

Defining and Validating Convergence Criteria for the Determination of Representative
Elementary Volume in Porous Media

by

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Author's Declaration

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Abstract

The representative elementary volume (REV) is a fundamental concept in the study of porous media, describing the minimum volume at which a material property can be considered statistically representative of the whole. Determining an REV is essential for linking pore-scale measurements, often obtained from high-resolution imaging, to continuum-scale models used in engineering and geoscience. In particular, accurate REV identification of porosity and tortuosity is critical, as these parameters govern transport processes such as flow, diffusion, and conductivity in porous structures.

This work presents a systematic methodology for identifying REV's based on a threshold criteria designed to reduce computational demands. An REV is defined as the volume in which at least 80% of 100 randomly sampled subdomains yield porosity or tortuosity values within 20% of the overall average. The method was applied to both synthetic datasets and real samples provided by Dong and Blunt, with subdomain volumes ranging from 10^3 to 100^3 voxels [1]. Of the 12 real samples analyzed, 7 satisfied the proposed criteria, and REV's were identified for both porosity and tortuosity. Samples that met the criteria exhibited smaller average pore sizes and higher porosity ratios, while outliers were explained using pore size distribution data.

To further assess robustness, predicted tortuosity values obtained using the correlation proposed by Tomadakis and Sotirchos were compared with ground truth measurements [2]. Several samples failed to reproduce the true values, indicating that even when an image contains an REV, it may not be internally self-consistent. While this may appear contradictory, it reflects the distinction between the stability of averaged values across subdomains and predictive accuracy of empirical correlations.

The results of this work demonstrate that REV's can be identified from relatively small fractions of the total image volume given that certain conditions are met, offering a balance between accuracy and computational efficiency. This framework provides a flexible approach for porous media characterization, with direct implications for hydrogeology, petroleum recovery, fuel cell design, and filtration technologies.

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Table of Contents

Author's Declaration	ii
Abstract	iii
Acknowledgements	iv
List of Figures	vii
List of Tables	xiii
List of Notation	xiv
1. Introduction	1
2. Background	6
2.1. Sources of Volumetric Images	6
2.2. Uses of Volumetric Images for Estimating Properties	6
2.3. Discussion of Representative Elementary Volume	7
2.4. Effective Diffusivity and Tortuosity	8
2.5. Tortuosity – Porosity Correlations	9
2.6. Tortuosity Distributions	13
3. Methodology	16
2.1 Image Acquisition	16
3.1. Image Generation	20
3.2. Determination of the Percolating Porosity	24
3.3. Image Processing	28
3.3.1. Identifying and Removing Invalid Voxels	28
3.4. Computing Tortuosity	29
3.5. Obtaining REV Data for Porosity and Tortuosity	32

3.6.	Computation of Pore Size Distribution	33
4.	Results	37
4.1.	REV Plots for Porosity and Tortuosity	37
4.2.	Determination of the REV	42
4.2.1.	Image A1 - Sandpack	44
4.2.2.	Image C1 - Carbonate	48
4.2.3.	Image S1 - Sandstone	52
4.2.4.	Image S6 - Sandstone	56
4.3.	Prediction of the Existence of an REV From Structural Information	60
5.	Tortuosity versus Image Resolution	65
6.	Predicting Tortuosity with REV Data	68
7.	Conclusions and Recommendations	74
8.	References	76
9.	Appendix A Image Generation Code	82
10.	Appendix B Image Analysis Code	83
11.	Appendix C Tables	101
12.	Appendix D Excluded Image Montages	104
13.	Appendix E Macro Image Montages	112
14.	Appendix F Tortuosity Prediction Plots	124
15.	Appendix G TS Model Coefficients	135

List of Figures

Figure 1 – A theoretical plot showing the dependence on sample porosity on sample volume, as proposed by Bachmat and Bear [3].	2
Figure 2 – A synthetic image and its associated REV porosity plot.	3
Figure 3 – Comparison of the predicted dependence of τ on ε according to the Bruggeman (Eq (2.4)) and Tomadakis- Sotirchos (Eq (2.5)) models. The values of 0.5, 1.0, and 0.25 correspond to the exponents used in the relevant correlations.	11
Figure 4 – (a) A generated image with a porosity of 70%. (b) and (c) depict the image after being subdivided into discrete slices of sizes 100 × 1000 and 200 × 1000 pixels, respectively.	14
Figure 5 – Variation of the tortuosity along the horizontal direction across the slabs in Figure 4. The blue data series corresponds to the slabs seen in Figure 4b and Figure 4c is the green data series.	15
Figure 6 – 3D renderings of the sample images obtained from Dong and Blunt, rendered in Paraview [32]. Images shown in a), b), c), d), e), f), g), h), i), j), k) and l) correspond to samples A1, C1, C2, S1, S2, S3, S4, S5, S6, S7, S8 and S9, respectively.	19
Figure 7 – Process of constructing of an image of randomly located by aligned fibers. Top row shows an example of a generated image with small n and medium rf , while bottom row shows an example of a generated image with large n with small rf . This depicts the step before extrusion.	21
Figure 8 – Top view (left), side view (middle) and rotated view (right) images of fibers aligned in 1D. Top row shows an example of a sample with fewer fibers having large diameter, while bottom row shows a sample with more fibers having smaller diameter. Images with $n = 100 \rightarrow 600$ and $rf = 3 \rightarrow 20$ were tested in this study. This depicts the step after extrusion.	22
Figure 9 – Sample images of fibers randomly oriented in the x-y plane but aligned along the z axis. Top row shows structure containing more fibers with small diameter, while bottom row	

shows structure containing fewer fibers with larger diameter. Images with $n = 100 \rightarrow 600$ and $rf = 3 \rightarrow 20$ were evaluated.	23
Figure 10 – Determination of percolation threshold by cluster labeling. Top row shows the case of small n and moderate rf , while the bottom row shows higher n and small rf . The left column is the original image, while the middle and right columns show the cases after dilating to $Rp - 1$ and Rp , respectively. The different colours in the void space indicate a different labeled cluster number.	25
Figure 11 – Variation of percolating porosity in the two directions perpendicular to the fiber axes with initial fiber size in image, where “Axis: 0” corresponds to the x-axis, and “Axis: 1” corresponds to the y-axis. Each image contains 100 fibers. The grey regions above the data points at each fiber size indicate the initial porosity of each set of images. The solid grey horizontal line located at 0.33 corresponds to the threshold reported by Tomadakis and Sotirchos [2].	26
Figure 12 - Percolating porosity as a function of initial fiber size in images with 400 initial fibers for the case of aligned fibers as shown in Figure 8.	27
Figure 13 – Distribution of percolating porosity as a function of fiber size for the case of fibers randomly rotated in-plane, as shown in Figure 9.	28
Figure 14 – Schematic of pore space used to determine tortuosity. Sample image of size 3 pixels by 3 pixels: a) yellow and purple denotes void and solid phases, respectively. Percolation occurs in the left-to-right direction and through the open face on the bottom. b) yellow denotes the highest solute concentration, purple corresponds to the lowest concentration and green depicts intermediate concentration in the void space.	30
Figure 15 – Segmentation of an image: a) subdivision using a regular grid and b) subdivision into random subdomains.	32
Figure 16 – The resulting 2D images of blobs obtained using the distance transform method (left) and local thickness method (right). The colour of the heat map indicates the size of the measurement, with hotter colours indicating a greater value.	34

Figure 17 – Plots of cumulative radial density function (orange) and cumulative pore size distribution (blue) for a 3D image of blobs.....	35
Figure 18 – Steps required to compute a local thickness; a) is the original image, b) depicts the voxels from the distance transform which have value of <i>R</i> or greater, c) draws spheres centered at each voxel identified in b), and d) repeats the sphere drawing process with each unique value identified by the distance transform and overlaps the result, creating a colour map with the hottest colour indicating the greatest value.	36
Figure 19 – The sample image of size 300 by 300 by 300 voxels and porosity of 70% characterized for its REV porosity and tortuosity in this study.	37
Figure 20 – REV porosity plot for structure shown in Figure 19. Each band corresponds to a subdomain volume of 103, 133, 163, 203, 253, 333, 503, 1003 from left to right, respectively.	38
Figure 21 – REV porosity plot for structure shown in Figure 19 obtained using a smoother domain of sub-volumes spanning from 103 to 2003	39
Figure 22 – REV tortuosity plot for Figure 19. Each band corresponds to a subdomain volume of 103, 133, 163, 203, 253, 333, 503, 1003 from left to right, respectively.....	40
Figure 23 – Violin plots for REV porosity and REV tortuosity data of Figure 19.....	41
Figure 24 – Violin plots for REV porosity and tortuosity data of Figure 19 after filtering.....	42
Figure 25 – 3D rendering of sample image A1.	44
Figure 26 – REV porosity data for image A1.	45
Figure 27 – REV tortuosity data for the x-axis on image A1.	46
Figure 28 – Frequency of adherence to criteria vs normalized volume of subdomain for image A1.	47
Figure 29 – A 3D rendering of sample image C1.	48
Figure 30 – REV porosity data for image C1.	49

Figure 31– REV tortuosity data for the x-axis on image C1.	50
Figure 32 – Frequency of adherence to criteria vs normalized volume of subdomain for image C1.	51
Figure 33 – A 3D rendering of sample image S1.....	52
Figure 34 – REV porosity data for image S1.....	53
Figure 35 – REV tortuosity data for the x-axis on image S1.	54
Figure 36 – Frequency of adherence to criteria vs normalized volume of subdomain for image S1.	55
Figure 37 – A 3D rendering of sample image S6.....	56
Figure 38 – REV porosity data for image S6.....	57
Figure 39 – REV tortuosity data for the x-axis on image S6.	58
Figure 40 – Frequency of adherence to criteria vs normalized volume of subdomain for image S6.	59
Figure 41 – Pore size distribution for sample image A1 [32]. The red dashed lines intersect at $y = 0.1$ and approximately $x = 7.5$	61
Figure 42 – Pore size distribution for sample image C1 [32]. The red dashed lines intersect at $y = 0.1$ and approximately $x = 11.5$	62
Figure 43 – Porosity ratio versus size value S for all samples examined in this study. Points in green indicate images that adhere to criteria for REV porosity and REV tortuosity defined in this study, while red points correspond to those images that do not adhere to these criteria. .	63
Figure 44 – Downscaling of the same base image at magnitudes of 1 (base image), 12 , 14 , 18 , 116 and 132 for a), b), c), d), e), and f) respectively.	66
Figure 45 – Tortuosity of downscaled images versus the downscaling factor for a) 2D image and b) 3D image.	67

Figure 46 – Tortuosity versus porosity for image A1. The dotted black line represents the predicted tortuosity from the proposed correlation by Tomadakis and Sotirchos. Each plot corresponds to the values obtained in this study for different subdomain volumes of a) 103 , b) 203 , c) 253 and d) 503	69
Figure 47 – Dependence of tortuosity on porosity, as generated from the correlation proposed by Tomadakis and Sotirchos.	70
Figure 48 – Comparison of predicted tortuosity value from the proposed correlation by Tomadakis and Sotirchos to the actual tortuosity calculated through the finite difference method [2]. Missing from here are images C2, S3 and S4, as the calculated tortuosity resulted in $\tau \gg 20$. The colours are purely for data point distinction and have no meaning.	71
Figure 49 – Percent error in tortuosity prediction compared to the ground truth value. The green bars indicate cases where an REV is obtained, while the red ones indicate cases where no REV is found.	72
Figure 50 – A montage of the relevant plots for image C2.	104
Figure 51 – A montage of the relevant plots for image S2.	105
Figure 52 – A montage of the relevant plots for image S3.	106
Figure 53 – A montage of the relevant plots for image S4.	107
Figure 54 – A montage of the relevant plots for image S5.	108
Figure 55 – A montage of the relevant plots for image S7.	109
Figure 56 – A montage of the relevant plots for image S8.	110
Figure 57 – A montage of the relevant plots for image S9.	111
Figure 58 – Macro plot for A1.	112
Figure 59 – Macro plot for C1.	113
Figure 60 – Macro plot for C2.	114
Figure 61 – Macro plot for S1.	115

Figure 62 – Macro plot for S2.	116
Figure 63 – Macro plot for S3.	117
Figure 64 – Macro plot for S4.	118
Figure 65 – Macro plot for S5.	119
Figure 66 – Macro plot for S6.	120
Figure 67 – Macro plot for S7.	121
Figure 68 – Macro plot for S8.	122
Figure 69 – Macro plot for S9.	123
Figure 70 – Tortuosity vs porosity data for C1.....	124
Figure 71 – Tortuosity vs porosity data for C2.....	125
Figure 72 – Tortuosity vs porosity data for S1.....	126
Figure 73 – Tortuosity vs porosity data for S2.....	127
Figure 74 – Tortuosity vs porosity data for S3.....	128
Figure 75 – Tortuosity vs porosity data for S4.....	129
Figure 76 – Tortuosity vs porosity data for S5.....	130
Figure 77 – Tortuosity vs porosity data for S6.....	131
Figure 78 – Tortuosity vs porosity data for S7.....	132
Figure 79 – Tortuosity vs porosity data for S8.....	133
Figure 80 – Tortuosity vs porosity data for S9.....	134

List of Tables

Table I – Fitting parameter for various fiber structures [2].	10
Table II – Tortuosity along the three axes in each sample image.	17
Table III – Pore structure properties of extracted AB networks on image samples from Dong and Blunt [32] [33].	18
Table IV – Summary of minimum subdomain volume size to remain within threshold of 20%.	60
Table V – Various calculated properties of each slab in image appearing in Figure 4b	101
Table VI – Various calculated properties of each slab in image appearing in Figure 4c	101
Table VII – Complete table of pore structure properties of extracted AB Networks on image samples from Dong and Blunt [32] [33].	102
Table VIII – All coefficient values solved for using numerical methods.	135

List of Notation

τ	Tortuosity
ε	Porosity
ε_p	Percolation threshold
α	Fitting parameter
ε_c	Porosity of a compressed sample
t_c	Applied thickness
ε_0	Porosity of the original sample
t_0	Thickness of the original sample
K_i	Directional absolute permeability, $i = x, y, z$
K_{avg}	Average permeability
F_i	Directional formation factor, $i = x, y, z$
F_{avg}	Harmonic mean of formation factor
L_i	Domain length, $i = x, y$
r_f	Fiber radius
R	Radius
R_p	Threshold radius at the point of no percolating clusters
$C_{A,i}$	Concentration of species A at point $i, i \rightarrow j, j = \# \text{ of pores}$
t	Time
D_{AB}	Diffusion coefficient of species A in medium B
n_A	Molar flux of species A
$N_{A,i}$	Molar flowrate of species A at point $i, i \rightarrow j, j = \# \text{ of pores}$
A_{eff}	Effective area for diffusion
$G_{i \rightarrow j}^d$	Lumped parameter of diffusive conductance
Δ_h	Forward difference operator
h	Spacing constant for forward difference
$P(r)$	Probability function with respect to r
S	Size value of image, based on pore size distribution

T Threshold value

$\frac{\varepsilon}{\varepsilon_p}$ Porosity ratio

1. Introduction

Computing transport properties of a porous material from a volumetric image, be it 2D or 3D, has become a common substitute for performing experiments. Several reasons exist for this practice, but it has become increasingly easy to acquire volumetric images as techniques such as x-ray tomography and focused ion beam imaging - scanning electron microscopy (FIB-SEM) are now common at most research facilities. Moreover, the computational power necessary to perform the needed simulations is readily available on standard desktop workstations. Finally, experiments can be time-consuming, prone to error and sometimes even impossible, such as finding the tortuosity of a fuel cell catalyst layer that is only $10\ \mu m$ thick and not self-supporting. Given the widespread use of volumetric images for this purpose, it is necessary to determine whether the computed transport properties are a valid substitute for experimentally obtained values and more generally what conditions must be met for this to be the case.

Geologists have faced this situation for many decades, but the problem they typically face is having to conduct experiments on small samples (typically $1 - 10\ cm$ diameter cylindrical plugs known as cores) that have been obtained from enormous reservoirs. In their case, the question is whether experiments performed on a small core yield properties which are representative of an entire reservoir where the properties vary spatially. Bachmat and Bear formalized this situation in 1986 when they described the concept of a representative elementary volume (REV) [3]. An REV is the volume of the smallest sample for which a measurement will yield a value that is representative of the entire sample. In their work, they discussed the REV in terms of the porosity with respect to volume, although it should be noted that such a plot can be made for any property of a medium other than the porosity. A typical relationship between sample volume and sample porosity is shown schematically in Figure 1 below. This plot shows 3 phases: (I) wide fluctuations in porosity at very small volumes where the samples contain a disproportionate amount of solid or void, (II) plateau in porosity considered to be the representative or true value at intermediate volumes where the samples consistently contain both solid and voids in the same proportions and (III) small variations in porosity in very large samples where the measurement

becomes influenced by the large-scale heterogeneity of the reservoir. This third stage is largely conceptual in nature since it is obviously not possible to obtain or test a core of this size.

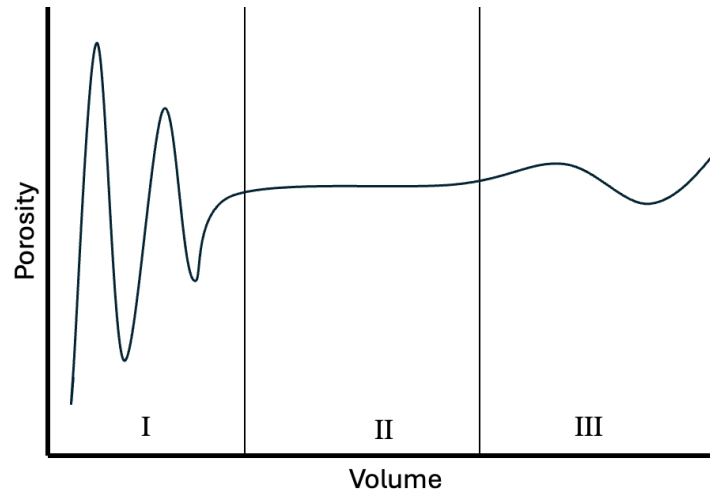


Figure 1 – A theoretical plot showing the dependence on sample porosity on sample volume, as proposed by Bachmat and Bear [3].

The experimental determination of such a plot would be tedious and time-consuming. On the other hand, it can be easily generated by analysis of a volumetric image of a sample. As an example, consider the image of blobs shown in Figure 2 (left) below. It is relatively trivial to extract many random subsections of this image (random size and location) and compute the porosity as the sum of void voxels over the total number of voxels for each subsection. Figure 2 (right) shows the variation in the porosity value as a function of the block size. For comparison, the true value for the entire image is given by the horizontal red line, determined by the quotient of the number of void voxels and the total number of voxels. This value likely differs from porosity measurements obtained through laboratory analysis which requires experimentation through determining the bulk volume or grain volume. At very small volumes, the porosity can take on any value between 0 and 1 because the sample volume may contain only voids, only solid voxels or any intermediate combination. Once the volume of the subsections reaches $\sim 40\%$ of the image size, the porosity obtained from the analysis consistently falls within 20% of the true value. The methods used to extract sub-sections and their subsequent analysis are discussed in more detail later in this work.

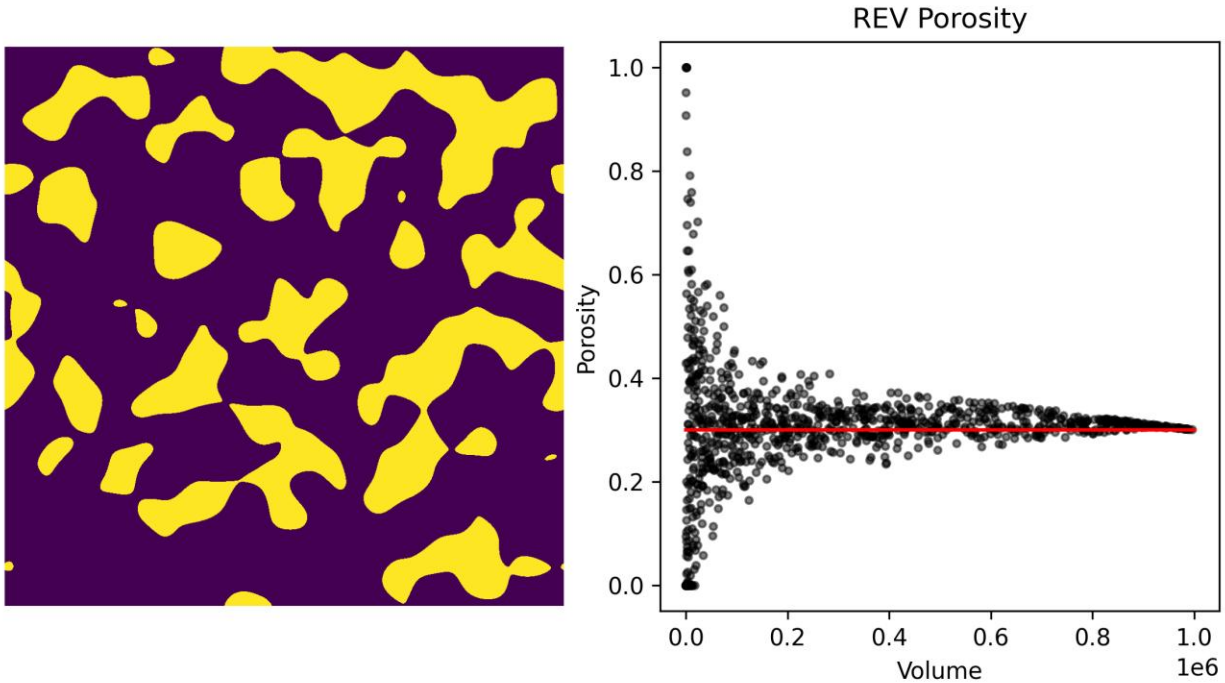


Figure 2 – A synthetic image and its associated REV porosity plot.

