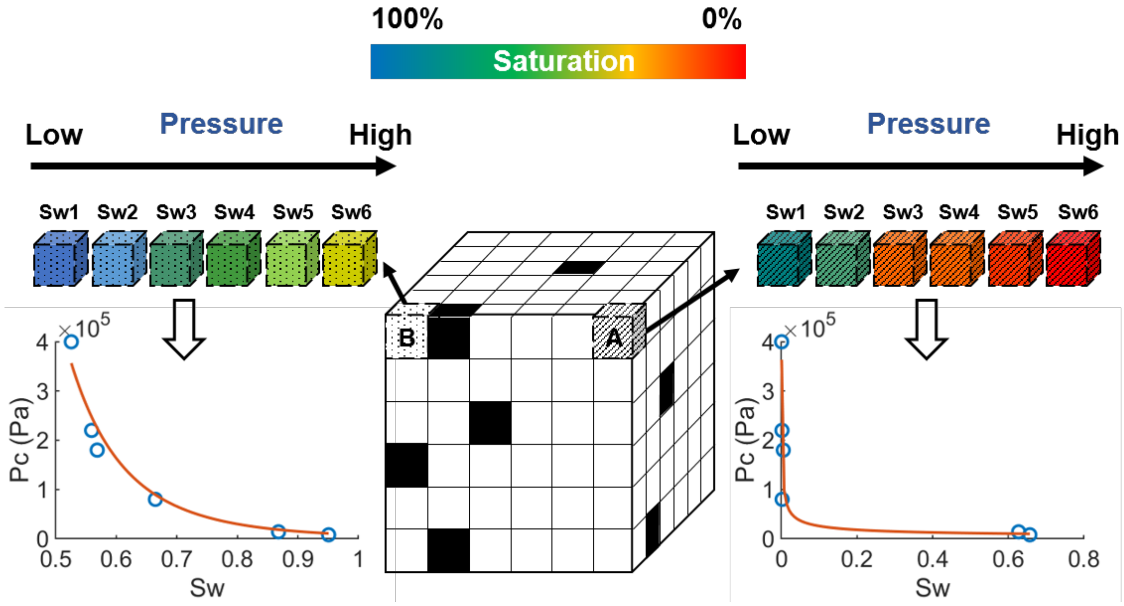
Multi-scale models of multiphase flow depend on the classification of regions with sub-resolution porosity. To identify these regions, and inform their description in the model, a recently proposed method is to segment a sub-resolution porosity map of the sample into different “sub-rock types”. We will refer to this as the “porosity-based” method. A crucial first step is to generate an accurate porosity map (Figure 4(b)). Figure S4 in supporting information depicts the histogram of the porosity distribution in the sample. Two thresholds (0.2 and 0.4) were manually selected to divide the sample into 3 microphase regions or 3 rock types (3RT), based on trial-and-error to obtain realistic simulation results for the capillary pressure curve (see further). The sub-rock typing result is shown in Figure 6.

The downside of porosity-based sub-rock typing is that it is based on the assumption that porosity is closely correlated to the multiphase flow properties of the microporosity. This is not necessarily the case. Therefore, we introduce a new method here to perform rock typing based directly on experimental multiphase flow data. To this end, we determined the invasion capillary pressure (Pct) distribution within the microporous phase. First, the saturation map at each drainage pressure step was calculated (Section 2.1.3). The saturation variation with the increase of pressure of every individual voxel was thus obtained. Next, these saturation maps were mean-filtered and downsampled by a factor 2 to reduce the noise dependency and computational load. Then, a Brooks-Corey-type P_c formulation (Brooks & Corey, 1964) was fitted to the capillary pressure-saturation data points of each voxel using a least-squares approach in Matlab. This yielded a relation of the following form for each voxel:

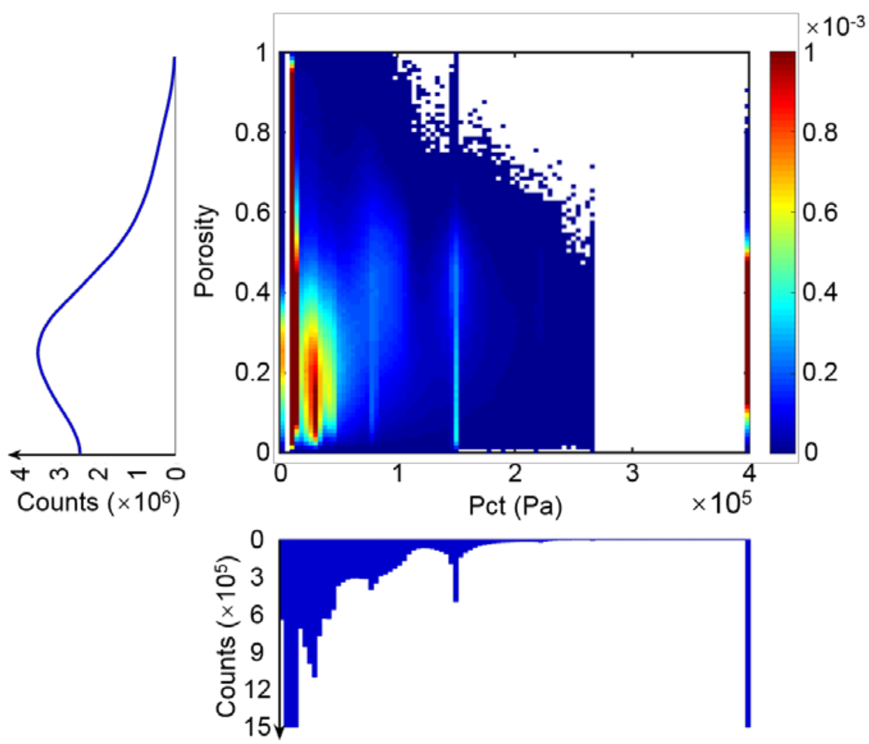
$$P_c = P_{ct}\left(\frac{1}{S_w}\right)^{\frac{1}{\lambda}} \tag{8}$$

Where P_c is the capillary pressure, P_{ct} is the fitted invasion capillary pressure, λ is a fitted parameter related to the pore size distribution and S_w is water saturation.

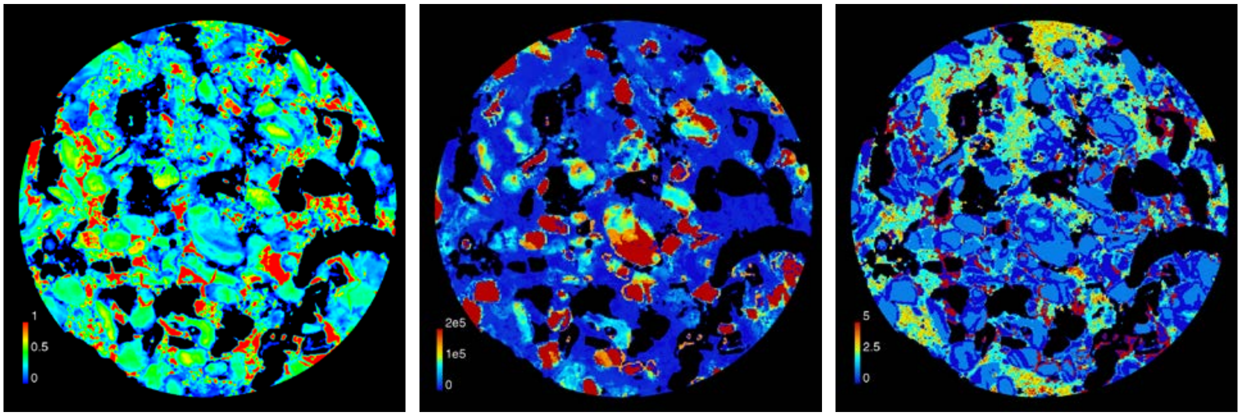
In this way, P_{ct} and λ values were derived for all microporous voxels. The fitted curves for two representative voxels are shown in Figure 5(a). Figure 5(c) presents the Pct map and the λ map, showing the 3D variation of the capillary pressure behavior in the sample. We primarily used the Pct map here due to its easier interpretability and lower noisiness than the λ-map. We considered both porosity and Pct together by performing a k-means clustering on the (ϕ, Pct) points of all the voxels (Figure 5(b)). This was used to divide the voxels into 5 clusters, representing 5 microporous subrock types, next to the microporous and solid voxels in the image.



(a)



(b)



(c)

Figure 5. Pct-based sub-rock typing workflow. (a) The diagram of data fitting of two representative voxels. (b) A plot of Pct versus porosity. (c) Porosity map (left), Pct distribution map (middle) and λ distribution map (right).

2.2.2 Pore network extraction and simulations

Two multi-scale PNMs of the sample were extracted using the porosity map and the sub-rock type maps as input. These PNMs consist of four types of network elements: resolved nodes (“pores”) and links (“throats”) that represent the macroporosity and unresolved (“Darcy”) nodes and links that represent the microporosity. The extraction is based on skeletonization and maximal ball clustering of the resolved pore space and each of the microporosity sub-rock types in order to find the centers of nodes and links, as described in Øren et al. (2019). These are then connected together to honour the connectivity of the multi-scale pore-space. Geometrical properties (e.g. inscribed radius, volume, shape factor) of the network elements are subsequently determined. For Darcy nodes and links, the geometrical properties are supplemented by the local porosity determined from the porosity map, and local petrophysical properties based on user input for each sub-rock type (see Section 2.2.3). Full details on the method can be found in Ruspini et al. (2021). We extracted two different PNMs of the same sample, based on respectively the porosity-based sub-rock typing map and the Pct-based sub-rock typing map (Figure 6). The properties of these PNMs are shown in Table 2. The total porosity was 26.2% with 5.6% contributed by macropores and 20.6% by micropores, which honours the micro-CT results (Table 1).

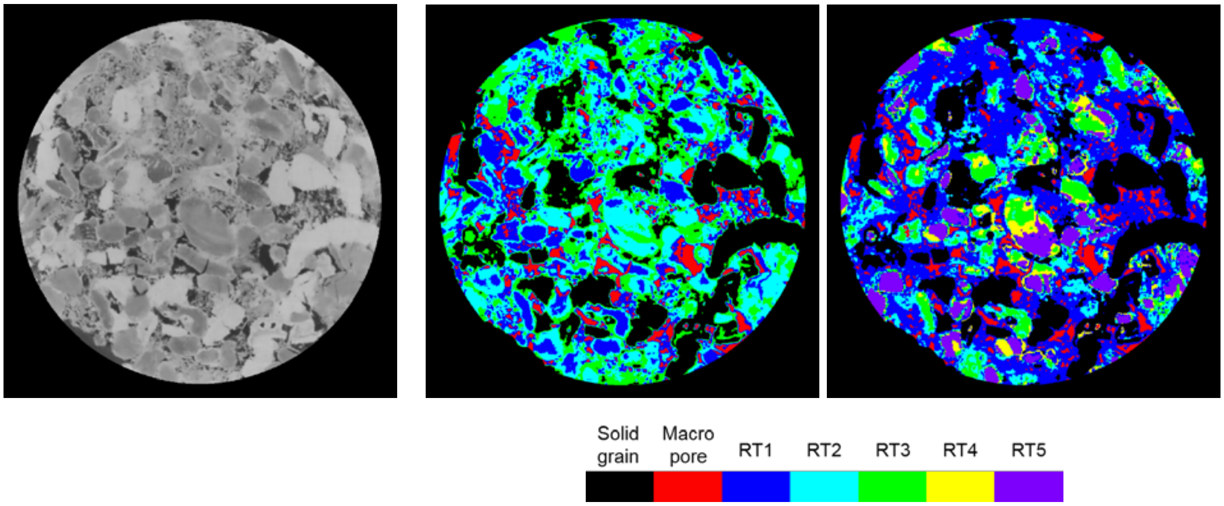


Figure 6. Dry image (left), porosity-based sub-rock typing result (middle) and Pct-based sub-rock typing result (right). The red and black in both sub-rock typing maps refer to macropores and solid grain. In porosity-based map: RT1, RT2 and RT3 show high, middle and low microporosity regions respectively. In Pct-based map: RT1 to RT5 represent lower to higher Pct microporous regions.