Of course, porosity is not the only property which can be analyzed as a function of volume. Any property which can be obtained from a full image can be obtained from sub-images and plotted as a function of sample size. All such plots should follow the same general trend of converging to a stable value as the sample size increases. However, not all properties will converge at the same size. Transport processes such as mass diffusion, heat conduction and fluid flow are influenced by long-range effects of the pore structure, such as up-stream constrictions. This essentially means that REV used to model diffusion must be larger than that used to determine porosity since diffusion is influenced by long-range features while porosity is a purely local value. Unfortunately, little attention has been paid to this phenomenon in the literature. Most studies have not even conducted an analysis of porosity based on the REV, let alone analyses of the transport property(ies) based on an REV. Garcia-Salaberri et al. conducted an REV study in gas diffusion layer (GDLs) materials used in fuel cells. Since GDLs are very thin ($< 400 \mu m$), the main concern in their work was not whether their image was large enough to serve as a satisfactory REV, but whether the GDLs themselves were thick enough to be reasonably represented as a

continuum [4]. In other words, they considered the question whether the continuum approximation can be applied to GDLs when modeling fuel cells. They determined the dependence of several effective properties (porosity, tortuosity, thermal conductivity and permeability) on image thickness and found that the simulations did not converge to a single stable value as the thickness of the modeled domain approached the thickness of the cross-section of the GDL. They interpreted this to mean that no REV was found from analysis in the thickness (i.e. through-plane) direction. For analysis of properties in the in-plane direction, the researchers found that at least 1 *mm* was required for the properties to reach stable values. We will show in the present thesis that reaching a stable value as a function of domain size does not necessarily mean that an REV is achieved. A stable value corresponds to the average of a distribution which may have a wide standard deviation, indicating that any given sub-sample may actually be far from the mean and therefore unrepresentative.

The aim of the present work is to develop a computational framework for determining if a given image is large enough to qualify as an REV of the sample from which it was taken. Specifically, this work addresses the following questions:

- Given a single image taken from a larger sample, can we determine if it is large enough to qualify as an REV without knowing the true value of the relevant transport and/or structural properties?
- Can a practical definition of an REV be established that allows one to conclude an image is “close enough”?
- If an REV is absent, can the image still be considered homogeneous enough to provide useful information?
- What conditions must be met for an REV to exist? For instance, are there certain physical properties of the image which can be used to predict if an REV is likely to be present?
- Since images with high resolution and small fields of view are likely to lack an REV, is it feasible to use image with lower magnification to perform tortuosity simulations?

It is expected that the outcomes of this work will benefit a wide variety of fields which rely on volumetric images to supplant experiments. This includes analysis of electrodes for Li-ion

batteries [5], redox flow batteries [6] and fuel cells [7], membranes for filtration [8] and sandstones and carbonate rocks for oil recovery, CO_2 sequestration and aquifer management [9].

2. Background

2.1. Sources of Volumetric Images

Volumetric images can be obtained by direct imaging of samples, reconstruction from 2D slices, or by synthetic generation from mathematical models. Typical techniques used to obtain such information include tomography and serial sectioning. Tomography acquires a series of non-destructive 2D projection images at different viewing angles. These projections are then computationally reconstructed into a 3D volume using algorithms such as filtered back-projections or iterative reconstruction [10]. Serial sectioning directly acquires consecutive slices of a material by physically removing thin layers from the surface. In focused ion beam-scanning electron microscopy (FIB-SEM), an ion beam is applied to a sample to mill away a nanometer-thick layer after which an SEM image of the newly exposed surface is obtained. This process is repeated over and over again to generate a stack of 2D cross-sections which is then compiled into a 3D dataset [11] [12].

An inherent trade-off exists between the achievable resolution and the size of the field of view (FOV). These parameters are inversely related because imaging systems are constrained by detector pixel count, acquisition time and data storage capacity [13]. Resolution enhancement is often pursued to capture finer details within a sample. However, if the FOV of the imaging system is too limited or the sample is not adequately representative, higher resolution may not yield meaningful insights. In such cases, the increased data volume in higher resolution images can lead to computational challenges and may not contribute to a more comprehensive understanding of the sample. Therefore, the utility of improved resolution must be evaluated. In some instances, a broader FOV with moderate resolution may be more beneficial than high-resolution imaging of a limited area. The review by Wildenschild and Sheppard highlights this specific relationship between resolution and FOV, where sample imaging can require acquisition times ranging from 15 minutes to 24 hours [14].

2.2. Uses of Volumetric Images for Estimating Properties

Volumetric imaging has become a pivotal tool for characterizing material and biological systems, providing three-dimensional insight into structures that are otherwise inaccessible. Beyond visualization, these images are increasingly used to quantify physical properties which can then be used in continuum models to predict macroscopic behavior. Statistical and physical modeling techniques have been developed to directly estimate material parameters from volumetric datasets. For example, models for microstructural characterization from 3D tomography can quantify pore structure, connectivity and other material parameters, which serve as input for continuum simulations to predict transport and mechanical properties [15]. In biological systems, mechanical properties have been extracted for use in finite element models to simulate tissue mechanics under physiological conditions, specifically rate of deformation [16]. In the case of electrochemical devices, Garcia-Salaberri et al. extracted transport properties from an image and used them in a continuum model of fuel cell operation [17]. They also conducted fuel cell simulations for the gas diffusion layer structure captured in the image and found that the prediction of the overall device performance was close to that determined from experiments, whereas the spatial distribution of degradation was much different.

Volumetric imaging has proven to be a powerful tool for determining the physical properties of materials, enabling researchers to link microstructural features to continuum-level behavior. While these studies demonstrate the broad applicability of volumetric imaging for property estimation, the focus of the present work will concentrate solely on tortuosity and porosity, as these parameters provide fundamental insight into transport phenomena and serve as the key metrics for evaluating representative elementary volume behavior in porous media.

2.3. Discussion of Representative Elementary Volume

In addition to the foundational work by Bear and Bachmat on the REV, more recent studies have sought to refine its application across a broader range of materials and physical properties beyond porosity [3]. Wu et al. introduced a novel criterion for determining REV in translucent porous media using light transmission techniques [18]. The study addressed limitations of traditional REV estimation methods and provided a more accurate approach for identifying the

minimum representative volume in materials where optical imaging can be applied. This work directly contributed to REV assessment in experimental contexts.

Costanza-Robinson et al. investigate the concept of REV in the context of porosity, moisture saturation and interfacial area [19]. The key conclusion from their work was that current REV methods may be routinely giving poor estimates of physical properties due to the difficulty in distinguishing between the end of phase I and the beginning of phase II on a porosity-volume plot (see Figure 1). Singh et al. proposed a texture-based characterization method called the “Gray-Level Size Zone Matrix”, allowing REV sizes to be estimated directly using greyscale images [20]. This bypasses the need for prior segmentation or extensive computational resources.

While the studies summarized here demonstrate significant advancements in both experimental and computational approaches to REV, they represent only a subset of the extensive work conducted in this field. Moreover, they are indirect, as they make the assumption of their measurements being accurate to the point of expanding to a continuum model, and can be unreliable when applied to novel images. A need clearly exists to develop a procedure to measure the REV directly and conclusively for a given image, especially for tortuosity which is an especially important property used in many applications.

2.4. Effective Diffusivity and Tortuosity

Diffusion of a solute through a porous medium is usually described by Fick’s law:

$$n_A = D_{eff} \frac{dC_A}{dz} \quad (2.1)$$

where n_A and C_A are the molar flux and concentration, respectively, of species A and D_{eff} is the effective diffusion coefficient of A through the medium. The effective diffusion coefficient is the volume-averaged diffusion coefficient through the porous domain. D_{eff} is always lower than the value through open space due to the blockages by the solid structure which comprises the porous medium. This reduction can be broken into 2 parts. The first contribution comes from the reduction in the amount of void space present, resulting in a direct proportional decrease in total

flux, as quantified by the porosity $\varepsilon = V_{void}/V_{bulk}$. The second contribution comes from the decrease of the flux due to the elongated pathways of the solute as it traverses the solid obstacles, which is expressed by the tortuosity τ . Unlike ε , τ does not have a simple definition and is usually defined as:

$$\frac{D_{eff}}{D_{AB}} = \frac{\varepsilon}{\tau} \quad (2.2)$$

Together, the inclusion of porosity and tortuosity yields the following form of Fick's law:

$$n_A = D_{AB} \frac{\varepsilon}{\tau} \frac{dC_A}{dz} \quad (2.3)$$

The determination of τ is the main challenge when modeling diffusion through a porous domain and so is commonly obtained from simulations based on volumetric images.

2.5. Tortuosity – Porosity Correlations

It is well known that conduction through a composite domain undergoes a phase transition at a critical volume fraction of the conducting medium. The effective conductivity is zero at volume fractions below this critical level, while it increases rapidly when the volume fraction increases above this value. This critical volume fraction known as the percolation threshold has been studied extensively, being defined for many different structure types [21] [22] [23]. Despite being analogous to conduction, correlations for effective diffusivity through porous materials almost universally neglect the existence of a threshold below which no conductivity occurs. The most common example of this problem is the almost universal use of the following simple power-law expression

$$\tau = \varepsilon^{-\alpha} \quad (2.4)$$

for the dependence of tortuosity on porosity. This relation is widely referred to as the Bruggeman correlation based on the work of Bruggeman to analytically derive values of α for common geometries (namely overlapping spheres and overlapping rods) [24]. The form of the power-law

expression implies that tortuosity becomes infinite as the porosity approaches 0. In fact, it is observed that the porosity does not have to decrease to zero in order for the voids of a domain to become disconnected. Nonetheless, an examination of the correlations collected in the extensive review by Ghanbarian et al. shows only one which explicitly accounts for a percolation threshold [25]. This lone exception is the one of Tomadakis and Sotirchos, who proposed the following correlation which not only included the percolation threshold ε_p (via the $\varepsilon - \varepsilon_p$ term) but also properly normalized the function via the $1 - \varepsilon_p$ term, i.e. [26],

$$\tau = \left(\frac{\varepsilon - \varepsilon_p}{1 - \varepsilon_p} \right)^{-\alpha} \quad (2.5)$$

They provided estimates for ε_p and α for various fiber structures including fibers randomly located in the X-Y plane but aligned in the Z direction (1D), fibers randomly rotated in the X-Y plane but fully parallel in the Z direction (2D) and fibers that randomly oriented in all three directions (3D). These values are summarized in Table I.

Table I – Fitting parameter for various fiber structures [2].

Orientation	X-Axis		Y-Axis		Z-Axis	
	ε_p	α	ε_p	α	ε_p	α
1D	0.33*	0.707	0.33*	0.707	0.0	1.0
2D	0.11	0.521	0.11	0.521	0.11	0.785
3D	0.037	0.661	0.037	0.66	0.037	0.66

* The percolation threshold for overlapping disks in 2D is closer to 0.31-0.32 according to the exhaustive list compiled in Wikipedia [27] [28].

The difference in the dependence of τ on ε according to the Bruggeman (B) and Tomadakis-Sotirchos (TS) models is quite stark, as shown in Figure 3. As expected, the tortuosity according to the TS model clearly rises to high values at higher porosity values than it does using the

Bruggeman model. Note the plots are obtained using values for the exponent α in the TS model that are lower than those used for the Bruggeman model. This has been done here to make the difference smaller than it would otherwise be if the same values are used in both models. Since it incorporates the important effect of percolation, the TS model will be used throughout this work. To use this model, however, one must know both the percolation threshold in addition to the exponent, which perhaps explains why the single-parameter Bruggeman model remains in favor.

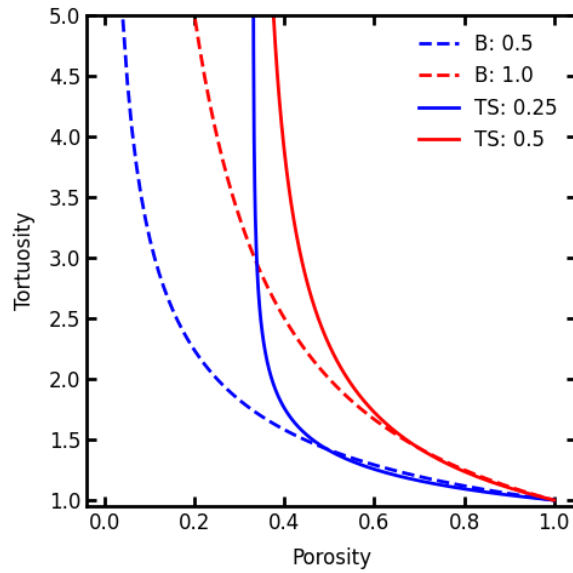


Figure 3 – Comparison of the predicted dependence of τ on ε according to the Bruggeman (Eq (2.4)) and Tomadakis- Sotirchos (Eq (2.5)) models. The values of 0.5, 1.0, and 0.25 correspond to the exponents used in the relevant correlations.

An advantage of using images to estimate tortuosity is that one can analyze and manipulate the image to extract additional helpful information. For instance, it is possible to determine the value of ε_p for a given image, and the methodology is detailed in section 3.2. This is useful for two reasons: (a) ε_p may not be readily available otherwise for the material under study and (b) ε_p is a statistical average taken over many realizations so the value for a given image may deviate greatly, allowing us to determine an appropriate range to be used within the TS model. As this

thesis focuses on determining tortuosity in sandstones from single images, both of these factors are important. It is therefore of interest to develop and validate a method for determining ε_p on the basis of a single image.

Experimental determination of the percolation porosity ε_p of a material requires characterizing samples having a range of porosities and identifying the porosity at which the void phase becomes contiguous. However, this can be rather challenging to do since the porosities of a given class of materials tend to fall within a narrow range. It is also not guaranteed that this range encompasses the percolation threshold. For instance, the porosities of fibrous structures typically lie between 0.6 and 0.8, depending on how the fibers are packed [29]. Similarly, the porosities of sandstones tend to fall between 0.1 and 0.3 [30]. An alternative way to accomplish this would be to alter or control the porosity of a sample by applying varying amounts of compression to reduce its thickness from an original value of t_0 to t_c . Provided the solid does not deform or break, then one can obtain the porosity ε_c of the compressed sample from the following expression:

$$\varepsilon_c = 1 - \frac{t_0}{t_c} (1 - \varepsilon_0) \quad (2.6)$$

where ε_0 is the porosity of the original sample [31]. However, this approach may be problematic. Firstly, it requires that the particles making up the samples not be damaged or altered in any way which is a questionable assumption. Secondly, the morphology of the void space is bound to change as it is compressed and so the percolating porosity obtained may or may not be relevant to the original material.

Analyzing images, however, provides several options that are not possible with physical materials. Firstly, one can generate artificial images with different numbers of particles, which can have different porosities if the particles are allowed to overlap. The radius of the particles can also be varied, which has the same effect on porosity. Tomadakis and Sotirchos combined both options in their various studies on this subject in the 1990s [2] [26]. Secondly, one can begin with a given image then dilate the solid progressively. Since this approach can be applied to images of real materials, it is preferable and used in this study. The methodology developed as part of this work is presented and validated in the next section.

2.6. Tortuosity Distributions

The motive behind determining the representative elementary volume of an image is to determine if the image is representative of the whole material from which it was obtained. This is essential if the transport properties obtained from the image are to be used to describe that of the sample as a whole. To illustrate the importance of checking for the existence of an REV, a simple example is presented here. Figure 4a depicts a 1000×1000 pixel image of a porous structure that is relatively homogenous in nature and has a porosity of 70%. This sample can be cut into slabs of discrete sizes and various properties can be determined for each slab.

A summary of the properties obtained from Figure 4b and 4c can be found in Table V and Table VI, respectively, appearing in Appendix C Tables. Figure 5 depicts the variation of the tortuosity over the domain of axis 1 across the entire sample shown in Figure 4, as well as the true tortuosity value of the whole image, where axis 1 is the horizontal direction. The tortuosity over each slab is significantly lower than the true value. Interestingly, this example shows that subdividing the original image into smaller slabs has deleterious effect on the estimate of the tortuosity. If the difference in the tortuosities of the various slabs is small, then the image may be considered homogenous. Conversely, if the differences are large, then each slab is structurally different and the image may be considered heterogenous.

As the slab size increases, the features of the smaller slabs are incorporated into the larger ones, resulting in a “more representative” subdomain of the whole image. A few interesting observations can be made in this regard. Firstly, as noted above, the smaller slabs all exhibit lower tortuosity than the true value. Thus, as the slabs become larger, they incorporate more of the ‘up-stream’ features of the structure that would hinder solute transport by diffusion. At the same time, the smaller slabs can slice through solids and create pathways by converting a dead-end cavern into an open channel and thereby artificially lower the tortuosity. This is not to say that slabs should be used to analyze tortuosity, but to clearly demonstrate why samples should be checked for REV when doing tortuosity calculations.

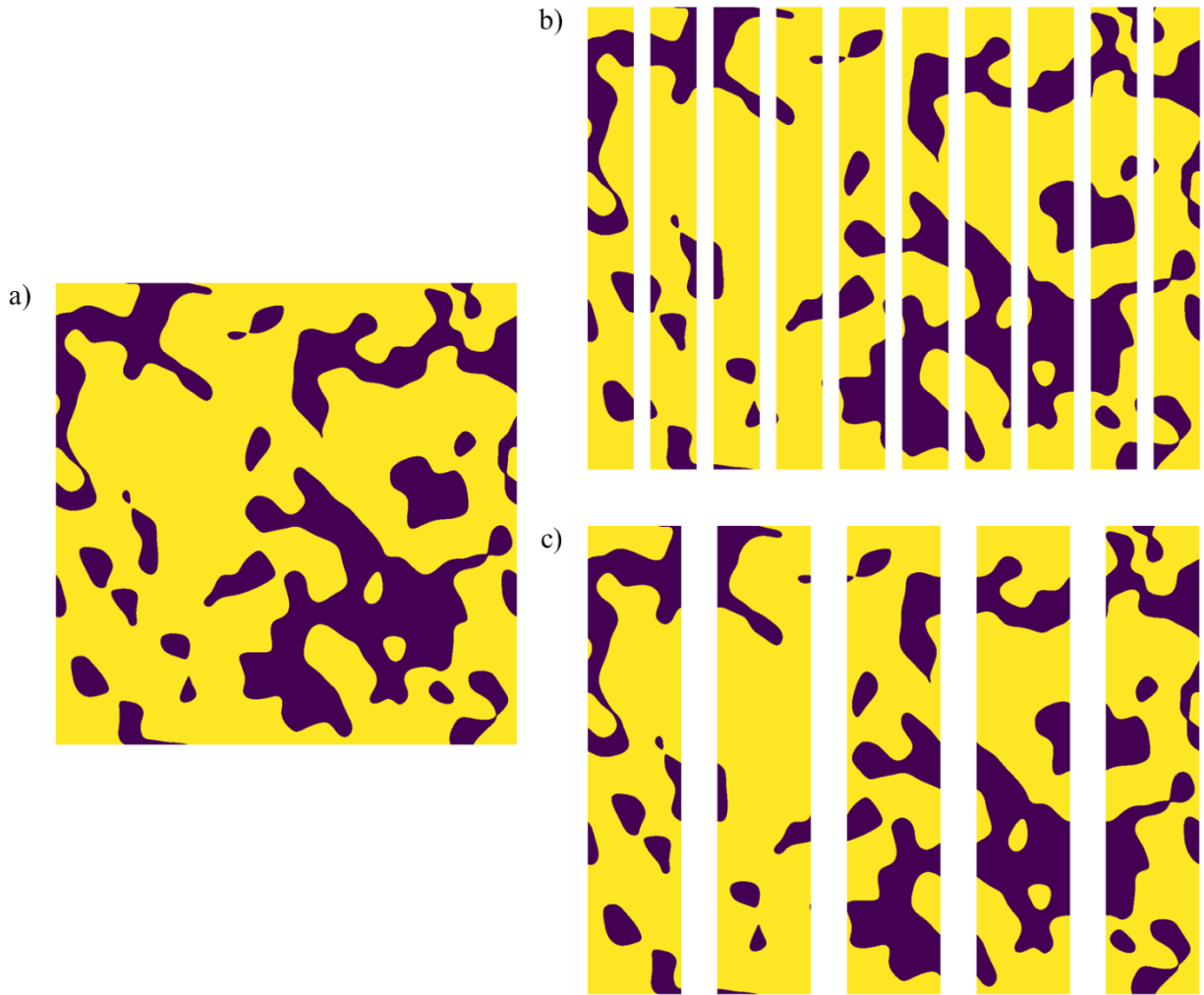


Figure 4 – (a) A generated image with a porosity of 70%. (b) and (c) depict the image after being subdivided into discrete slices of sizes 100×1000 and 200×1000 pixels, respectively.

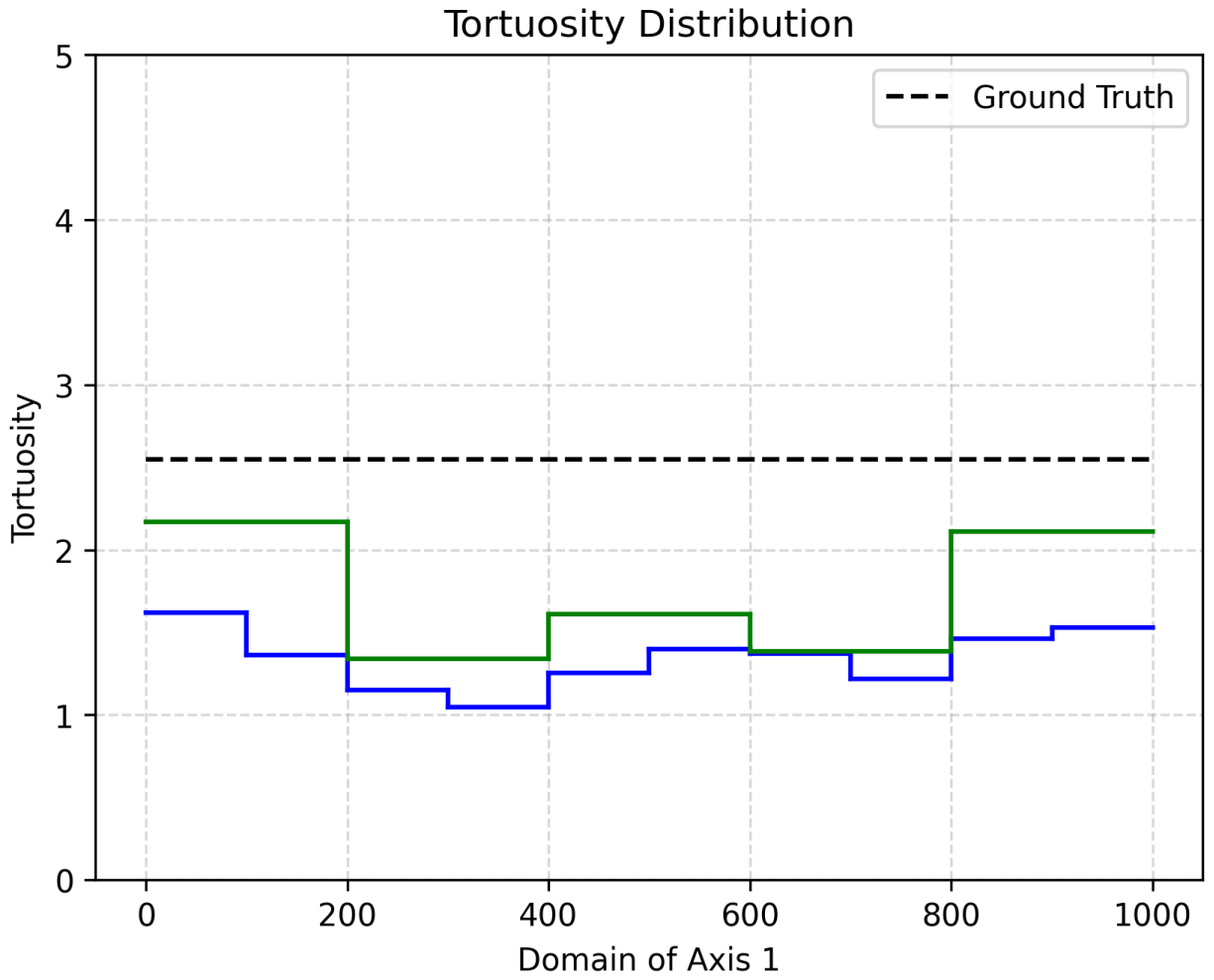


Figure 5 – Variation of the tortuosity along the horizontal direction across the slabs in Figure 4. The blue data series corresponds to the slabs seen in Figure 4b and Figure 4c is the green data series.

3. Methodology

2.1 Image Acquisition

Image of real rock samples have been acquired from the study by Dong and Blunt on network extraction. The images with a name starting with “S” were imaged by the Synchrotron micro-CT scanner, whereas the remaining images used a desktop micro-CT system, as described by Dong [1]. The known properties obtained from each sample image are listed in Table II and Table III. The tortuosity values shown in Table II have been determined in our laboratory as a part of this study independently from the work done by Dong and Blunt. 3D renderings of each image are presented in Figure 6, generated using the original data files provided online.

The tortuosity determined from the formation factors obtained by Dong and Blunt are similar to those independently obtained in Table II, with notable differences being the characteristically high tortuosity samples (C2, and S4). Two significant figures are shown here for simplicity of comparison.

Table II – Tortuosity along the three axes in each sample image.

	Tortuosity		
Sample Name	x	y	z
A1	2.43	1.98	1.90
C1	5.77	4.66	7.16
C2	34.25	16.76	25.63
S1	7.54	5.34	5.11
S2	3.09	2.79	2.67
S3	11.64	6.93	8.63
S4	18.71	11.61	12.17
S5	3.35	3.08	2.97
S6	3.09	2.67	2.45
S7	2.79	2.32	2.40
S8	2.21	2.03	2.04
S9	4.01	4.40	3.63

Table III – Pore structure properties of extracted AB networks on image samples from Dong and Blunt [32] [33].

Samples	A1	C1	C2	S1	S2	S3	S4	S5	S6	S7	S8	S9
Resolution (μm)	3.85	2.85	5.35	8.68	4.96	9.1	8.96	4	5.1	4.8	4.89	3.4
Size	300 ³	400 ³	400 ³	300 ³	300 ³	300 ³	300 ³	300 ³	300 ³	300 ³	300 ³	300 ³
Porosity (%)	42.9	23.3	16.8	14.1	24.6	16.9	17.1	21.1	24	25	34	22.2
K_x (mD)*	6,773	1,289	136	2,138	4,198	744	439	6,847	13,175	7,915	14,999	2,283
K_y (mD)*	9,232	2,282	289	2,597	4,883	1,200	596	6,396	13,976	9,254	15,666	2,790
K_z (mD)*	9,664	1,138	139	2,816	5,174	733	587	6,202	14,660	9,271	14,897	3,506
K_{avg} (mD)*	8,556	1569	188	2,517	4,751	892	541	6,481	13,937	8,813	15,187	2,860
F_x*	5.58	27.94	281.8	50.41	12.52	62.4	104.2	15.74	13.34	10.58	6.42	17.69
F_y*	4.4	21.46	136.2	38.07	11.03	39.19	67.78	14.4	11.78	9.48	6.05	20.22
F_z*	4.29	35.88	214	36.37	10.88	50.23	69.6	14.17	11.52	9.41	6.21	15.74
F_{avg}*	4.69	27.21	192.8	40.76	11.43	48.82	77.49	14.74	12.17	9.79	6.22	17.7
τ_x*	2.39	6.51	47.34	7.11	3.08	10.55	17.82	3.32	3.20	2.65	2.18	3.93
τ_y*	1.89	5.00	22.88	5.37	2.71	6.62	11.59	3.04	2.83	2.37	2.06	4.49
τ_z*	1.84	8.36	35.95	5.13	2.68	8.49	11.90	2.99	2.76	2.35	2.11	3.49

* K_x , K_y , and K_z are the directional absolute permeability in the x , y and z directions, respectively. K_{avg} is the average permeability of the three directions. F_x , F_y and F_z are the formation factors in the x , y and z directions, respectively. F_{avg} is the harmonic mean of formation factors in the three directions. τ_x , τ_y , and τ_z are the tortuosities in the x , y , and z directions, calculated from the formation factors.

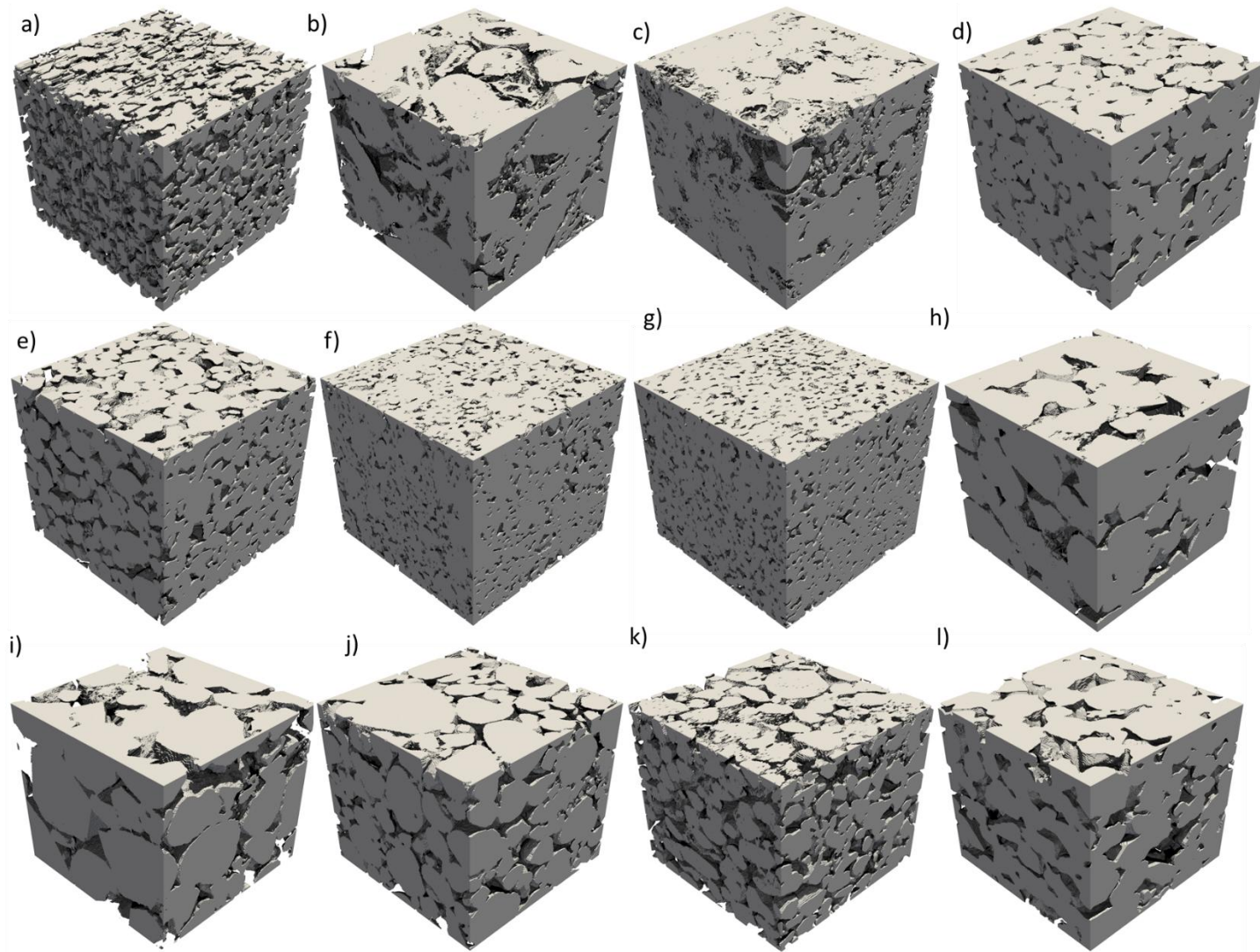


Figure 6 – 3D renderings of the sample images obtained from Dong and Blunt, rendered in Paraview [32]. Images shown in a), b), c), d), e), f), g), h), i), j), k) and l) correspond to samples A1, C1, C2, S1, S2, S3, S4, S5, S6, S7, S8 and S9, respectively.

3.1. Image Generation

A major part of this work is to develop an algorithm to determine the percolating porosity of a given image. To ensure that this algorithm operates correctly, it is necessary to first apply it to images for which percolating porosity values are known before applying it to the samples described in the previous section. Since Tomadakis and Sotirchos provide this information for several different fiber types, these have been chosen as the test cases here [2] [26].

Images of aligned fibers are relatively easy to generate since this only requires first producing a 2D image of overlapping disks and then extruding it to form a 3D image, as shown in Figure 7. The first step is to select n pixels randomly in a 2D image of the specified domain size ($L_x, L_y = 300, 300$). As the locations of the pixels are randomly selected, the locations of the fibers are therefore random. Then the points are dilated to the desired fiber radius r_f , resulting in all fibers having the same radii. This is accomplished by applying a distance transform relative to the chosen pixels, then applying a threshold to locate pixels further than r_f from the nearest point to define the void space. In order to avoid edge effects, pixels are chosen from a domain of size $(L_x + 2r_f, L_y + 2r_f)$ before carrying out the dilation step and removing r_f pixels from all sides to obtain the required domain size. Finally, the 2D image is extruded to form a 3D image, similar to those shown in Figure 8. The extrusion of the 2D image is completed through stacking the image in the third axis, essentially replicating the 2D image to the specified size ($L_z = 300$).

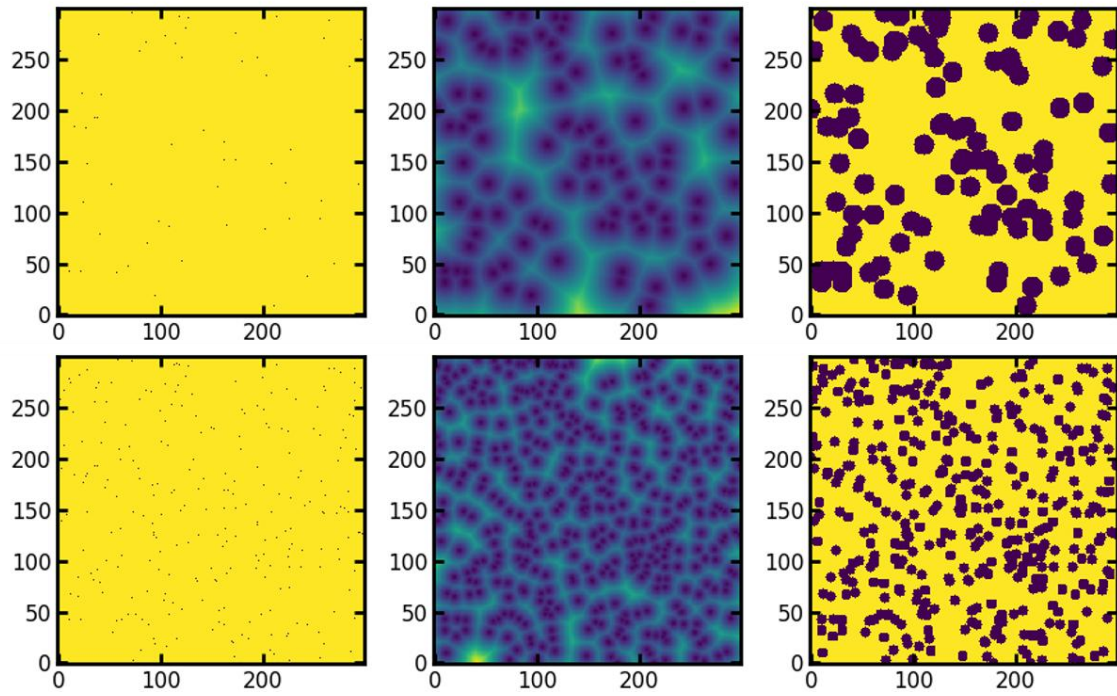


Figure 7 – Process of constructing of an image of randomly located by aligned fibers. Top row shows an example of a generated image with small n and medium r_f , while bottom row shows an example of a generated image with large n with small r_f . This depicts the step before extrusion.

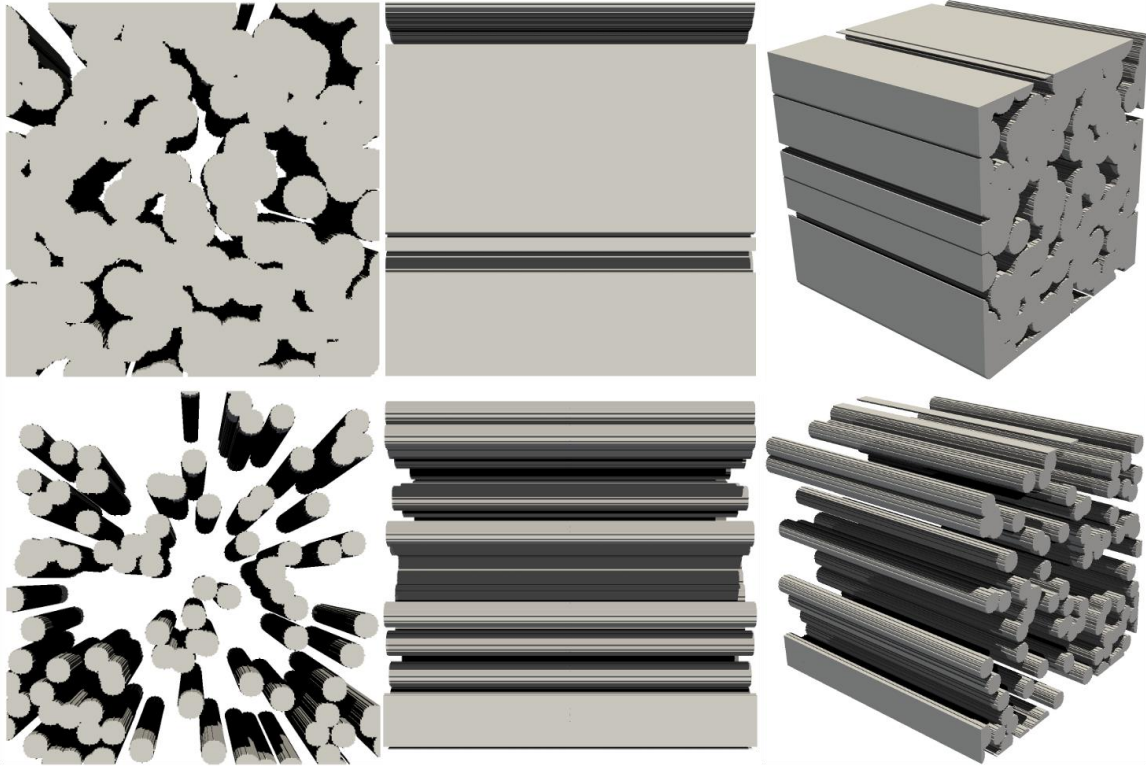


Figure 8 – Top view (left), side view (middle) and rotated view (right) images of fibers aligned in 1D. Top row shows an example of a sample with fewer fibers having large diameter, while bottom row shows a sample with more fibers having smaller diameter. Images with $n = 100 \rightarrow 600$ and $r_f = 3 \rightarrow 20$ were tested in this study. This depicts the step after extrusion.

Compared to aligned fibers, it should be noted that the generation of images of randomly rotated fibers is significantly more complicated. In a recent study, Beckman et al. surveyed the problems associated with the commonly used methods, which typically result in a non-uniform fiber density across the domain [34]. This problem was in fact discussed by Bertrand over 100 years ago and is sometimes called Bertrand's paradox. Specifically, the random drawing of chords on a circle which circumscribes the domain will not produce a uniform density of lines within the domain. Beckman et al. proposed a simple method which was empirically demonstrated to produce uniform densities [34]. First, a ray is drawn from the center of the domain at a random angle ($0 \rightarrow 2\pi$) and random length ($0 \rightarrow (\sqrt{L_x/2 + L_y/2})^2$). A fiber is then formed by drawing a perpendicular line at the endpoint to each of these rays, the length of which spans the whole image domain. This process is repeated in order to draw as many lines as desired. A 3D image is

generated by first assigning each line a random location along the 3rd axis ($-r_f \rightarrow L_z + r_f$). Each line is then dilated using the same distance transform-based approach used in the case of aligned fibers. Examples of the structures formed by this process for different values of n and r are shown in Figure 9. the domain size is increased by $2r_f$ in all directions to avoid edge effects prior to dilation and then trimmed to the original desired size in the final step.



Figure 9 – Sample images of fibers randomly oriented in the x-y plane but aligned along the z axis. Top row shows structure containing more fibers with small diameter, while bottom row shows structure containing fewer fibers with larger diameter. Images with $n = 100 \rightarrow 600$ and $r_f = 3 \rightarrow 20$ were evaluated.

Tomadakis and Sotirchos also analyzed images with fibers randomly oriented in all three dimensions, but comparisons were not made to this case since a robust way to generate images that avoid the Bertrand paradox was outside the scope of the present work. For this reason, this work focuses on images with aligned fibers.

3.2. Determination of the Percolating Porosity

To determine the percolating porosity of an image, the solid is dilated progressively (i.e. 1 layer of voxels at a time). This is accomplished by obtaining the distance transform relative to the solid phase in each image, then applying thresholds ranging from $R = 1 \rightarrow R_p$ where R_p is the radius of the dilation at which no percolating cluster remains. Percolation is checked after each dilation by labeling all void voxels with their cluster number, then examining whether the faces on opposing sides of the domain have at least one cluster label in common. If no percolating cluster(s) is found, then the percolation threshold lies somewhere between R_p and $R_p - 1$. This process is illustrated in Figure 10 for two images with different fiber radii and number of fibers, with the color in the void space representing the cluster number. The middle column shows the case when $R = R_p - 1$ and the right column show $R = R_p$.

It is important to note that there are other methods of determining the percolating porosity of an image. Dilation was selected as it is the only method which can truly be applied to real image samples which already exist, and is consistent with the method used by Tomadakis and Sotirchos [2].

The void space is fully connected in the structures shown in the left and middle columns of Figure 10. In the middle structures, a few pockets of isolated void space can be seen. On the other hand, a percolating path no longer exists (either from left to right or top to bottom) in the structures on the right, as seen by the lack of a connecting cluster spanning from the left face to the right face. Consequently, the percolation threshold lies somewhere between these two states due to the discrete nature of the dilation process. However, for the sake of consistency through this work, the percolating porosity ε_p is calculated at $R = R_p - 1$ by finding the fraction of all void voxels, percolating or not, to the total number of voxels in the image.

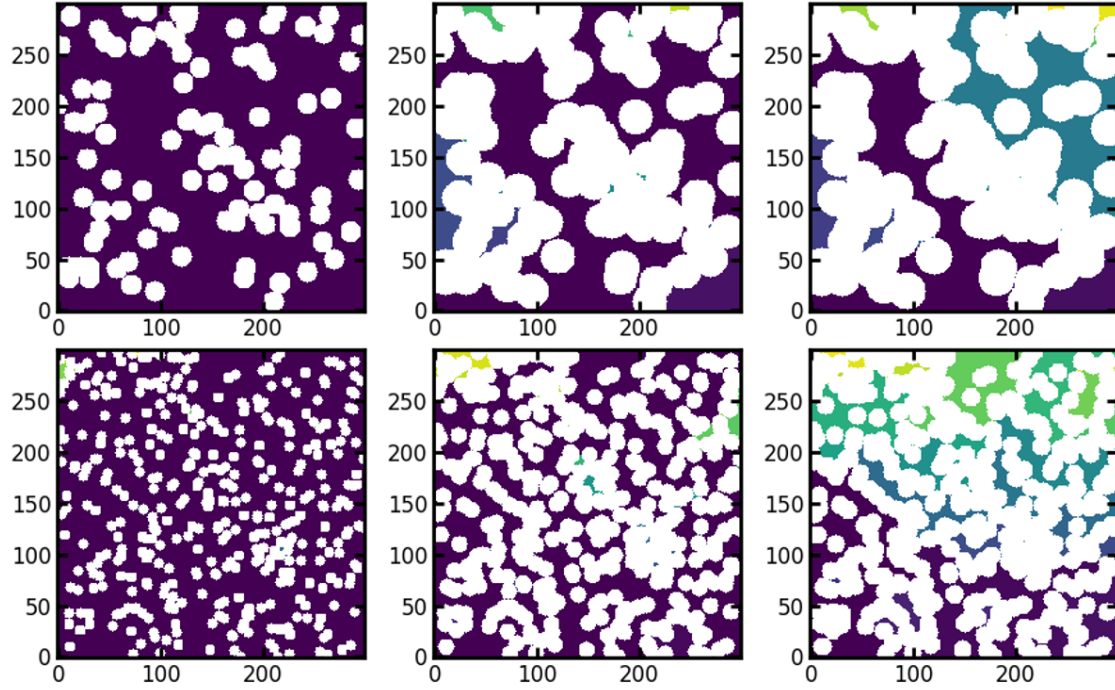


Figure 10 – Determination of percolation threshold by cluster labeling. Top row shows the case of small n and moderate r_f , while the bottom row shows higher n and small r_f . The left column is the original image, while the middle and right columns show the cases after dilating to $R_p - 1$ and R_p , respectively. The different colours in the void space indicate a different labeled cluster number.