After extraction, the resulting PNMs were used to predict permeability and pore-scale fluid distributions during drainage. Permeabilities were calculated by assigning a conductivity value to each element (based on Poisseuille flow in resolved network elements and Darcy's law in Darcy elements, taking the local microporosity's permeability) and solving a set of mass balance equations (Ruspini et al., 2021). Drainage was simulated quasi-statically by calculating an intrusion capillary pressure for each network element, and then performing an invasion-percolation (i.e. progressively invading accessible network elements in ascending order of their intrusion capillary pressure). Invasion capillary pressures for resolved pores and throats were calculated by assuming triangular, square or cylindrical cross-sectional shapes (Mason & Morrow, 1991). In Darcy elements, the invasion pressure was found from input capillary pressure curves of the sub-rock type (scaled according to the local porosity and permeability using the Leverett-J-curve). The simulation took fluid connectivity through wetting layers into account, and assumed a fluid to be connected through a Darcy element as long as the local relative permeability to the fluid was larger than zero. Full details are provided in Ruspini et al. (2021).

Table 2. Properties of extracted PNMs

Properties	Porosity-based model	Pct-based model
Nodes	666543	658120
Links	4334582	5006058
Darcy pore	4898310	5561272
Total porosity	0.2625	0.2624
Resolved porosity	0.0564	0.0563
Unresolved porosity	0.2061	0.2061

2.2.3 Petrophysical properties

The petrophysical properties taken into account to represent unresolved porosity in each Darcy node of the PNM are porosity, permeability, relative permeability and capillary pressure curve (P_c-curve). The local porosity in each element was determined from the porosity map. Compared with the traditional way of assigning an average porosity value to the whole microporosity phase, the introduction of the porosity map captures more realistic porosity heterogeneity. The permeability for each node was calculated from a power correlation $k = a * \varphi^b$, where a and b are supplied as input values for each sub-rock type. Parameter b was set to 3.37 for all types based on a nm-scale imaging study performed by Menke et al. (2019) on microporosity in Estaillades. Since the microporosity's permeability values affect the intrusion capillary pressure curve of Darcy nodes through Leverett-J scaling, parameter "a" was tuned to match the output P_c-curve of the PNM simulations with our experimental P_c-curve measurement (Section 2.1). Note that anchoring simulations to available experimental data is common practice for multi-scale models, in order to allow better predictions of more difficult-to-obtain properties.

The determination of the relative permeability curve for each rock type is a challenging task, as this property is difficult to measure directly. Here, the Brooks-Corey model (Brooks & Corey, 1966) was used to assign the same relative permeability curves to all Darcy elements, in order to decrease its uncertain influence on the drainage simulation results. Approaches to obtain more accurate relative permeability curves for different micro-regions are the subject of future investigations.

For the porosity-based PNM, the Brooks-Corey-type P_c formulation (Brooks & Corey, 1964) was fitted to the experimental Pc-measurement to obtain P_c-curves for each microporosity type. The fitted curve was split into three parts, corresponding to the three microporosity regions from the porosity map (see Section 2.2.1). The saturation range of each of these parts was then rescaled to a range between 0 and 1, to serve as input P_c-curves for the sub-rock types, where the curve with the lowest Pc-range was assigned to the rock type with the highest porosity. Note that this workflow represents a coarse fit of the input properties to the experimental Pc-data (see e.g. Bultreys et al. 2015), but that this may not generally yield good results for all samples, and that there is no set way to divide the experimental Pc-curve into the individual sections (in this work, this was done by trial-and-error, until a satisfactory fit was found between the simulated and the experimental Pc-curves). For the Pct-based PNM, the input P_c-curves of each rock type were calculated directly from the imaging data, that is, the average saturation within each sub-rock type was determined at each capillary pressure step. This significantly reduced the input uncertainty of the simulations compared to the porosity-based workflow.

3 Results

3.1 Simulation results

The permeability values simulated with the Pct-based model and porosity-based model were 69.93 mD and 9.54 mD respectively, compared to literature values of 95.5 mD to 283.6 mD (Alyafei et al., 2015; Bultreys et al., 2015; Nono et al., 2014) and minipermeameter values 202.4 ± 86.9 mD. To validate the experimental workflow and the image analysis results from it, we compared the drainage results with a capillary pressure curve obtained using mercury intrusion capillary pressure (MICP) method (Bultreys et al., 2015), rescaled to the water-decane interfacial tension (48.3 mN/m) and contact angle (0^o). As shown in Figure 7, the evolution of the saturation from the imaging with the capillary pressure imposed in our experiment agreed well with the MICP data, indicating that the experimental operation and data processing methods were reasonable and reliable. Furthermore, the simulated capillary pressure curves also showed a good match with our experiment, and the input parameters were thus considered to be reasonable for the further pore-by-pore evaluation of the model.

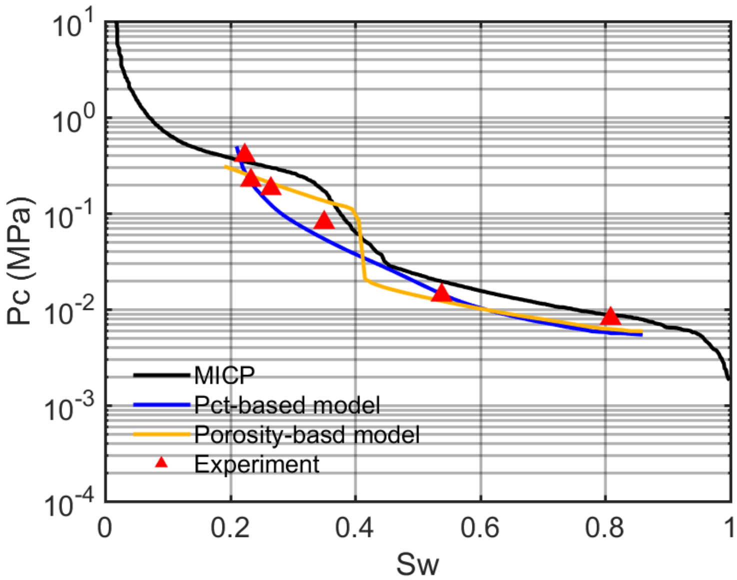
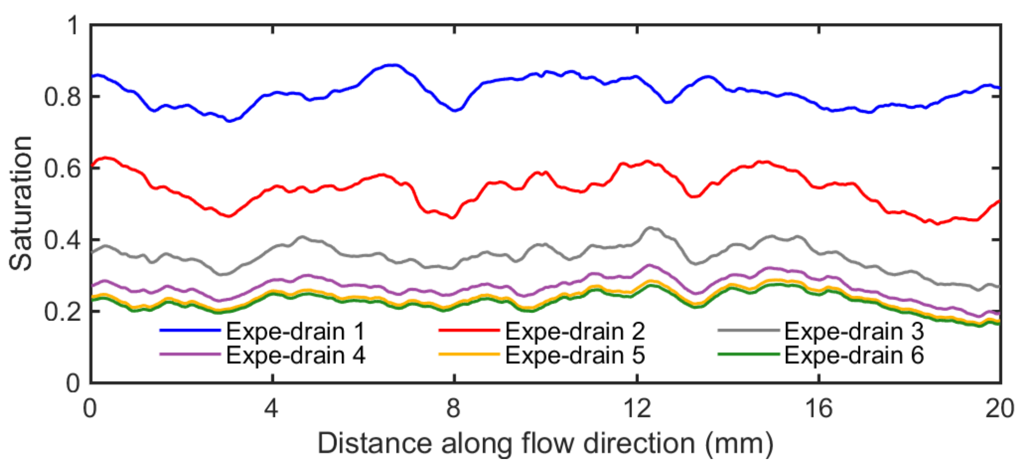