Figure 11 shows the result of the above process by presenting the variation of the percolating porosity with the initial fiber size. The percolating porosity at each fiber size is determined on the basis of 50 images, each of which has dimensions 300×300 pixels and contains 100 fibers. Also shown on the plot is the distribution of percolating porosities for each initial fibre size and the average value indicated by the horizontal tick marks near the center of each distribution. The grey regions above the data points at each fiber size indicate the initial porosity of each set of images. The solid grey horizontal line located at 0.33 corresponds to the threshold reported by Tomadakis and Sotirchos, although it should be mentioned that the accepted value is closer to 0.31, which agrees with the tick marks on each distribution [27].

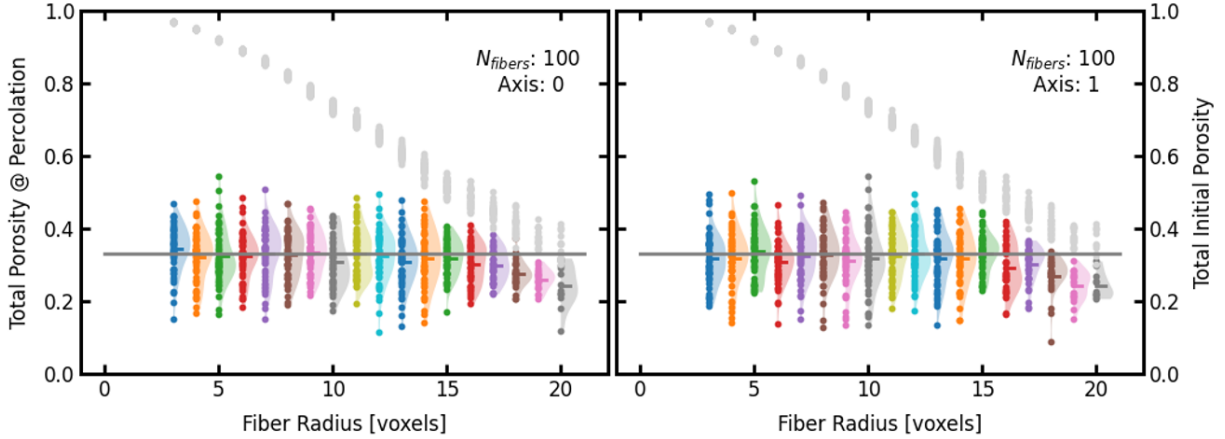


Figure 11 – Variation of percolating porosity in the two directions perpendicular to the fiber axes with initial fiber size in image, where “Axis: 0” corresponds to the x-axis, and “Axis: 1” corresponds to the y-axis. Each image contains 100 fibers. The grey regions above the data points at each fiber size indicate the initial porosity of each set of images. The solid grey horizontal line located at 0.33 corresponds to the threshold reported by Tomadakis and Sotirchos [2].

As shown in Figure 11, the initial porosity approaches the percolating porosity as the fiber radius increases due to the large fibers occupying a substantial fraction of the image and exceeding the percolation threshold. Not surprisingly, this effect is more pronounced when the number of initial fibers increases. This is clearly evident in Figure 12, which shows the results when 400 fibers are placed in the initial image. Nonetheless the average percolating porosity for this case remains in agreement with the case for $N = 100$, at $\sim 0.31 - 0.32$, at least until the initial image itself is no longer percolating.

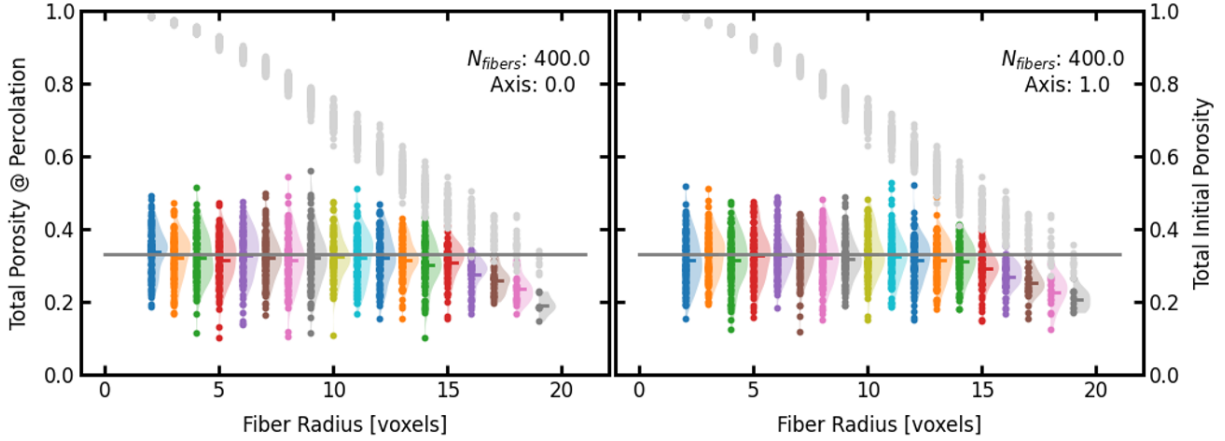


Figure 12 - Percolating porosity as a function of initial fiber size in images with 400 initial fibers for the case of aligned fibers as shown in Figure 8.

The above analysis confirms that the developed method to determine the percolation threshold on a given image is valid since it produces values in agreement with known values. However, the results clearly show that the percolation threshold actually spans a rather large range, even for the simple case of overlapping disks. For instance, the results shown in Figure 11 demonstrate that the percolating porosity can vary between 0.2 and 0.5. Thus, a major conclusion from this analysis is that the commonly used assumption of a percolation porosity of 0.33 for a structure composed of randomly aligned fibers may be highly erroneous, as demonstrated by Figure 11. This reinforces the notion that a unique percolation value should be found for each image. Note that this problem is not relevant when fitting experimental data since the sample on which experiments are usually conducted are many times larger than the domain represented by a typical tomography image. Larger domains are more likely to follow the statistical distribution.

The same analysis was applied to images with fibers randomly rotated in plane, yielding the results shown in Figure 13 for the case of $n = 100$. The grey line indicates the value of $\varepsilon_p = 0.11$ which was reported by Tomadakis and Sotirchos. Interestingly, they report the same value for all 3 directions, while the results shown here indicate a slight difference between the two in-plane directions (Axis = 0, 1) compared to the through-plane direction (Axis = 2). For the in-plane direction parallel to the fibers, the threshold is closer to 0.08, while the value is 0.11 for the

through-plane direction perpendicular to the fibers. It seems reasonable to expect differences in these two directions, considering the anisotropic morphology of the void space. However, the difference should not be large, as these results indicate. This agreement further reinforces the conclusion that the proposed method developed in this study to determine the percolating porosity is suitable.

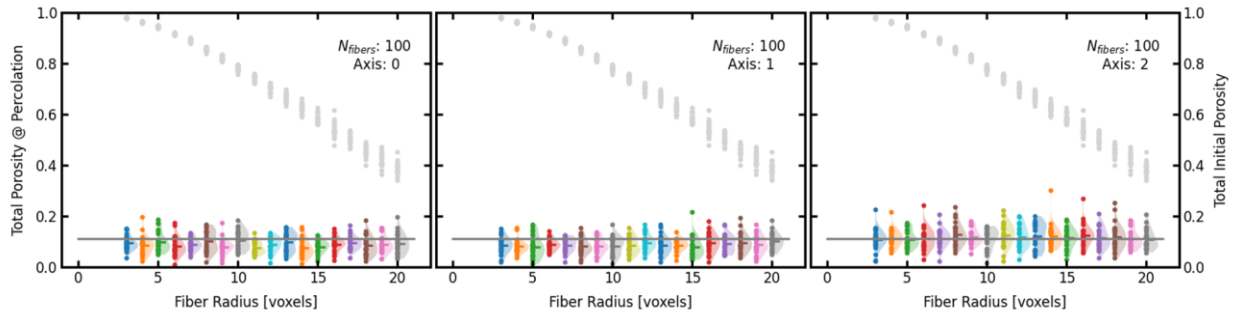


Figure 13 – Distribution of percolating porosity as a function of fiber size for the case of fibers randomly rotated in-plane, as shown in Figure 9.

3.3. Image Processing

The various image processing procedures and operations carried out in this study were done using both Python and Julia software. The scripts used to process images can be found in Appendix B Image Analysis Code.

3.3.1. Identifying and Removing Invalid Voxels

In the analysis of porous media, not all void volumes contribute to transport processes such as diffusion. A particular subset of these volumes referred to as closed pores consists of isolated or dead-end voids that do not form part of the continuous percolating network of interest. These regions can trap fluid but do not facilitate flow or diffusion through the material, leading to biases in computed transport properties if they are not properly identified and excluded. Closed pores may occur within the bulk of the medium as disconnected pockets or at the surface as incomplete

channels that open only to the surroundings. When voxel images are used for quantitative analysis, the presence of such invalid voxels introduces noise into porosity and tortuosity measurements, artificially inflating void space without contributing to connectivity. In some cases, the particular numerical solver for the coefficient matrix will be unable to resolve, as detailed in section 3.4. Consequently, a crucial step in preprocessing porous media data is to systematically detect and remove invalid voxels, ensuring that only the effective pore space is retained. This is accomplished in this study using the same method that is used to check for percolation. Namely, each void in the image is labelled according to which cluster it belongs. Any cluster number which does not appear in both the inlet and outlet faces of the entire space is considered closed and therefore removed from the domain prior to computing the tortuosity.

3.4. Computing Tortuosity

To determine the tortuosity of an image, Fick's law of diffusion is applied. A sample image will be used to demonstrate this, as shown in Figure 14.

In general, Fick's Law can be written as Equation (3.12) in the x-direction.

$$\frac{\partial C_A}{\partial t} = D_{AB} \frac{\partial^2 C_A}{\partial x^2} \quad (3.1)$$

The molar flux n_A and molar flowrate N_A of solute species A through the voids are given in Eqns **Error! Reference source not found.** and (3.3) below:

$$n_A = D_{AB} \frac{dC_A}{dx} \quad (3.2)$$

$$N_A = D_{AB} A_{eff} \frac{dC_A}{dx} \quad (3.3)$$

For this work, all systems are assumed to be under steady state conditions, where n_A and N_A are zero.

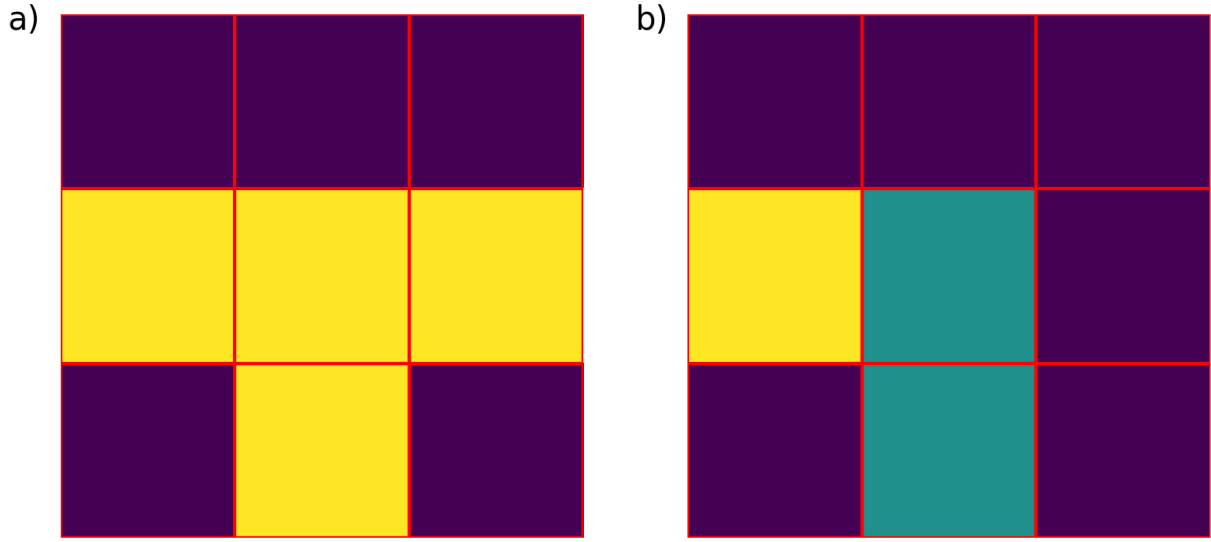


Figure 14 – Schematic of pore space used to determine tortuosity. Sample image of size 3 pixels by 3 pixels: a) yellow and purple denotes void and solid phases, respectively. Percolation occurs in the left-to-right direction and through the open face on the bottom. b) yellow denotes the highest solute concentration, purple corresponds to the lowest concentration and green depicts intermediate concentration in the void space.

Using the finite difference method to approximate a first-order differential equation results in Eqns (3.4) and (3.5). The forward-difference approach is used to approximate the derivative of function f at each position x . Thus, the difference in f at position x is given as Equation (3.7).

$$N_{A,i \rightarrow j} = D_{AB} A_{eff} \left(\frac{C_{A,j} - C_{A,i}}{x_j - x_i} \right) \quad (3.4)$$

$$N_{A,i \rightarrow j} = G_{i \rightarrow j}^d (C_{A,j} - C_{A,i}) \quad (3.5)$$

$$G_{i \rightarrow j}^d = \frac{D_{AB} A_{eff}}{x_j - x_i} \quad (3.6)$$

$$\Delta_h[f](x) = f(x + h) - f(x) \quad (3.7)$$

where $G_{i \rightarrow j}^d$ is the lumped parameter of diffusive conductance.

Equation (3.5) can be used to generate the coefficient matrix for the configuration shown in Figure 14 a), as well as the relevant boundary conditions. In this case, the boundary conditions being applied are such that the concentration at the entry face is $C = C_{in}$ and exit face is $C = 0$. Each pixel is labelled with a number between 1 and 9 starting from left to right and moving from top to bottom. Thus, the first void pixel in Figure 14a is numbered as pixel 4. The following mass balance can be written for pixel 4, as follows:

$$G_{4 \rightarrow 5}(C_5 - C_4) + G_{4 \rightarrow 1}(C_1 - C_4) + G_{4 \rightarrow 7}(C_7 - C_4) = C_{in} \quad (3.8)$$

$$G_{13 \rightarrow 14}(C_5 - C_4) = C_{in} \quad (3.9)$$

where C_{in} is the boundary condition being applied.

Similarly, a mass balance can be written for the neighbouring void pixel 5 as follows:

$$G_{5 \rightarrow 4}(C_4 - C_5) + G_{5 \rightarrow 6}(C_6 - C_5) + G_{5 \rightarrow 2}(C_2 - C_5) + G_{5 \rightarrow 8}(C_8 - C_5) = 0 \quad (3.10)$$

With the mass balance written for each pixel, the coefficient matrix can be created. In this case, it would be a sparse 9 by 9 matrix, which can then be solved by various means. In general, the mass balance for a single internal pixel can be written as Equation (3.11), and for an edge pixel as Equation (3.12).

$$\sum_j G_{j \rightarrow i} x_j - \sum_j G_{j \rightarrow i} x_i = 0; i = a; j = b, c, \dots d \quad (3.11)$$

$$\sum_j G_{j \rightarrow i} x_j - \sum_j G_{j \rightarrow i} x_i = C_{in} \text{ or } C_{out}, i = a; j = b, c, \dots d \quad (3.12)$$

where i is the number of the voxel being analyzed, j is the number of the neighbouring pixels, and a, b, c , and d are the pixel numberings. This definition can be trivially expanded to three dimensions, where each pixel is now considered a voxel. Note that solid voxels can be omitted from the coefficient matrix and mass transfer between solid voxels and void voxels prohibited or the G value can be set to a very low value to ensure negligible diffusion occurs through the solid voxels. The former approach is used in this study since it reduces the number of unknowns to be solved and thus saves computational time.

3.5. Obtaining REV Data for Porosity and Tortuosity

Obtaining REV data requires extracting sub-sections from the main image and analyzing each separately. The selection of subdomains from the larger image must be considered carefully since the method of sampling directly influences the reliability of the results. Two general approaches are described here. The first involves the construction of a grid of uniformly sized subdomains that span the entire image, as shown in Figure 15 a. This method ensures complete spatial coverage and enables direct comparison between subdomains of equal dimension. The second approach relies on randomly selecting square or cubic subdomains for 2D or 3D images at various locations and sizes (Figure 15 b). Random sampling provides insight into the statistical variability of the structure and allows the analysis of scale effects, particularly in determining how the porosity and tortuosity converge toward stable values as the sampled volume increases.

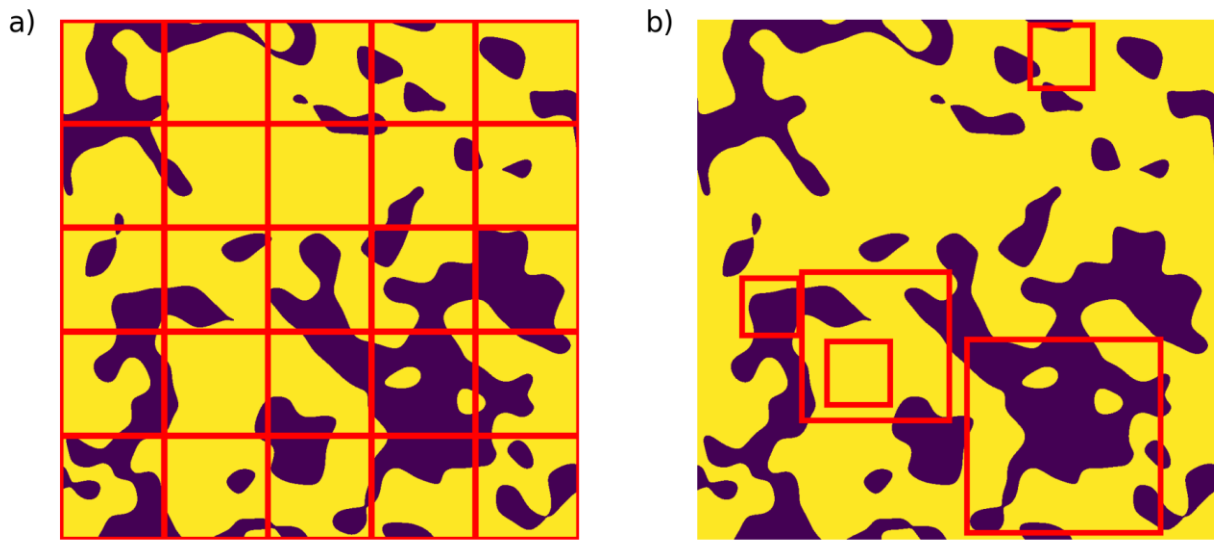


Figure 15 – Segmentation of an image: a) subdivision using a regular grid and b) subdivision into random subdomains.

Using segmentation by subdivision according to a regular grid (Figure 15a), only a single-sized subdomain is studied at once, whereas segmentation into random subdivisions shown in Figure 15b leads to an REV plot containing different subdomain sizes, as discussed in Section 4.1. Additionally, if a material has spatial heterogeneities which are periodic or aligned with the grid,

this can result in biases that are avoided by random sampling since each subdomain is selected independently over the entire image. Both methods are used in this study for different reasons.

Since each block can be processed independently, the block analysis becomes readily parallelizable. The bottleneck in terms of computing speed in almost every scenario is the capabilities of the hardware being used. To fully take advantage of parallelizability, the supported platform must have multi-threading enabled, with a high number of cores to handle the tasks.

3.6. Computation of Pore Size Distribution

The pore size distribution is a key property of porous materials as both the pore size and distribution affect the transport processes [35] [36]. Only a few ways exist to experimentally measure a pore size distribution, but several options are available to determine one from an image. The two main options are the distance transform or the local thickness method. These are illustrated in Figure 16. The distance transform labels each voxel in the void phase with the distance to the nearest solid voxel. This can be interpreted as the radius of the largest circle that can be drawn centered on each voxel before encountering a solid voxel. The local thickness labels each voxel with the radius of the largest circle that overlaps it. Both have the same range of values, but they have a different distribution of values. The distance transform has many voxels containing small values near the walls, but these are not relevant to the size distribution since all images have these in common. The local thickness method on the other hand yields a more representative distribution of values with regions of large void space containing many voxels, as shown by the red and orange regions in Figure 16 (right).

Once an image has been analyzed using the distance transform or local thickness method, one can extract statistical distributions from the data obtained. Torquato discusses this in detail in his textbook [37]. The use of the distance transform yields what is called the radial density function (RDF), while analysis of the image obtained from the local thickness method provides the pore density function (PDF). Both functions range from the same values of radii but contain different distributions. Once the pore size distribution is known, it is possible to derive the cumulative density function $F(r)$ expressing the probability of finding a voxel larger than r , i.e.,

$$\int_r^\infty P(r')dr' = F(r) \quad (3.13)$$

where $P(r)$ is the probability of finding a voxel with a radius of r . When r decreases to zero, $F(r)$ necessarily includes all of the voxels in the sample and so

$$\int_0^\infty P(r)dr = 1.0 \quad (3.14)$$

The cumulative density functions based on the distance transform and local thickness method for a 3D image are shown in Figure 17. A useful feature of the cumulative distribution is that one can easily find the fraction of pores smaller than a given size. For instance, we can easily determine that 20% of the voxels have a size of 18 or larger in the PDF, or 12 or larger in the case of the RDF.

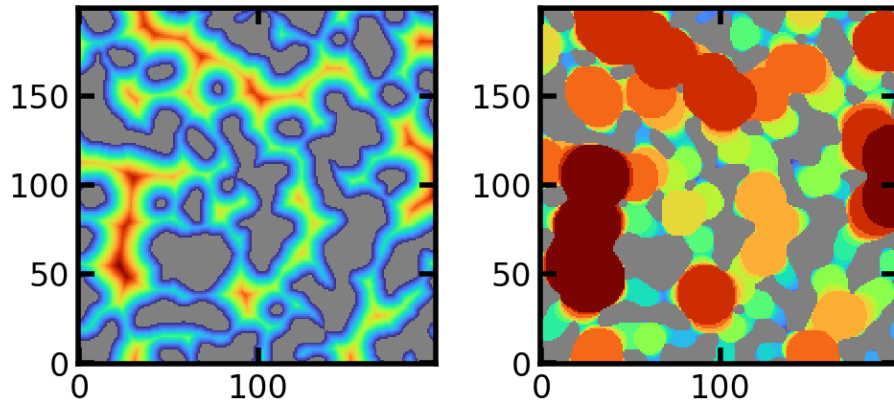


Figure 16 – The resulting 2D images of blobs obtained using the distance transform method (left) and local thickness method (right). The colour of the heat map indicates the size of the measurement, with hotter colours indicating a greater value.

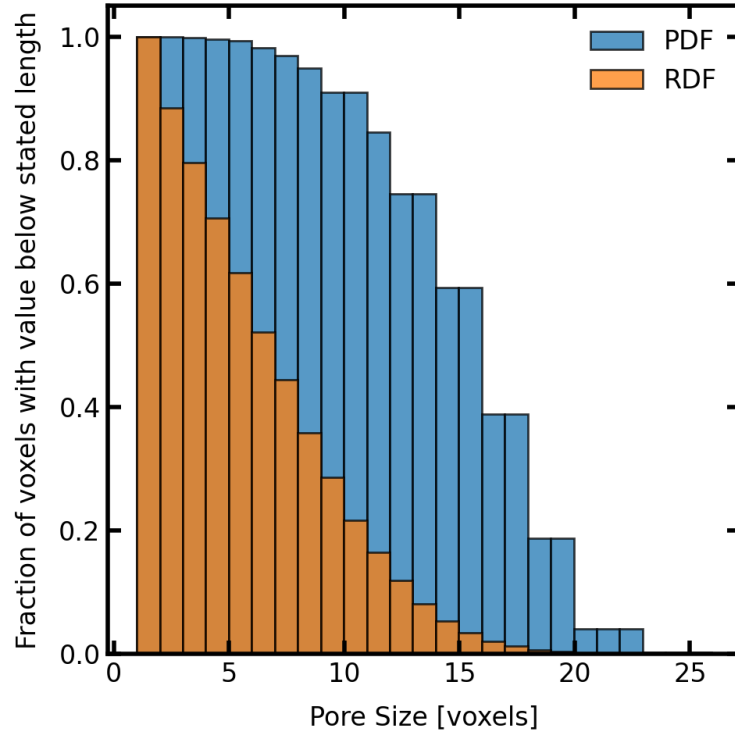


Figure 17 – Plots of cumulative radial density function (orange) and cumulative pore size distribution (blue) for a 3D image of blobs.

The computation of distance transforms is somewhat complicated and has been the subject of much research over the years [38] [39]. Functions for distance transforms are available in most programming systems. Since the local thickness method is not as commonly used, a custom implementation has been developed in this study. The steps are shown in Figure 18. It starts with the application of the distance transform and finding all pixels that are larger than a given size R , as shown in Figure 18b. A circle of radius R centered at each surviving pixel is then drawn to produce the image shown in Figure 18c. This process is repeated for each value of R and spheres are combined into a single image by inserting values of R into a voxel if R is greater than the value currently present to create an array which spans all radii identified within the distance transform. The final result is the one shown in Figure 18d.

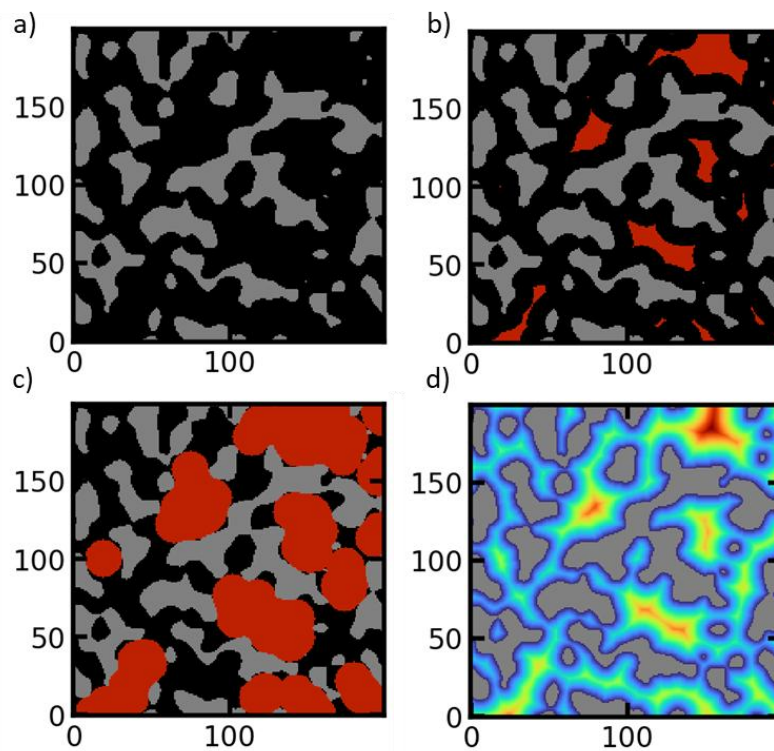


Figure 18 – Steps required to compute a local thickness; a) is the original image, b) depicts the voxels from the distance transform which have value of R or greater, c) draws spheres centered at each voxel identified in b), and d) repeats the sphere drawing process with each unique value identified by the distance transform and overlaps the result, creating a colour map with the hottest colour indicating the greatest value.

4. Results

4.1. REV Plots for Porosity and Tortuosity

The calculated porosity and tortuosity of each block subdomain can be plotted against its normalized volume fraction. The resulting plot is a REV plot for porosity. Figure 20 shows a plot of REV porosity versus $\log_{10} \left(\frac{V_B}{V_T} \right)$ where V_B is the volume of the subdomain and V_T is the total volume of the sample for the image shown below in Figure 19. The x-axis in this plot provides a measure of the volume of the subdomain block.

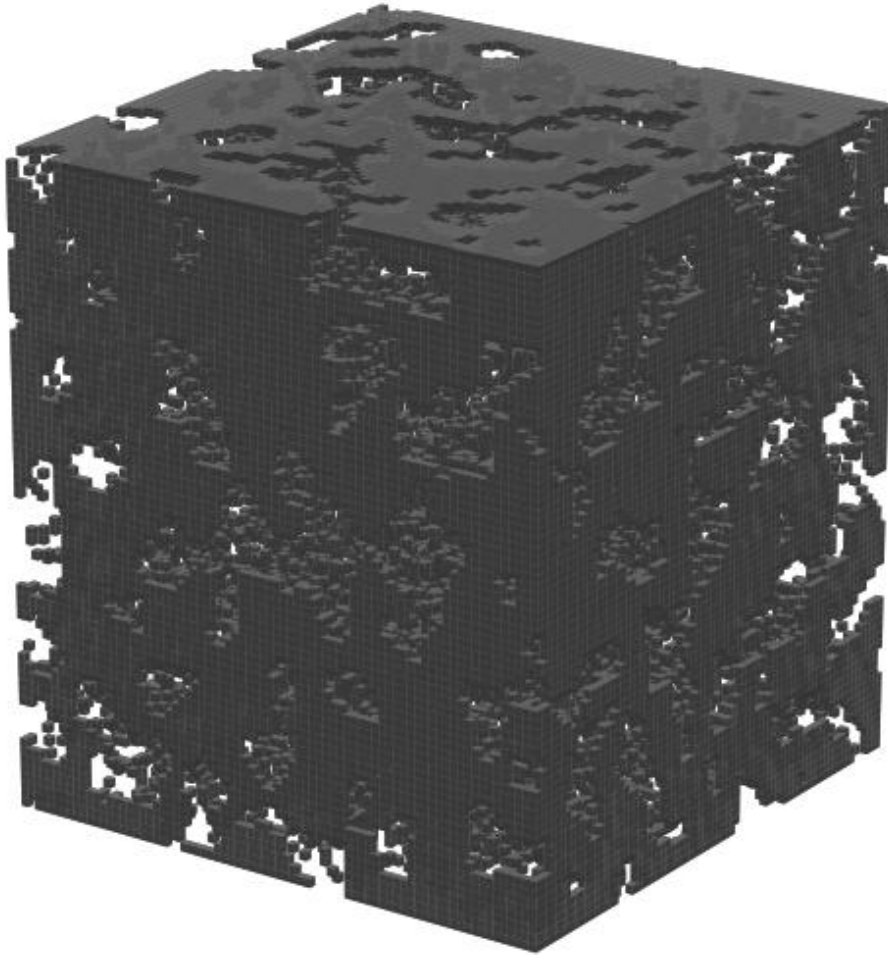


Figure 19 – The sample image of size 300 by 300 by 300 voxels and porosity of 70% characterized for its REV porosity and tortuosity in this study.

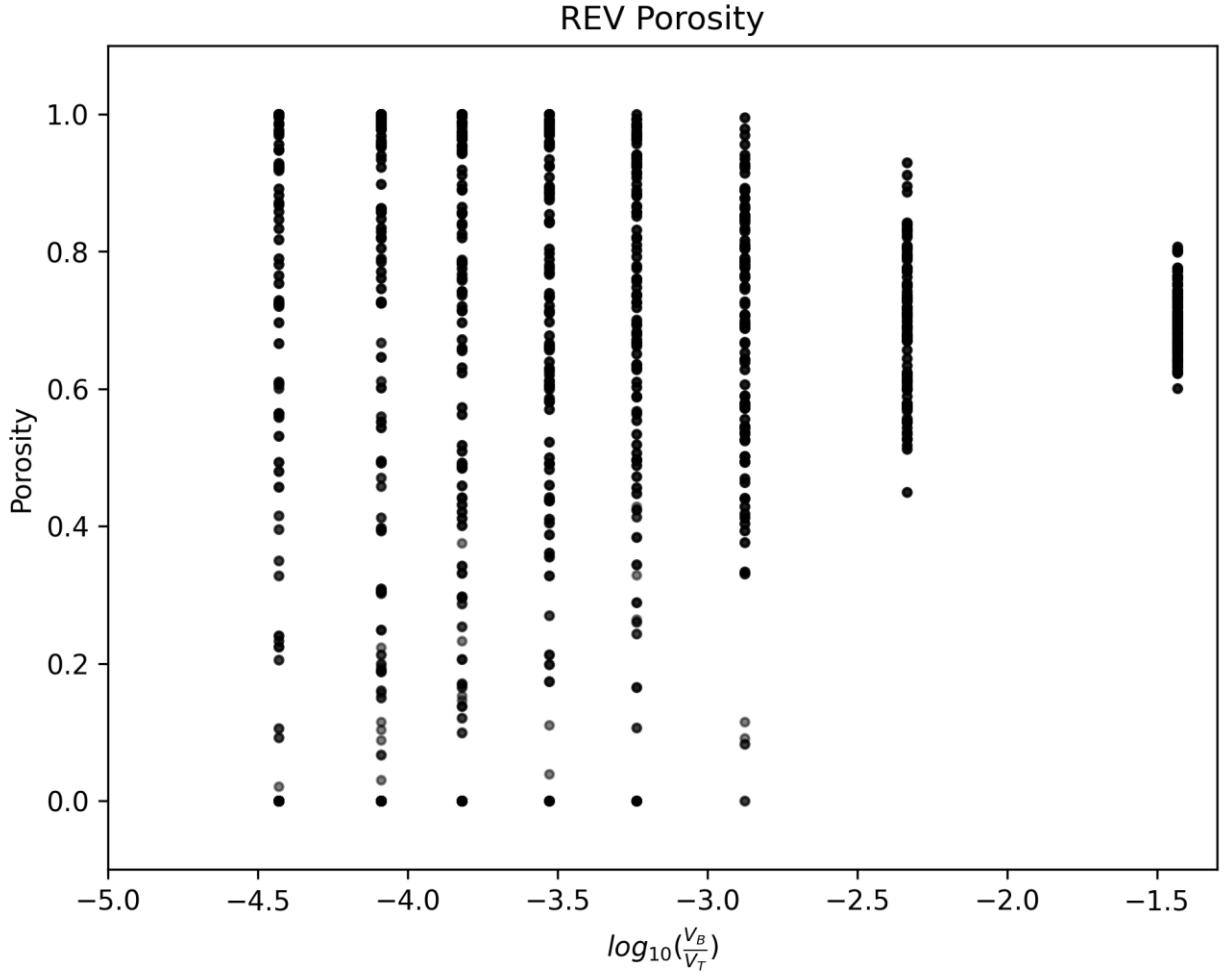


Figure 20 – REV porosity plot for structure shown in Figure 19. Each band corresponds to a subdomain volume of 10^3 , 13^3 , 16^3 , 20^3 , 25^3 , 33^3 , 50^3 , 100^3 from left to right, respectively.

Determining the porosity of blocks is trivial and fast, whereas determining tortuosity is considerably more computationally expensive, as detailed in Section 3.4. To reduce computational demand, the subdomain volumes considered were limited to 10^3 , 13^3 , 16^3 , 20^3 , 25^3 , 33^3 , 50^3 and 100^3 voxels. This restriction results in a plot that exhibits the discrete bands observed in Figure 20 corresponding to the volume of the subdomains that are constrained to be perfect cubes with edge lengths x and volumes x^3 . Alternative methods of generating subdomain volumes that are not limited to cubes or specific subdomain volumes yield more continuous data and “fill in” the gaps in the plot, as illustrated in Figure 21. Future studies may further explore the use of a continuous domain of sub-volumes to determine REV.

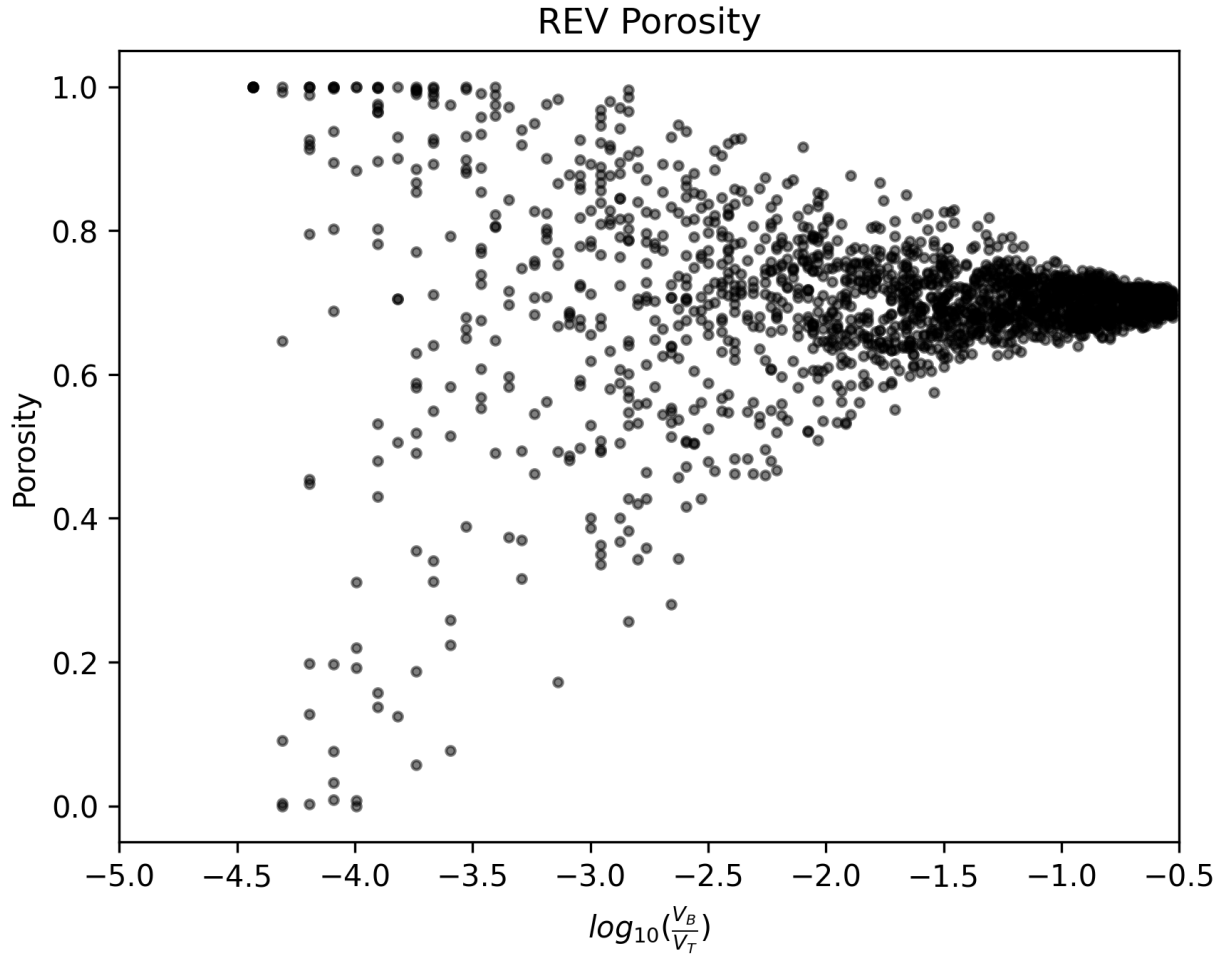


Figure 21 – REV porosity plot for structure shown in Figure 19 obtained using a smoother domain of sub-volumes spanning from 10^3 to 200^3 .

The same procedure can be followed for tortuosity as the metric of interest to yield the resulting REV plot presented in Figure 22. The y-axis has been normalized to $1/\tau$ in this plot since this constrains the range of possible values between 0 and 1 and enables an easier side-by-side comparison with porosity REV plots. Conveniently, subdomains with very high tortuosity values are normalized to be near zero values, but can still be distinguished.

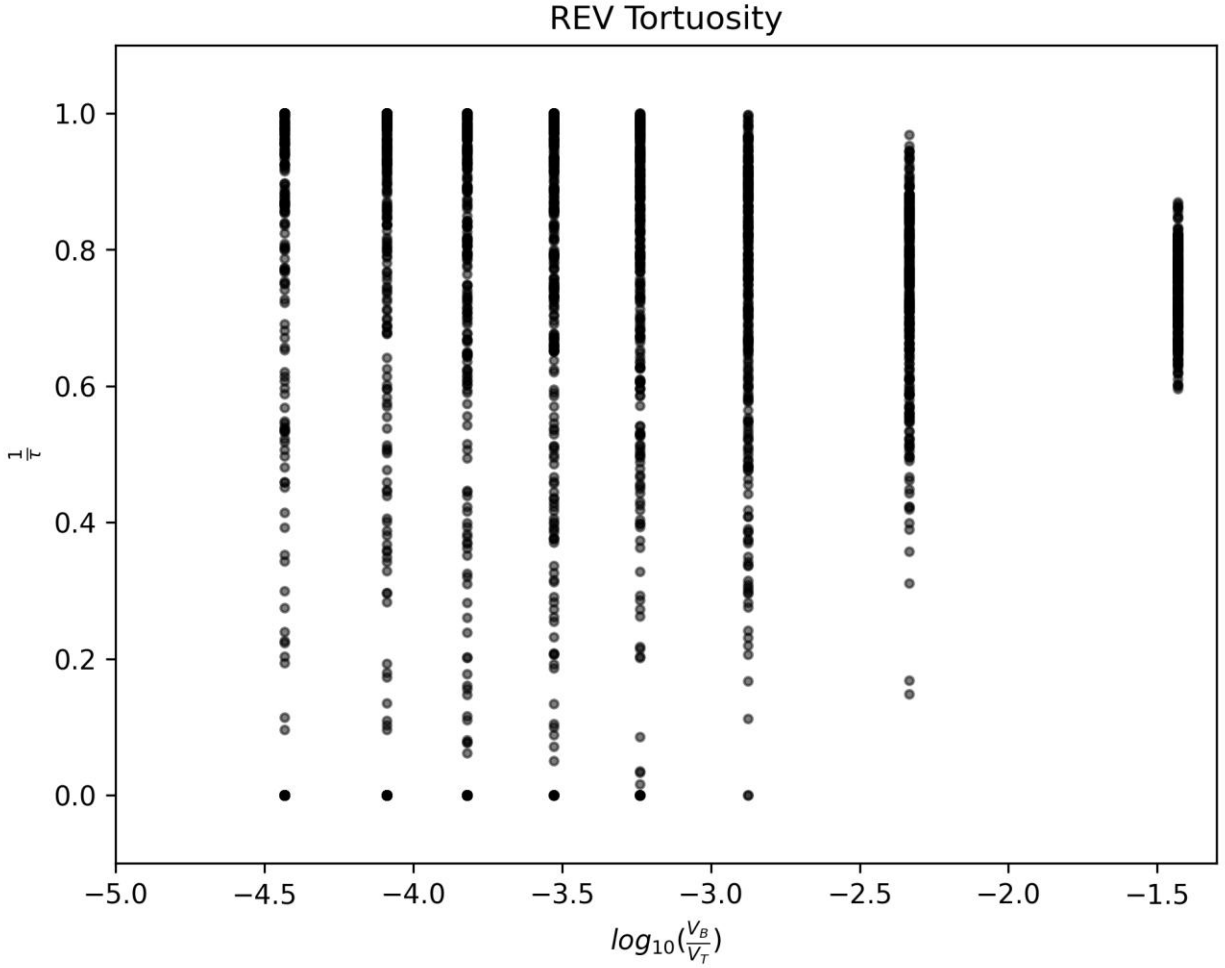


Figure 22 – REV tortuosity plot for Figure 19. Each band corresponds to a subdomain volume of $10^3, 13^3, 16^3, 20^3, 25^3, 33^3, 50^3, 100^3$ from left to right, respectively.