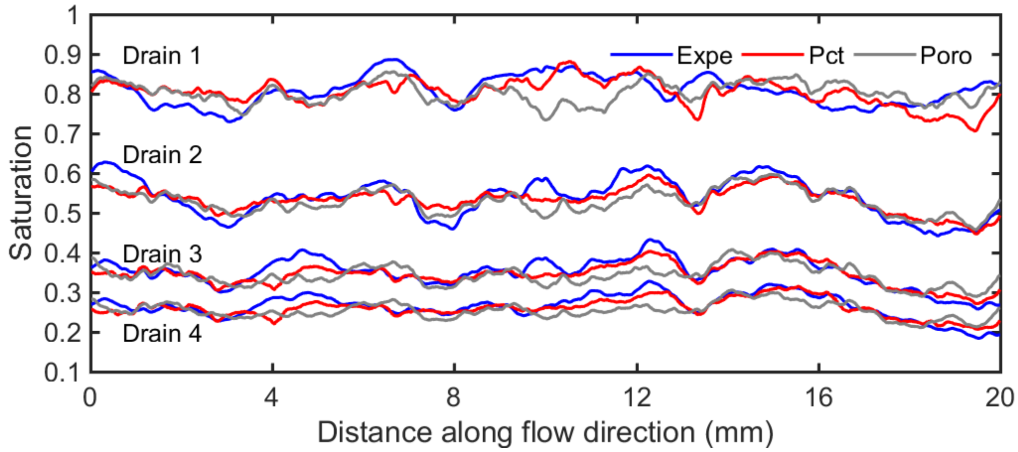
Figure 7. Comparison of capillary pressure curve obtain from MICP experiment, our drainage experiment, and simulations.

3.2 Model validation of fluid distributions

Figure 8 shows the slice-average probile of the brine saturation along the flow direction in the sample. Visual comparision indicates that the distribution simulated by the Pct-based model generally fits more closely to the experimental measurements.



(a)

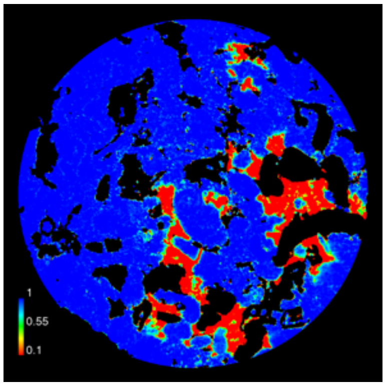
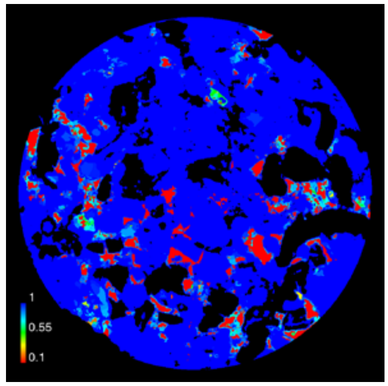
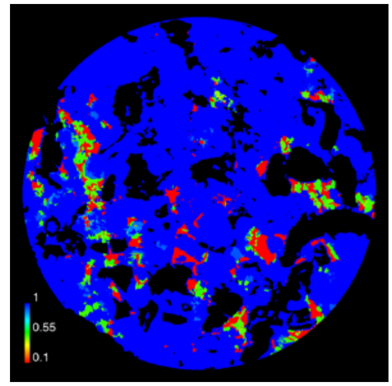
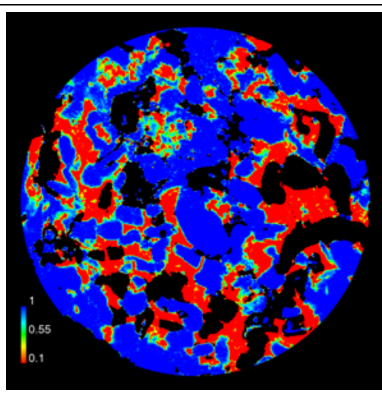
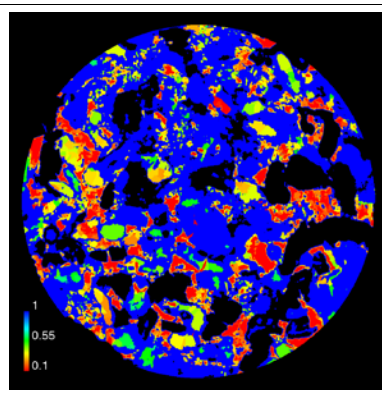
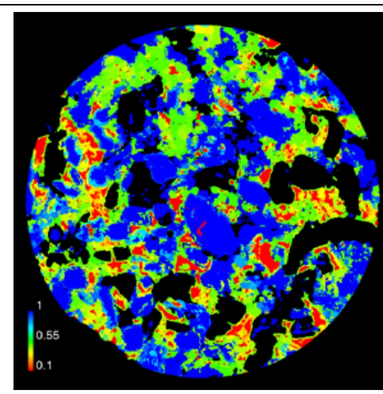
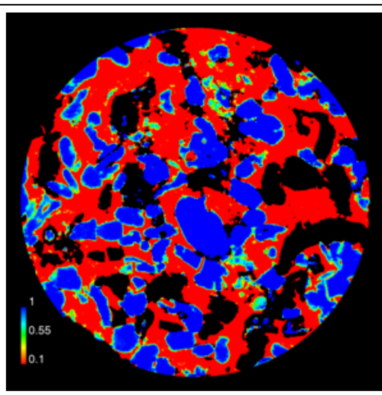
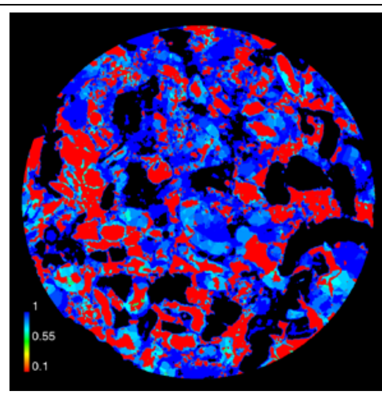
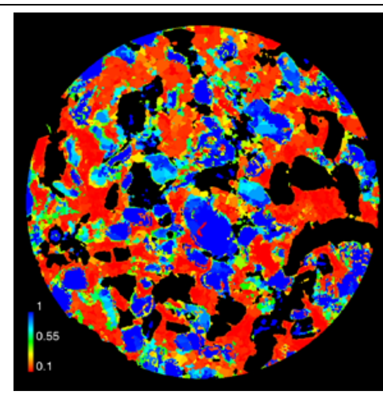