A limitation of the above plot is that the frequency of each measurement is difficult to discern since many data points coincide. An alternative method to present the REV data shown in Figure 23 is as a so-called violin plot which shows the distribution of porosities obtained for each subdomain volume. The colours of each plot are chosen simply for contrast and have no meaning. The amplitude at each point of the distribution gives the density of data points obtained at that subdomain volume.

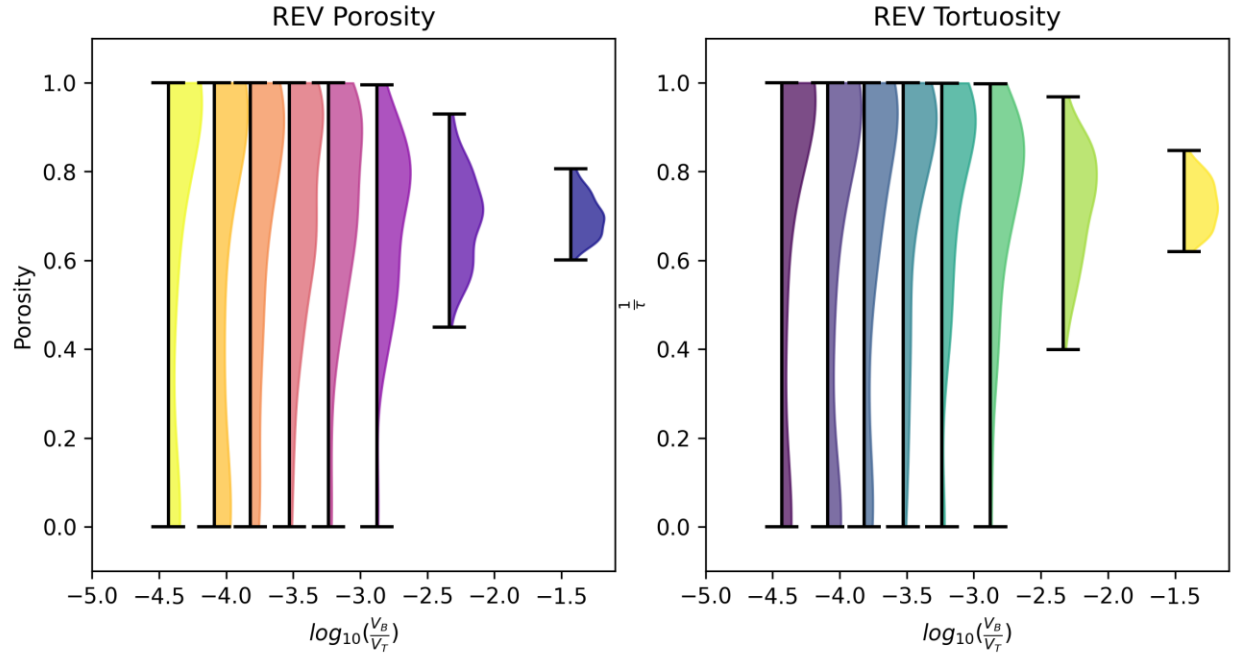


Figure 23 – Violin plots for REV porosity and REV tortuosity data of Figure 19.

To produce a meaningful REV tortuosity plot, certain data points must be filtered out. Data points which do not meaningfully contribute to diffusion across the material should be discarded since they can cause the bimodal behaviour of the tortuosity at $y = \frac{1}{\infty} = 0$. This bimodal behavior occurs from many subdomains being nearly entirely solid, resulting in extremely tortuous paths. Additionally, subdomains which are entirely void space are discarded since the only subdomains of interest are those which contain actual structural information about the original image. An entirely void subdomain may compose a larger subdomain which contains information about the solid phase, but as it could describe any other void volume, the analysis of the block is not necessary. To focus only on subdomains which share characteristics to the original image, subdomains are filtered for porosities which fall within $\pm 20\%$ of the average value, which tends to be the same as the porosity of the original large image. The first two data exemptions are essentially moot at this point, but the justification for excluding the data is necessary. The resulting filtered data are presented below in Figure 24.

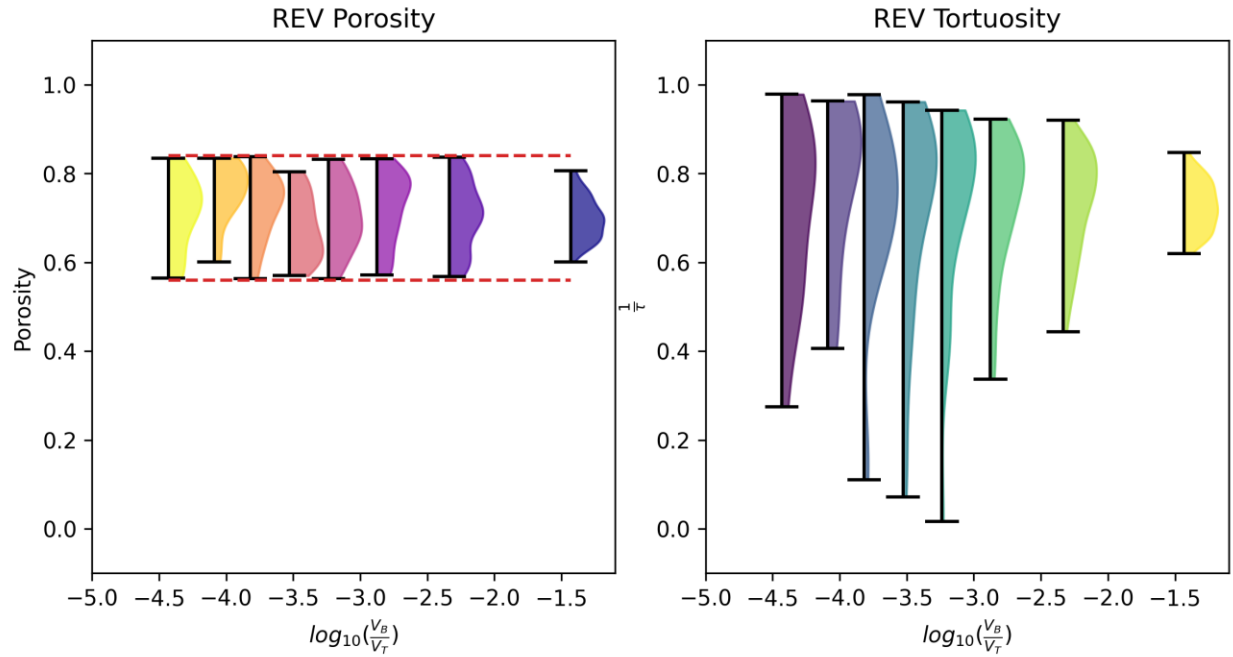


Figure 24 – Violin plots for REV porosity and tortuosity data of Figure 19 after filtering.

The dotted red lines indicate the threshold of $\pm 20\%$. The filtering of the data trims the data points at the extremes ($y = 0$ and 1) of the REV tortuosity plot and eliminates the bimodal behaviour in the resulting distributions.

4.2. Determination of the REV

The conceptual definition of an REV is fairly straightforward as discussed in the Introduction. The REV is the volume above which the measurement of the property of interest becomes stable. However, in practice one must define “stable”. For instance, it could be defined as the average value becoming constant within a certain threshold or the standard deviation between the measured property values shrinking below some value. Essentially, this requires defining a criterion for stability and then defining a threshold value for that criterion to be considered stable. Several criteria have been considered in this study, but a simple definition has ultimately been chosen: an REV is reached when 80% of the randomly selected subdomains are within 20% of the average value. This simple method does not require fitting any distributions or normalizing

data in any way and is easy to understand intuitively. Of course, one could change the specific values for the thresholds to be more or less stringent (i.e. 90% of the points lie with 10% of the average), but the 80-20 rule is used here.

To test this criterion for stability, the images obtained from the work of Blunt and Dong are analyzed in detail below [1]. This involves determining the porosity and tortuosity of randomly located subdomains having different sizes. The fraction of valid subdomains falling within 20% of the average value is then plotted versus $\log_{10}(\frac{V_B}{V_T})$. For the porosity data, 10000 randomly located subdomains are incremented 1 voxel at a time to cover the range in size from 10^3 to 100^3 voxels and analyzed at each interval. In the case of the tortuosity measurement, the subdomain sizes considered are $10^3, 13^3, 16^3, 20^3, 25^3, 33^3, 50^3$ and 100^3 and 100 randomly located subdomains are selected for each subdomain size. These sizes are selected to provide sufficient datapoint density, while maintaining reasonable image processing times. Selected images of interest of samples A1, C1, S1 and S6 are discussed in detail in this section here. The remaining image renderings and associated property plots of the other samples examined in this study are included in Appendix D Excluded Image Montages.

4.2.1. Image A1 - Sandpack

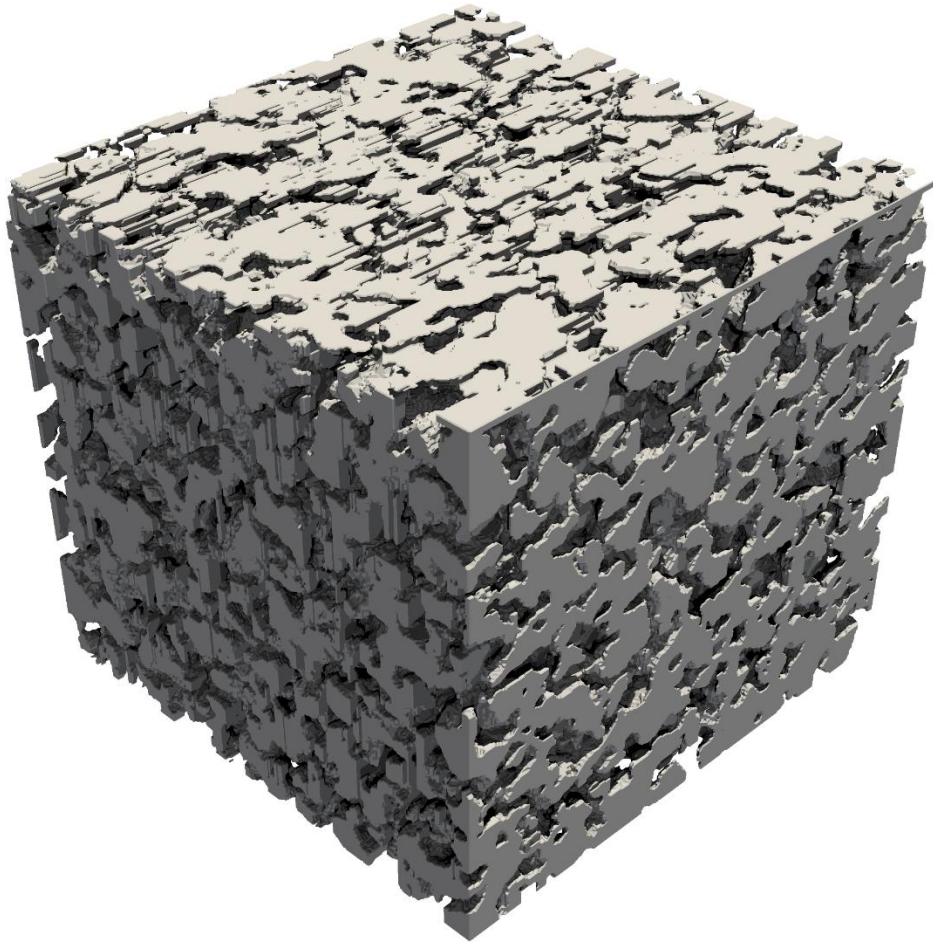


Figure 25 – 3D rendering of sample image A1.

Image A1 has the dimensions of $300 \times 300 \times 300$ voxels. The REV data for A1 are presented in Figure 26 and Figure 27. Only the tortuosity in the x-direction is shown in Figure 27 since the sample is isotropic. Despite its appearance, sample A1 has not been assumed to be isotropic. Detailed analysis of this sample in all three directions has been conducted and confirms its relatively isotropic nature with respect to tortuosity.

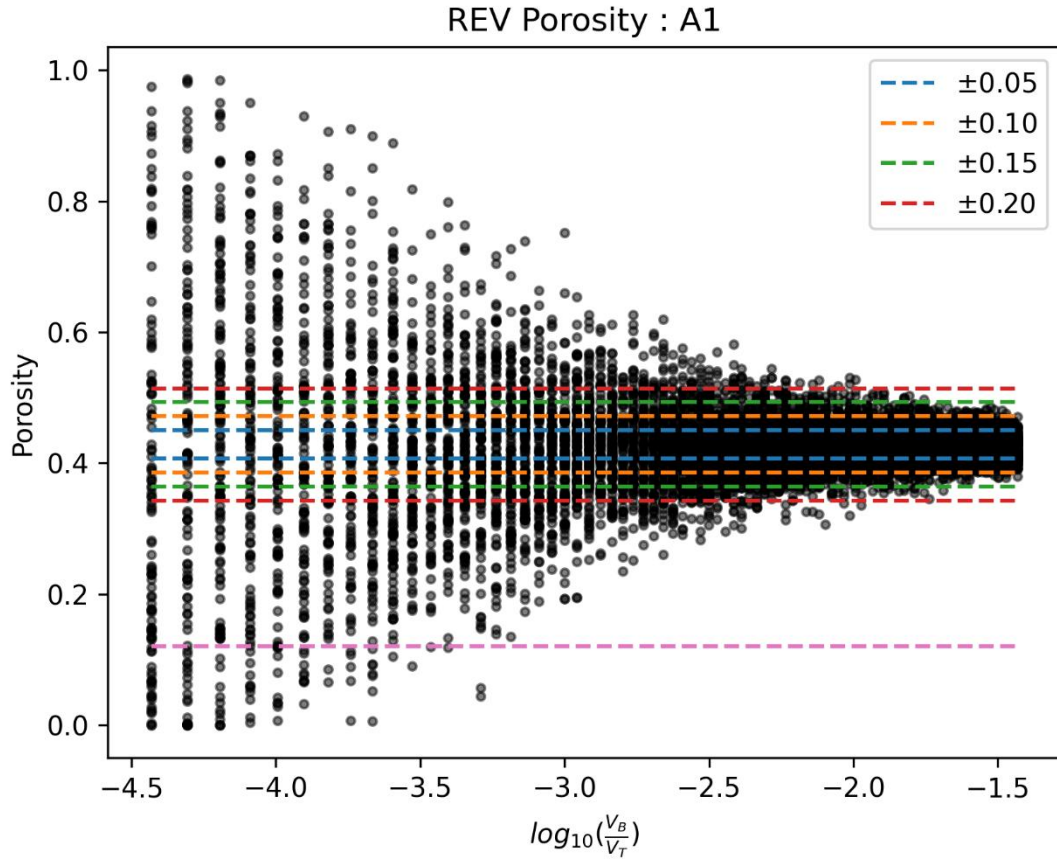


Figure 26 – REV porosity data for image A1.

Due to the large quantity of data to be presented, a simple scatter plot is simpler to interpret than a violin plot. These are incorporated with the violin plots in Figure 26 and 27. Each pair of matching colour dashed lines represents the upper and lower bounds imposed by the threshold, with the red lines representing $\pm 20\%$ of the average porosity, green lines representing $\pm 15\%$, orange lines representing $\pm 10\%$, and blue lines representing $\pm 5\%$. The percolation threshold is also plotted as the pink dashed line. From visual inspection, it is clear that the relative number of points within the thresholds increases as the subdomain volume size increases. The precise volume size where this occurs can be determined by plotting the frequency f of points within the threshold against the normalized volume fraction. This is shown for both porosity and tortuosity in Figure 28.

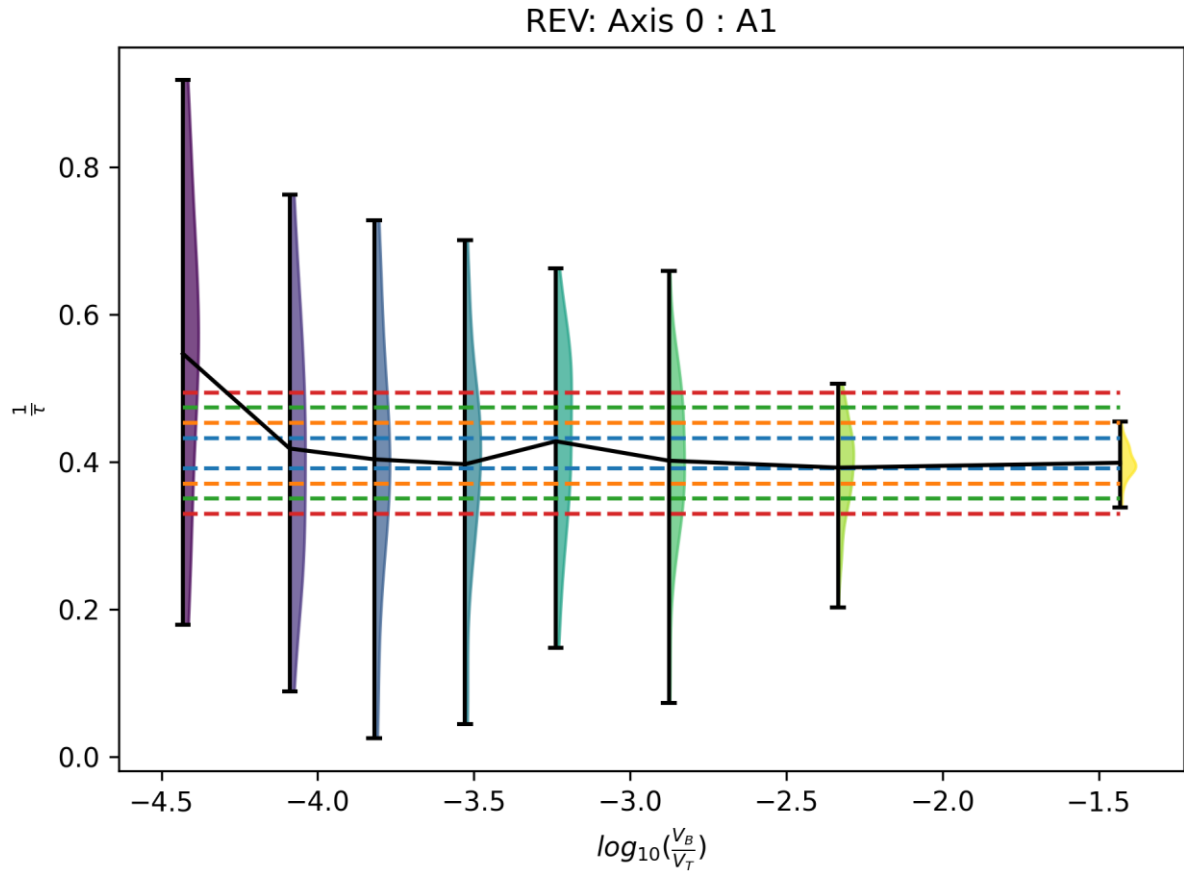


Figure 27 – REV tortuosity data for the x-axis on image A1.

Figure 27 has similar features to that of Figure 26 with one notable difference. The black line indicates the mean value of $1/\tau$ within each data bin. An attempt has been made to determine the convergence criterion based on the stability of this value. However, as will be shown with the next sample, stability is not guaranteed in every case. The same analysis can be performed on the REV tortuosity data. It is only for the two largest subdomains that the majority of the points lie within the thresholds.

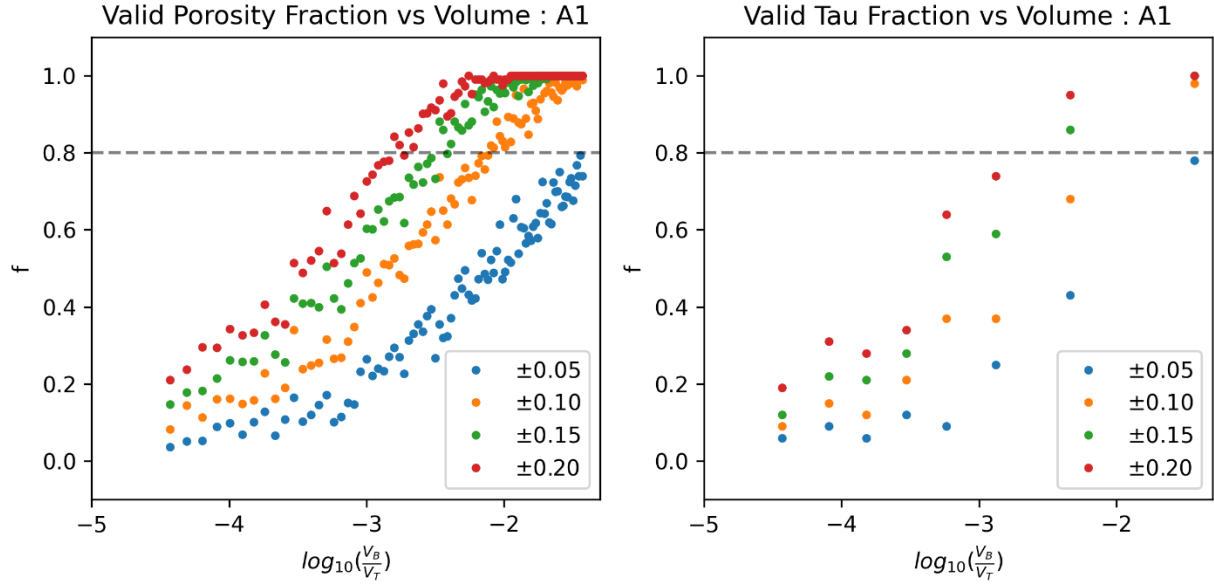


Figure 28 – Frequency of adherence to criteria vs normalized volume of subdomain for image A1.

Each colour of data series corresponds to a specific threshold value. From visual inspection, the smallest volume of subdomain which complies with the criterion occurs at $x = \sim -2.8$ and $x = \sim -2.5$ for porosity and tortuosity respectively, which corresponds to a subdomain volume of approximately 35^3 voxels and 44^3 voxels. Convergence for porosity is fast since small volumes relative to the whole volume accurately represent the bulk porosity. At larger subdomain volumes, the majority of subdomains account for the bulk porosity, regardless of the threshold value.