(b)

Figure 8. Brine saturation slice-average profiles along fluid flow direction. (a) Experimental results. (b) Comparision of experiment and model predictions at 1 to 4 drainage steps.

The simulations were then compared to each step of the imaging experiment at a matching total saturation. Figure 9 shows the comparison between saturation distributions of the experiment and the two model cases. In the first and second drainage stage, due to the low capillary pressure, large macro pores and well connected micropores are invaded by oil, while other macro pores remain uninvaded or partially invaded. From the third capillary pressure on, the displacement takes place almost completely in the microporous regions. This general trend was captured by both models. However, visual inspection of the fluid saturation maps shows that the new Pct-based model performs significantly better than the classical porosity-based model in predicting the fluid distribution.

The observed discrepancy in the porosity-based model is related to the fact that the porosity-based model (similarly to most classical multi-scale models) assumes that regions with higher porosity have larger pore sizes and are more easily drained. Contrary to this classical assumption, the experiment shows that the sub-rock type with the lowest average porosity has the lowest water saturation at high capillary pressure steps (Figure 10). While the model contained enough degrees of freedom for it to be tuned to the sample-averaged capillary pressure curve in Figure 7, this is not the case for the pore-scale distribution of the fluids. Matching this distribution is known to be a crucial issue to obtain reliable relative permeability curves from the model (Bultreys et al., 2020; Gharbi & Blunt, 2012; Ruspini et al., 2017). Comparison to the novel Pct-based method, which is directly based on the breakthrough pressure of each pore and provides a much better match, shows that the fluid distribution discrepancy can be resolved by avoiding the basic assumption that higher porosities are related to lower intrusion capillary pressures in the sub-rock typing.

Step	Experiment	Porosity-based model	Pct-based model
1			
2			
3			

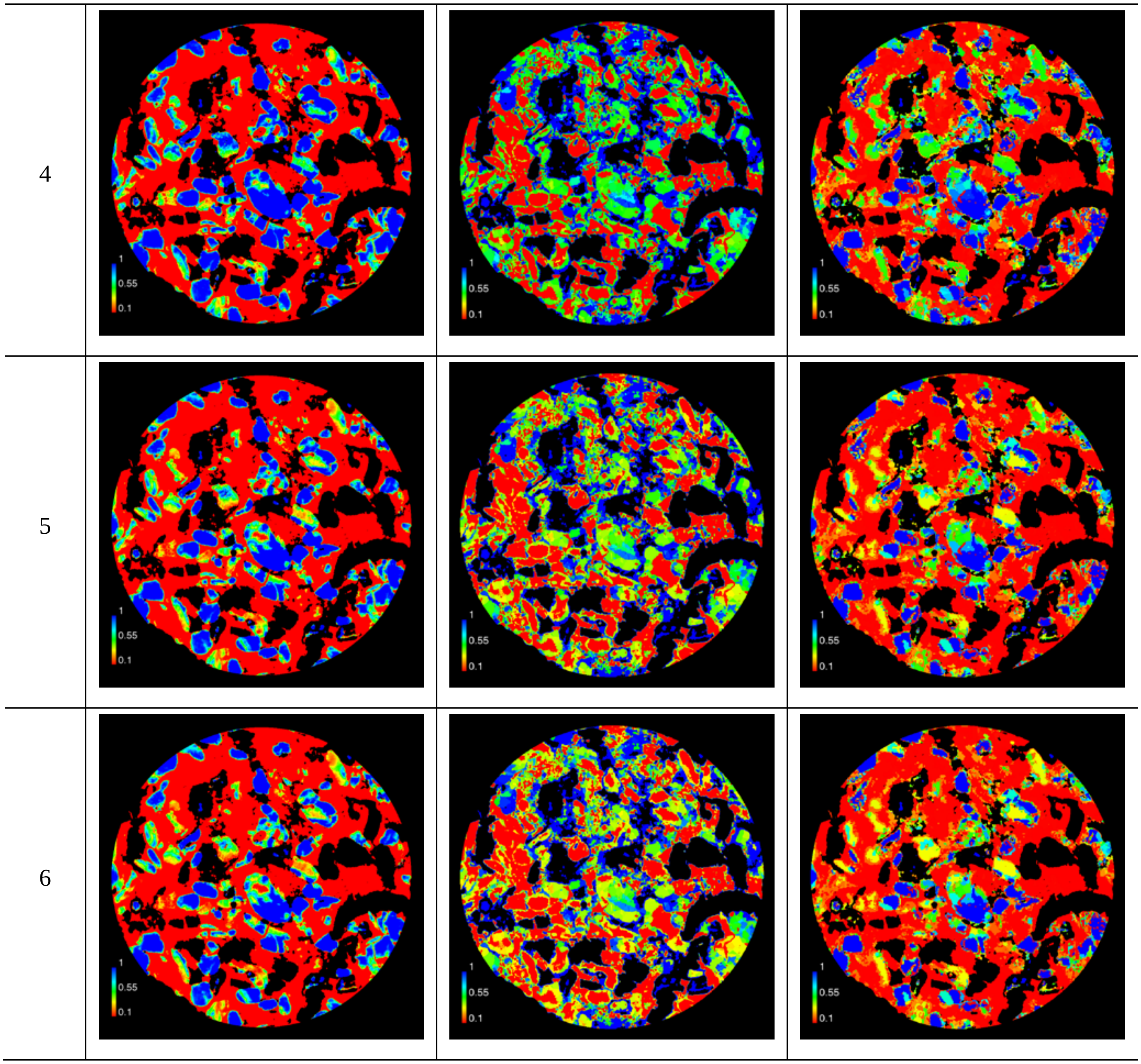


Figure 9. Saturation map comparison at each drainage pressure. The left column is experimental results. The middle and right column are simulation results in porosity-based and Pct-based pore network model.