4.2.2. Image C1 - Carbonate

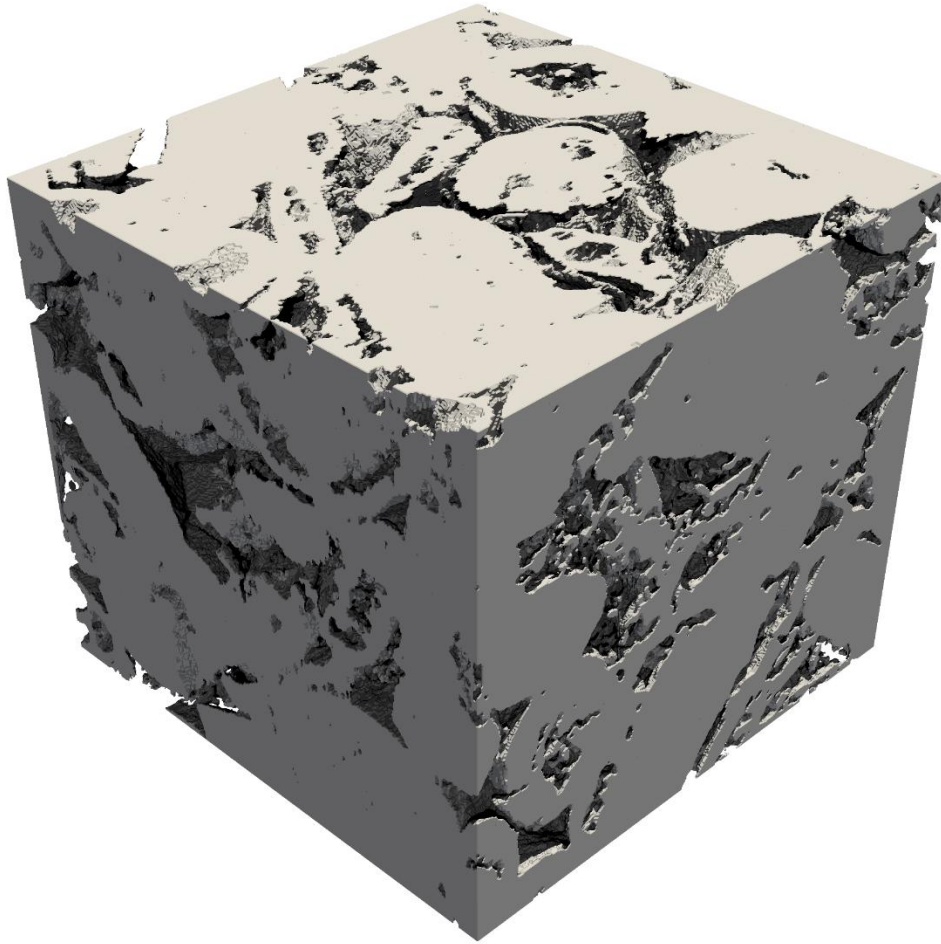


Figure 29 – A 3D rendering of sample image C1.

Image C1 has the dimensions of $400 \times 400 \times 400$ voxels. The REV data for C1 are presented in Figure 30 and Figure 31. Similar to the previous sample, only data regarding the REV tortuosity along the direction of axis 0 is shown as the properties along the other directions are not significantly different.

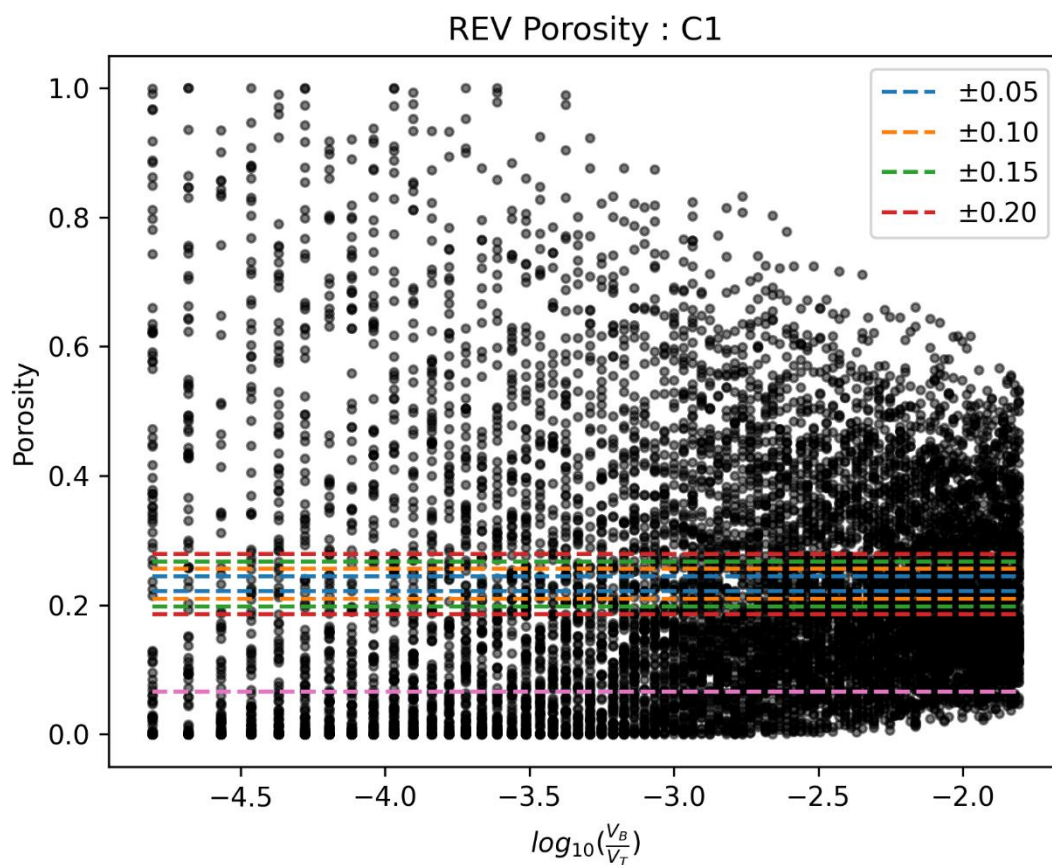


Figure 30 – REV porosity data for image C1.

The REV porosity data in Figure 30 display very different behaviour than that of image A1. While the measured porosities are converging toward a single value as the subdomain volume increases, the rate with which it does so is very slow.

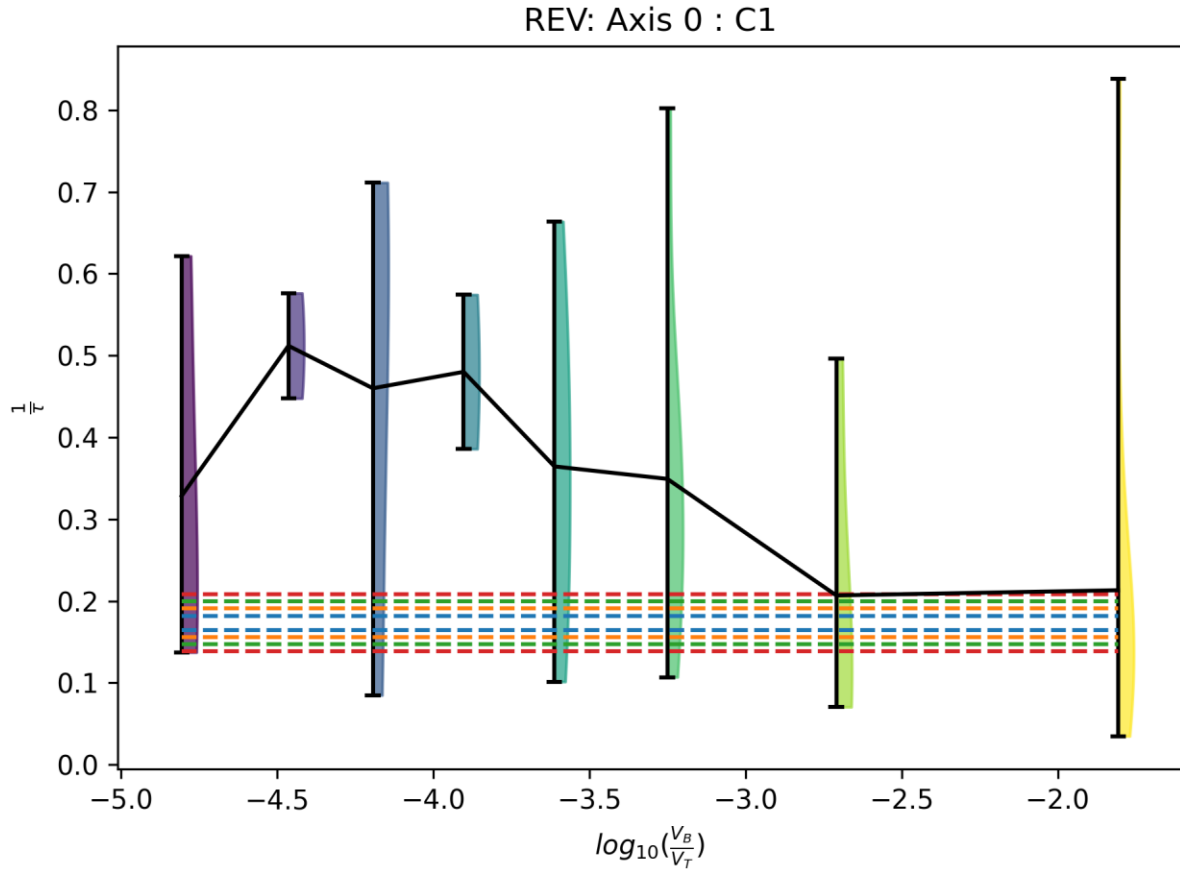


Figure 31– REV tortuosity data for the x-axis on image C1.

After filtering for relevant porosity subdomains, the tortuosity of the remaining blocks is distributed fairly evenly within each bin, as indicated by the data bins showing no strong preference for any particular value at smaller subdomain volumes (Figure 31). It is worth noting that the apparent narrowing of threshold values is misleading.

The average tortuosity value becomes stable in the final two tested subdomain volumes, which may indicate the existence of a reasonable REV. However, the mean (black line) lies outside of all of the specified thresholds and so it fails our definition of attaining the REV, as is also evident in Figure 32. All data series fail to meet the REV criteria although the trend of increasing frequency as the subdomain size increases is still observed. Logically, this suggests that the true REV size is

larger than the largest tested subdomain volume and may be substantially larger than the entire image, indicating that this structure may not have a REV.

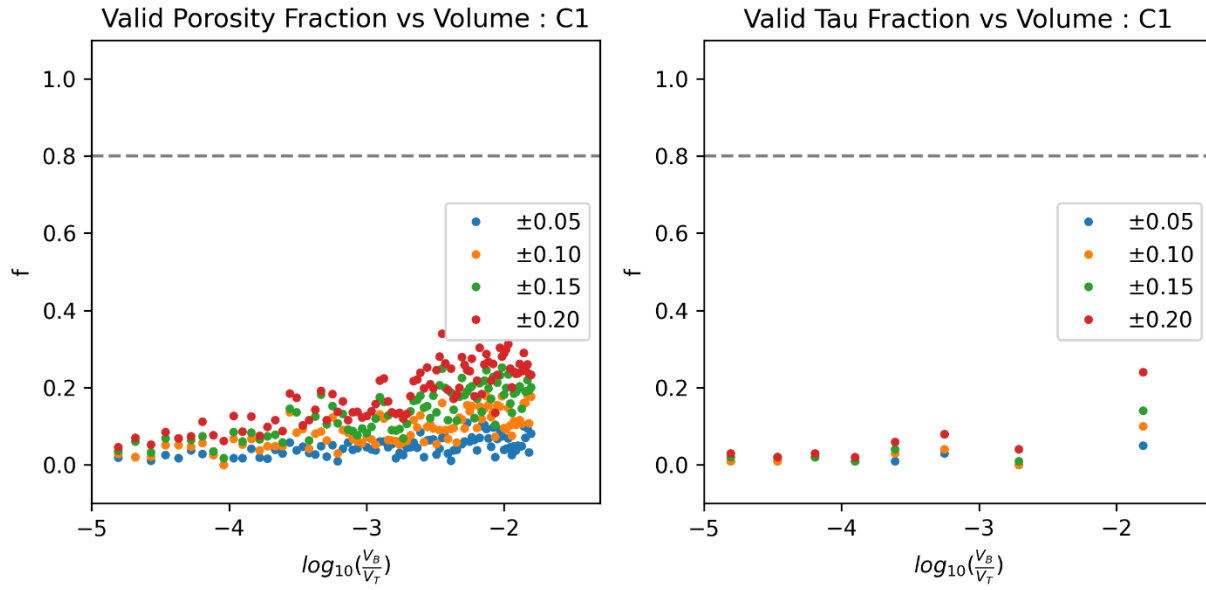


Figure 32 – Frequency of adherence to criteria vs normalized volume of subdomain for image C1.

4.2.3. Image S1 - Sandstone



Figure 33 – A 3D rendering of sample image S1.

Image S1 has the dimensions of $300 \times 300 \times 300$ voxels. The REV data for S1 can be seen in Figure 34 and Figure 35. As with the previous samples, only REV tortuosity information for axis 0 is shown as the properties along the other directions exhibit no significant differences.

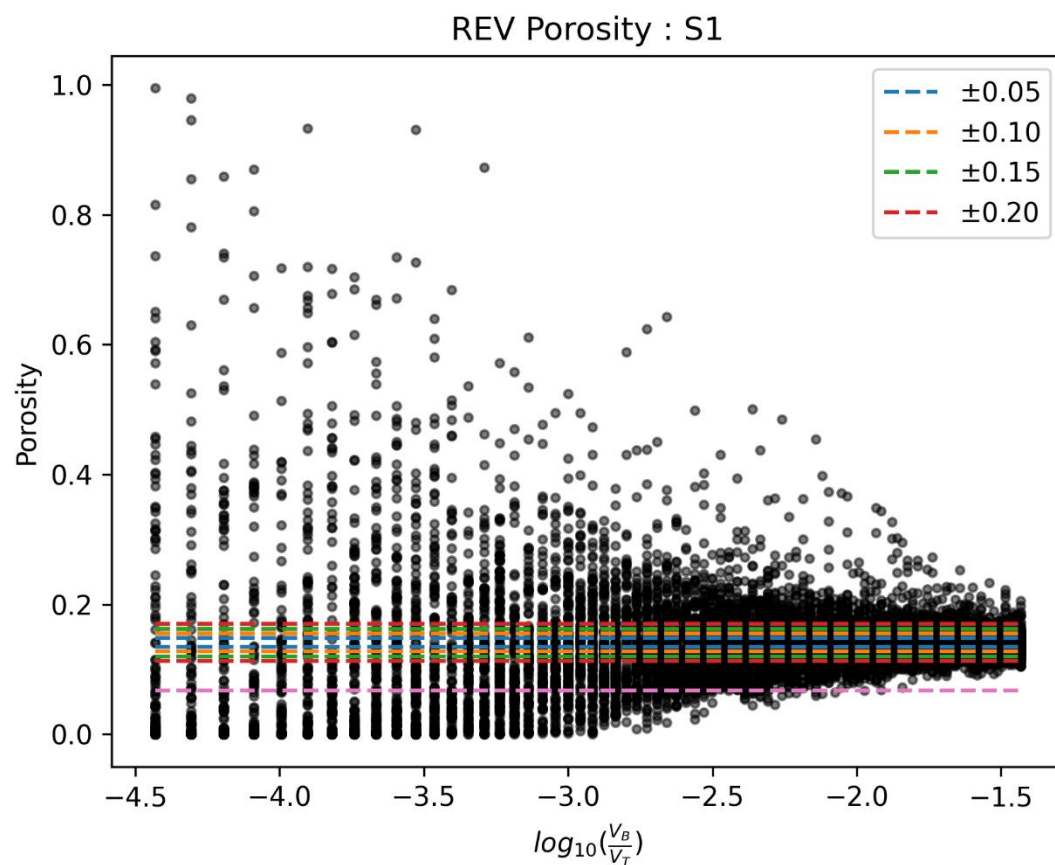


Figure 34 – REV porosity data for image S1.

From Figure 34, the porosity of S1 appears to converge toward the true value of 0.141. The percolating threshold is calculated to be 0.07 so this image sample can be considered “far” from disconnecting after a phase of dilations as described in Section 3.2.

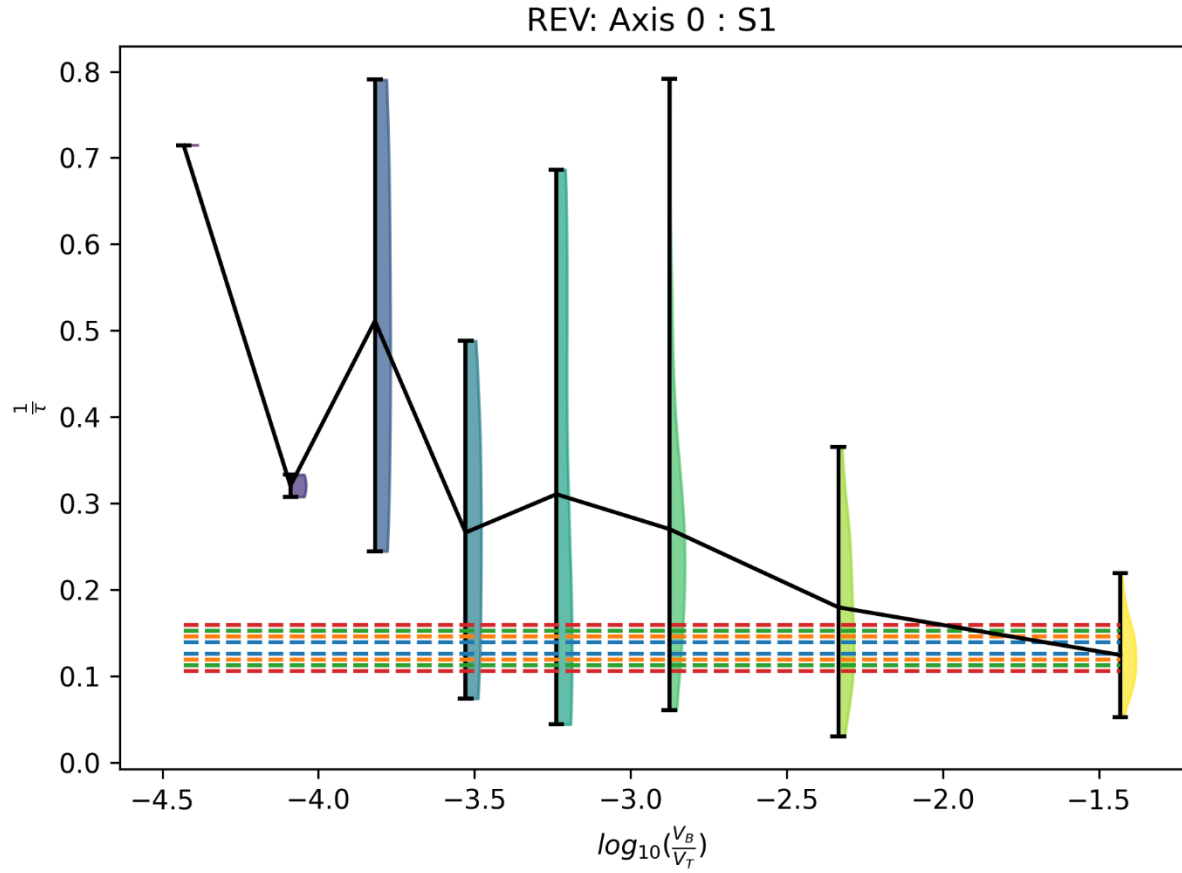


Figure 35 – REV tortuosity data for the x-axis on image S1.

The bins for the REV data do not contain a large amount of data points due to the filtering described in Section 4.1. However, this appears to only affect the smallest sampled subdomain since the remaining bins show the expected behaviour of converging to a single average value. Most of the tortuosity data points within the largest tested subdomain fall within the applied threshold, as evident in Figure 36 (right). The average tortuosity value within each tested volume does not stabilize, but a reasonable REV exists for this image, as seen in Figure 36.

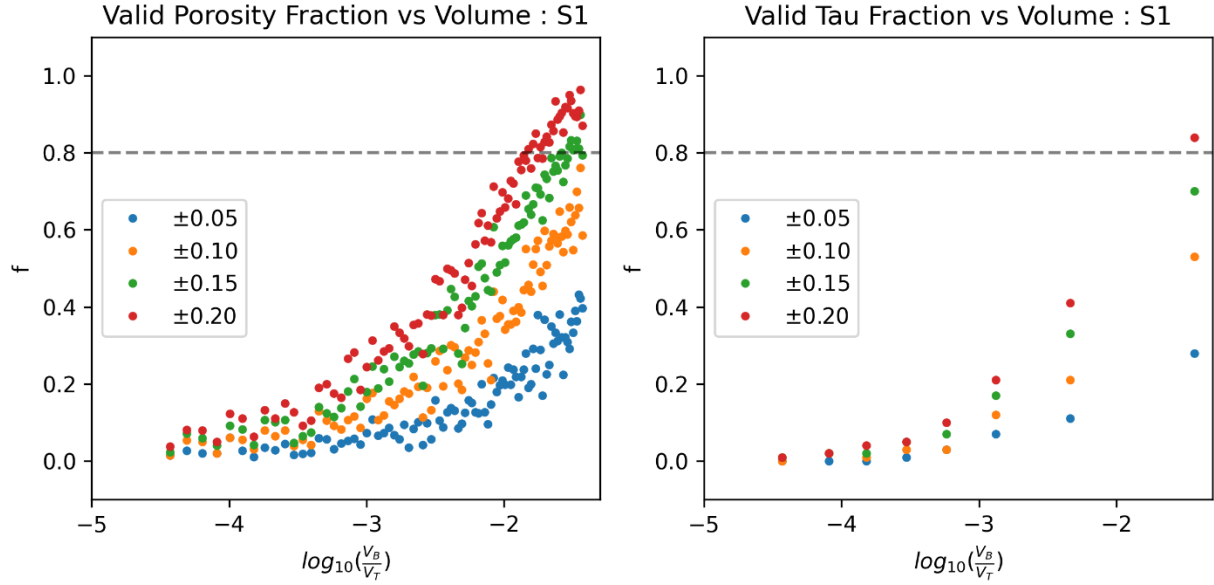


Figure 36 – Frequency of adherence to criteria vs normalized volume of subdomain for image S1.