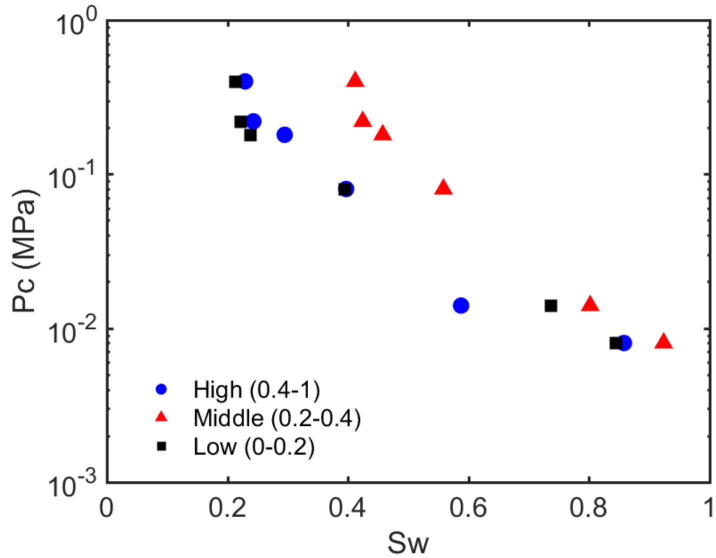


Figure 10. Average experimental saturation for the 3 micro-phase regions determined by the porosity-based sub-rock typing, for each capillary pressure step. These are the high (0.4-1), middle (0.2-0.4) and low (0-0.2) porosity regions respectively.

3.3 Saturation error

To investigate the accuracy of the predicted saturations further, we compared the simulations to the experiment directly on the image by calculating the squared saturation error in each voxel: $\left(S_{w\_exp} - S_{w\_mod}\right)^2$. Cross-sections of these saturation error maps are are shown in Figure 11(a). The Pct-based model generally shows higher accuracy than the porosity-based model, especially unresolved regions at high capillary pressures.

The saturation error in certain open pores and in pores just above the image resolution is relatively large in the beginning of drainage in both models (pressure steps 1-3). To explain this, Figure 12 shows the pore radius distribution of water filled macropores and throats in the experiment and in the Pct-based model. We define the discrepancy of the filling state as the percentage of network elements that were occupied by a different fluid in the simulation than in the experiment (Bultreys et al., 2018). If more than half of the fluid within a single pore or throat was wetting phase, the pores or throats were considered to be wetting phase occupied, otherwise, they were classified as non-wetting phase filled. As expected, the non-wetting phase invaded large open pores and throats in the beginning, and almost all the brine within them was displaced before increasing to the fourth pressure. Similar to single-scale models (Bultreys et al., 2018), the pores and throats with intermediate size had the largest filling discrepancy. At the first drainage pressure, the occupancy for pores with large radius (>12 μm) had a close match. However, the simulation predicted that all small pores were wetting-filled while the experiment did not show this behaviour. The throat filling error also reached 18.14% in this step. As shown in previous studies (Bultreys et al., 2018), the experimental fluid distribution and filling states at the pore scale are generally not fully reproducible, even in repeated experiments. Some of the pore-by-pore errors are likely caused by wrong intrusion pressure predictions in throats that are only just above the resolution. Furthermore, we only imaged the central part of the sample and the boundary conditions are therefore not exactly the same in the model and the experiment, which increased the pore-by-pore uncertainty of the simulation.

To quantitatively compare the saturation errors at each drainage step, we calculated the absolute average root mean square error (δ_{Abs}) and the volume weighted average root mean square error (δ_{VolWei}) of the models over the entire image:

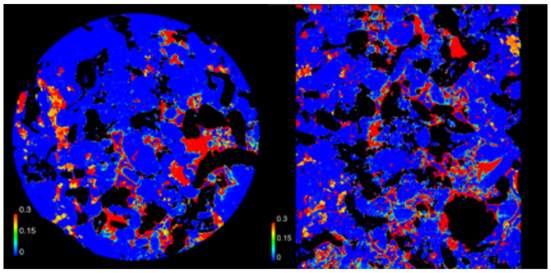
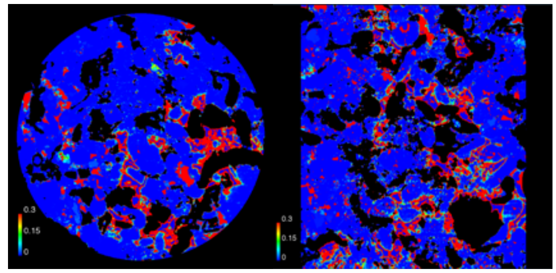
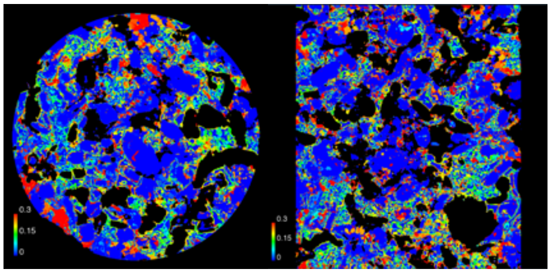
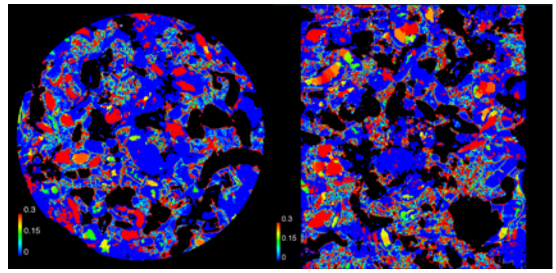
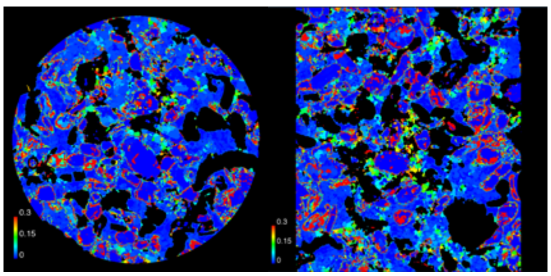
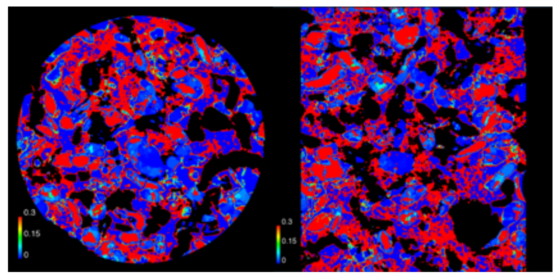
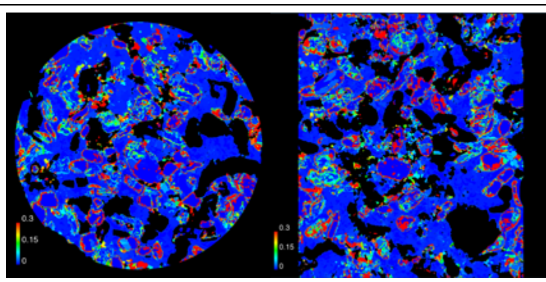
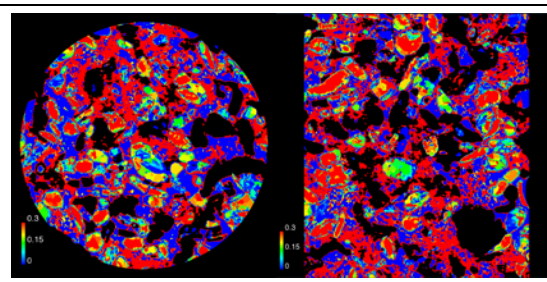
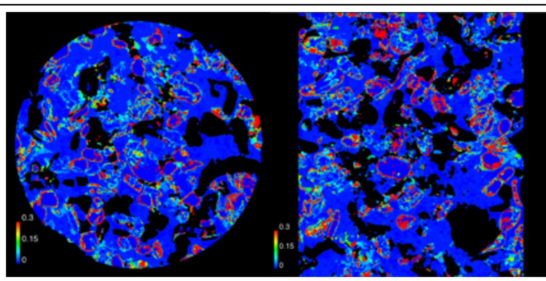
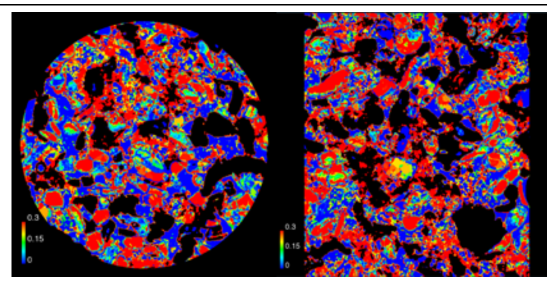
$$\delta_{Abs} = \sqrt{\frac{\sum\left(S_{w\_exp} - S_{w\_mod}\right)^2}{N}} \tag{9}$$

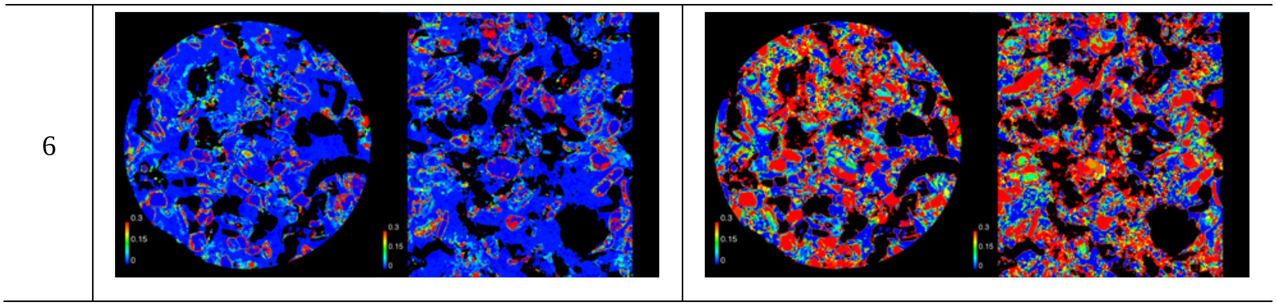
$$\delta_{VolWei} = \sqrt{\frac{\sum\left(\left(S_{w\_exp} - S_{w\_mod}\right)\cdot\varphi\right)^2}{N}} \tag{10}$$

Where S_{w_exp} and S_{w_mod} are brine saturation of each voxel from experimental measurments and simulations respectively, φ is the corresponding porosity of each voxel, N is the total number of pore voxels.

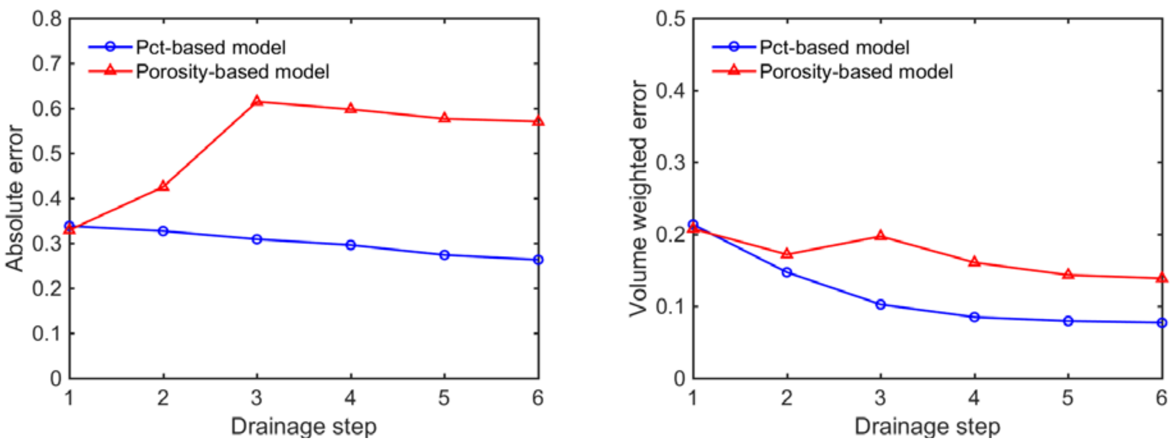
Figure 11(b) indicates that the saturation error in the porosity-based model at high drainage pressures is significantly higher than that at low pressures, while the Pct-based model shows a smoother trend and lower errors, decreasing from 0.34 to 0.26 with the increase of pressures. The volume-weighted error in the porosity-based model is almost twice as high as in the Pct-based model in drainage steps 3 to 6.

Step	Pct-based model error map		Porosity-based model error map	
	X-Y plane	X-Z plane	X-Y plane	X-Z plane

1		
2		
3		
4		
5		

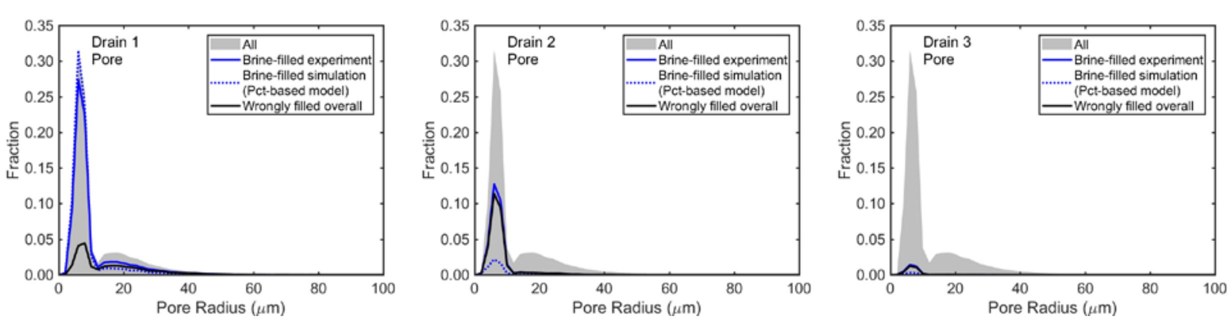


(a)



(b)

Figure 11. Saturation error. (a) Saturation error map. The left two columns (X-Y plane and X-Z plane maps respectively) are saturation discrepancy between experiment and Pct-based model simulations. The right two columns (X-Y plane and X-Z plane maps respectively) are saturation discrepancy between experiment and porosity-based model simulations. The balck is solid grain. The blue color represents the simulated saturation error is very small, while the red color denotes the error is large. (b) Absolute saturation error (left) and volume weighted saturation error (right) predicted by the two models.



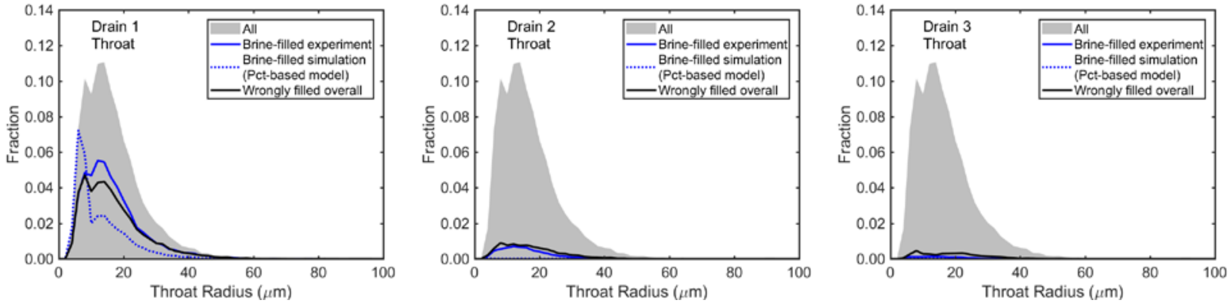


Figure 12. Water-filled open pore (top) and throat (bottom) size distribution after each drainage step.

4 Conclusions

In this work, we proposed a multi-scale PNM validation workflow using drainage experiments imaged with micro-CT, to study the factors that influence the uncertainty of pore-scale modelling and simulation. The differential imaging technique was used to quantify the porosity map and the saturation distribution during capillary-dominated drainage in an Estaillades limestone sample. A "classical" porosity-based and a novel invasion-capillary-pressure-based sub-rock typing methods were used to characterize the microporosity, followed by a multi-scale PNM extraction. The continuum scale properties and pore-scale multiphase distribution from the two models were then compared to experimental data.

We showed that the P_c-curves simulated by both models matched our image-based capillary pressure curve and an MICP curve of the rock type. The porosity-based model performed poorly in simulating multiphase fluid distribution at the pore-scale, while the novel Pct-based model significantly improved the prediction of pore filling states. This indicated that the multiphase transport behavior within sub-resolution pores was poorly correlated to the sub-voxel porosity. Further research should indicate if this is due to micropore geometry variations or due to dynamic effects inside the microporosity, e.g. inhomogeneous drainage due to extremely low brine conductivities that slow down the invasion to very long time scales. The methodology presented in this work was proven to be a robust approach in decreasing the uncertainty of pore-scale modelling and can be extended to other complex reservoir rocks modelling, to provide more insights on, for example, CO_2 sequestration and reservoir management.

Despite the improved results obtained with the Pct-based method, the determination of input petrophysical properties for microporous flow zones is still challenging and was shown to be a key factor affecting the reliability of the simulation. Furthermore, this current "best-fit" model is generated based on the fact that we have the full information of the drainage experiment. While this may be useful as a hybrid workflow to calculate properties that are difficult or impossible to measure in unsteady-state experiments, notably relative permeability, performing the experiment itself is time-consuming and complex. Therefore, further work should point out if the Pct-based rock-typing can serve as a baseline to develop more straightforward sub-rock typing methods.

Acknowledgments, Samples, and Data

Veerle Cnudde and Arjen Mascini (Ghent University) are gratefully acknowledged for their advice and support during the experiment and the analysis. Shan Wang holds a PhD scholarship funded by the China Scholarship Council (CSC Grant 201906440157). Tom Bultreys is a postdoctoral fellow of the Research Foundation–Flanders (FWO) and acknowledges its support under grant 12X0919N. The special research fund of the Ghent University (BOF-UGent) is acknowledged for the financial support to the UGCT Centre of Expertise (BOF.EXP.2017.0007). Leonardo Ruspini would like to thank the Norwegian Research Council for partially supporting this research (grant 296093). The data is made available on the Digital Rocks Portal (www.digitalrocksportal.org).

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