From Figure 36, the minimum subdomain volume which adheres to the criteria are 70^3 and 99^3 for porosity and tortuosity, respectively. Although S1 has the lowest porosity within the dataset, the data yield a valid REV for both characteristics. The existence of a reasonable REV size must therefore be dependent on factors in addition to the porosity of the image, which will be discussed in section 4.3.

4.2.4. Image S6 - Sandstone

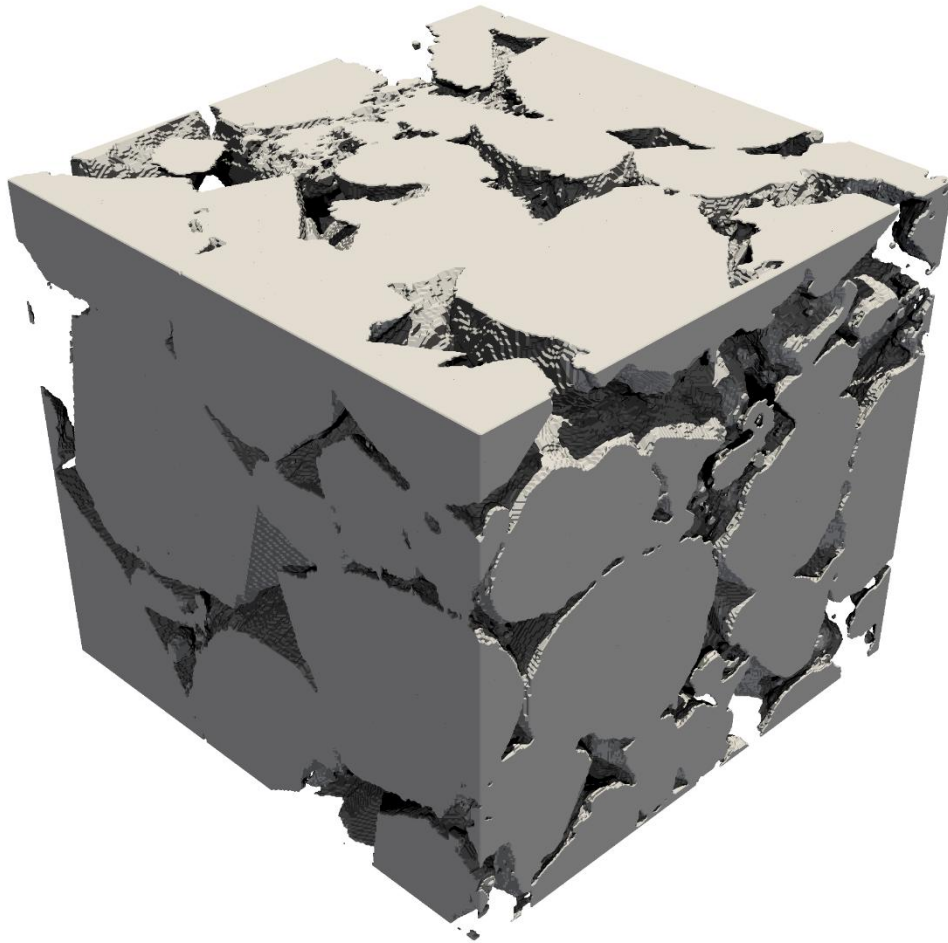


Figure 37 – A 3D rendering of sample image S6.

Image S6 has the dimensions of $300 \times 300 \times 300$ voxels. The REV data for S6 can be seen in Figure 34 and Figure 35. As with the previous samples, only REV tortuosity information for axis 0 is shown as no significant difference is observed in the other directions.

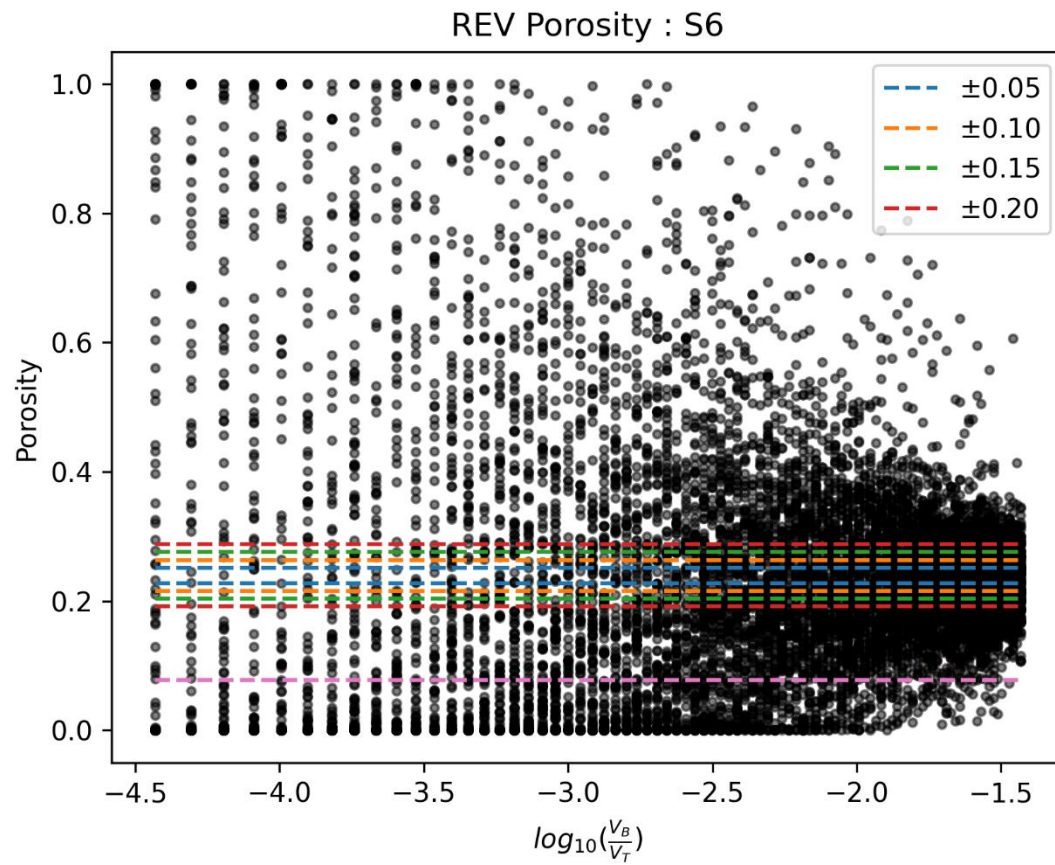


Figure 38 – REV porosity data for image S6.

The REV porosity plot for S6 is similar to that of C1, where the data vary over a large range even at the largest tested subdomain. This indicates that no REV in porosity is obtained for the data shown here, as also in Figure 40.

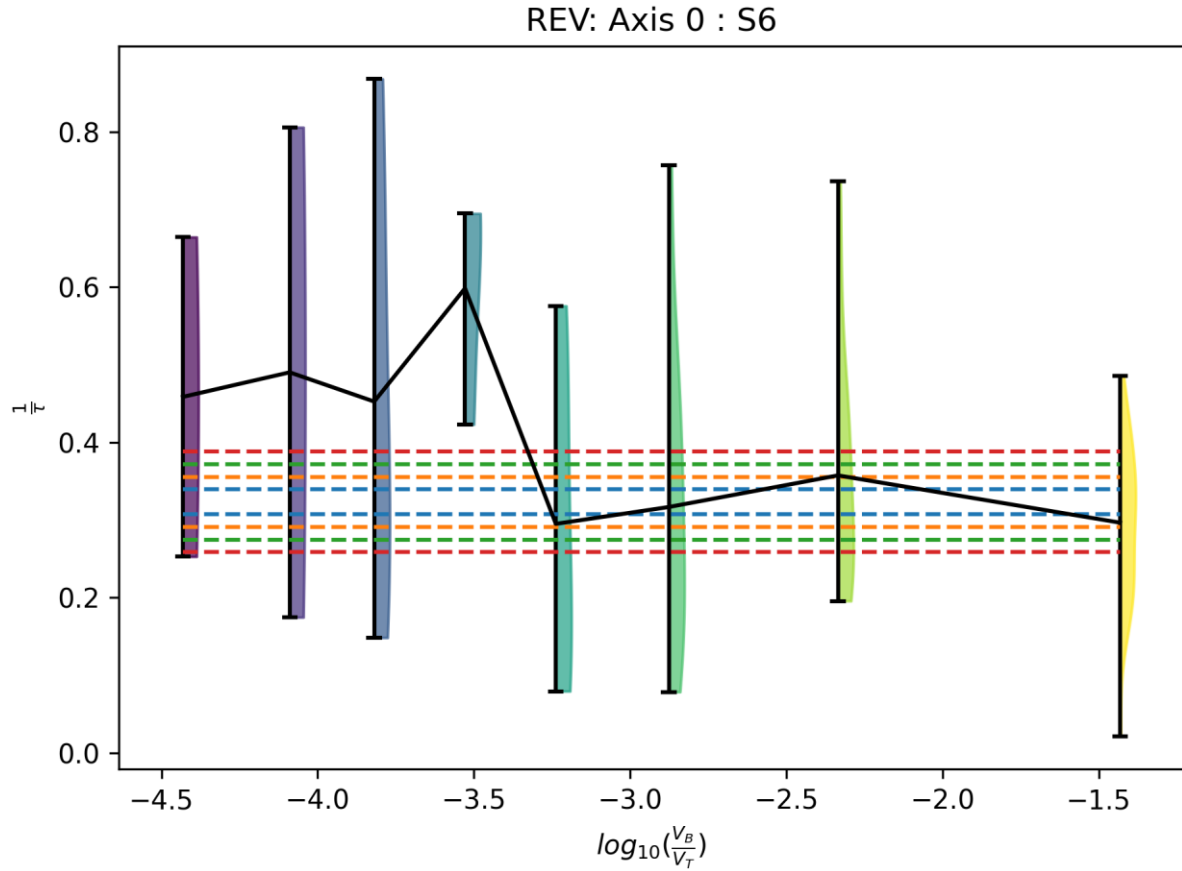


Figure 39 – REV tortuosity data for the x-axis on image S6.

The REV tortuosity data are similar to that of S1 in that the smaller subdomains show no particular bias to any given value. The mean value for tortuosity stabilizes and remains within the thresholds in the higher volume subdomains. This may indicate increasing statistical self-consistency in that each randomly selected subdomain is more likely to have the same tortuosity. However, in contrast to the previous example, even the average value does not appear to be stabilizing.

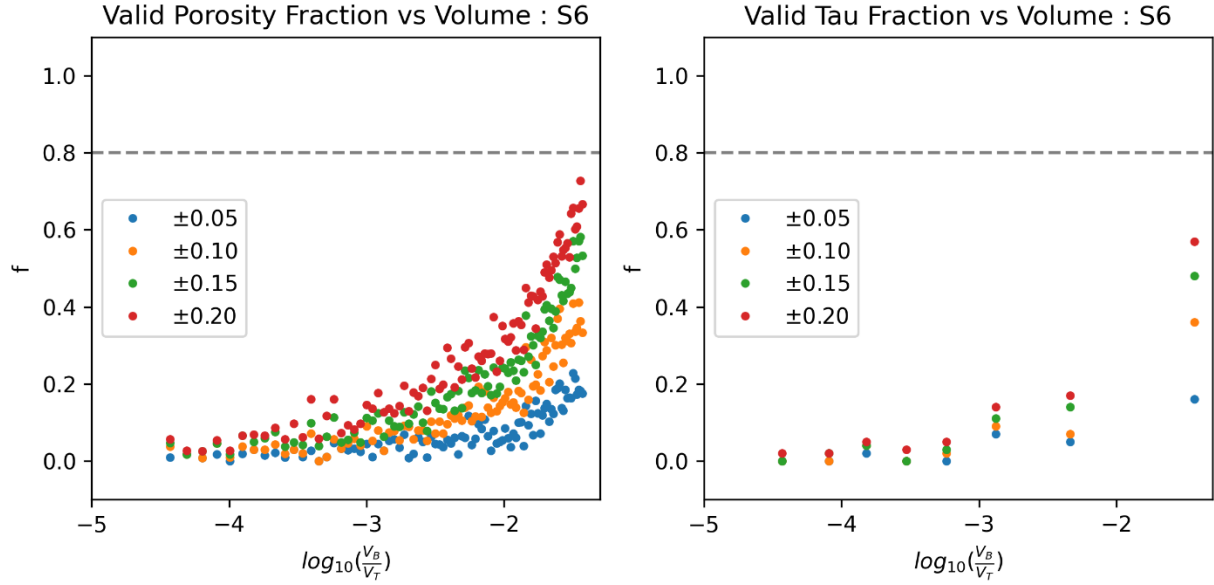


Figure 40 – Frequency of adherence to criteria vs normalized volume of subdomain for image S6.

From Figure 40, an REV for porosity or tortuosity is not found, but both properties clearly appear to be converging as the subdomain volume increases. Following the previous examples, the porosity of the original image is “far” from disconnecting after a phase of dilations, with $\varepsilon = 0.24$ and $\varepsilon_p = 0.08$, indicating again that other factors must contribute to determining the REV.

A summary of the above results and images not shown here can be found in Table IV, which gives the image subdomain size at which an REV is reached according to the 80-20 criteria. A “—” indicates that an REV is not obtained.

Table IV – Summary of minimum subdomain volume size to remain within threshold of 20%.

Sample Name	Convergence Size	
	Porosity	Tortuosity
A1	35 ³	44 ³
C1	—	—
C2	—	—
S1	70 ³	99 ³
S2	55 ³	65 ³
S3	48 ³	95 ³
S4	41 ³	88 ³
S5	—	—
S6	—	—
S7	95 ³	95 ³
S8	60 ³	65 ³
S9	—	—

From these data, no connection is evident between adhering to criteria for porosity and tortuosity REV. The size at which the data converge to an REV for porosity does not correlate with the size at which the REV for tortuosity is attained, although the size at which the REV for tortuosity is always greater than or equal to the corresponding size for porosity.

4.3. Prediction of the Existence of an REV From Structural Information

One reason as to why some images may pass while others fail the REV criterion is that some images have relatively large pores so that small block sizes do not properly capture the void space. This effect can be quantified by measuring the average pore size of the images obtained from pore size distribution information. In order to classify an image based on its average pore size, we coin the term “size value” denote it as S . This quantity is defined as the diameter which 90% of pores are equal to or smaller in size. From the cumulative density function, this can be obtained through visual inspection by extending a horizontal line at $y = 0.1$ and determining the pore diameter in voxels. An example of this determination for image A1 in Figure 41 yields a size of 7.5 voxels.

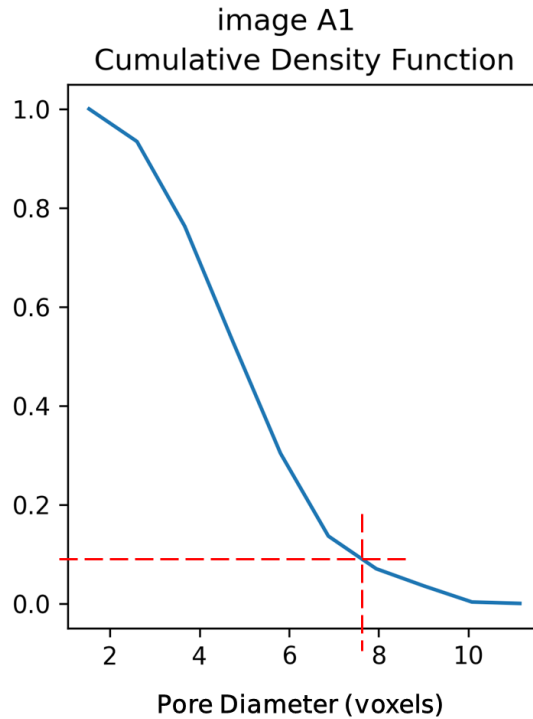


Figure 41 – Pore size distribution for sample image A1 [32]. The red dashed lines intersect at $y = 0.1$ and approximately $x = 7.5$.

While larger values of S generally imply wider pores and may increase the likelihood of pore overlap and interconnection, this metric alone does not directly measure their connectivity. Since

connectivity is dependent on pore size, arrangement and abundance of throats, two porous materials with the same average pore size can exhibit vastly different levels of connectivity. Figure 42 shows the pore size distribution for image C1 which does not yield an REV based on the criteria defined in this study.

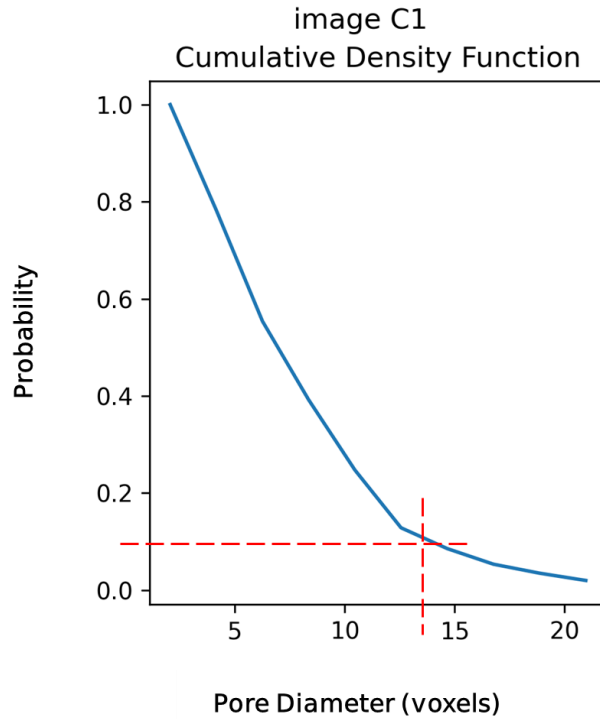


Figure 42 – Pore size distribution for sample image C1 [32]. The red dashed lines intersect at $y = 0.1$ and approximately $x = 11.5$.

Since S alone describes pore size, and not connectivity, it is not sufficient to indicate if an REV exists, so the effect of other parameters has been investigated. An obvious choice is the percolating porosity that has been obtained for all samples using the method described previously. However, the use of this property alone is also inconclusive, as it only provides detail regarding connectivity. When considering both S and the percolating porosity together a trend begins to emerge. This is evident from Figure 43 which shows a plot of percolating porosity normalized by sample porosity versus the size factor S . Each data point is colored according to whether or not an REV could be found in the image (green indicates adherence to the criteria for

REV porosity and REV tortuosity defined in this study, whereas denotes non-adherence) and a clear trend emerges.

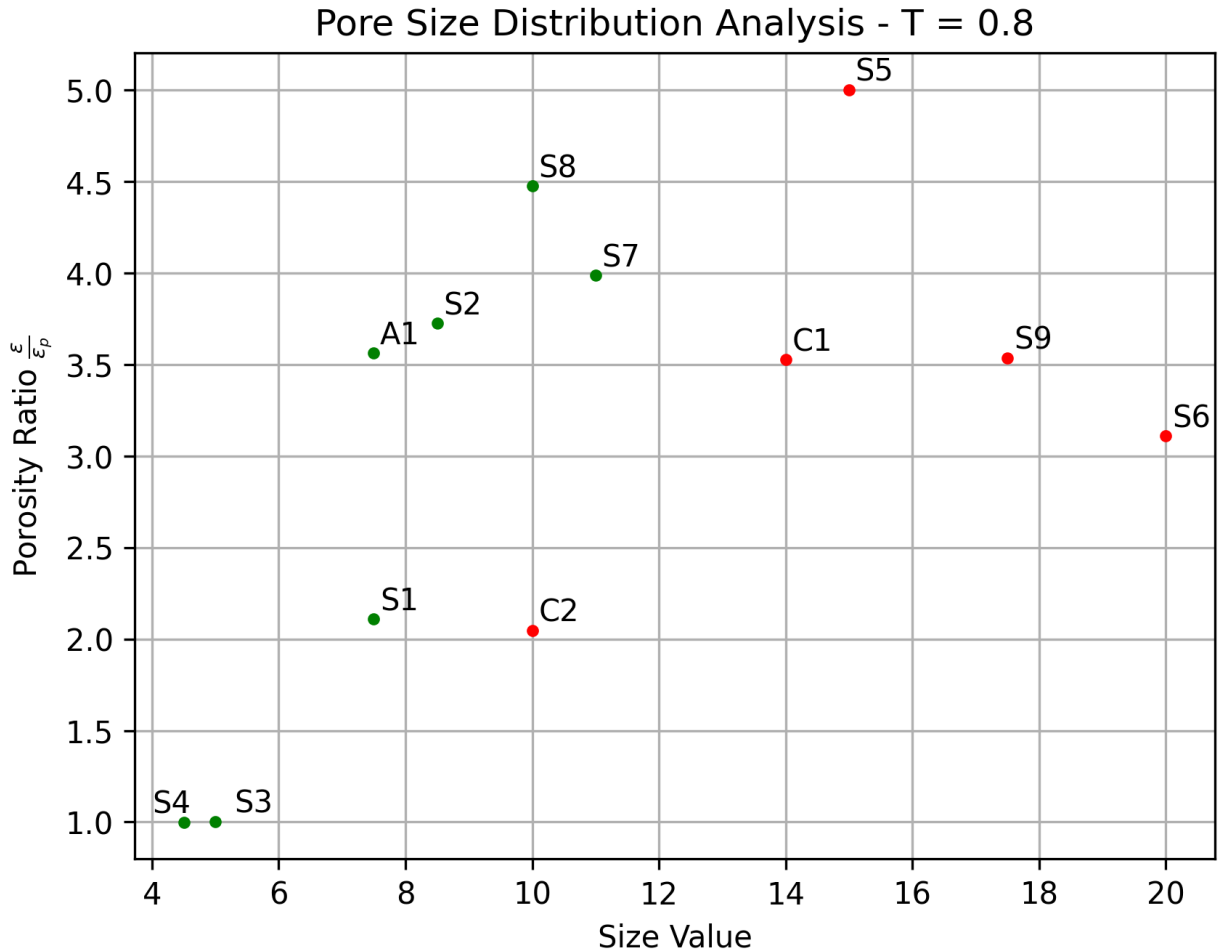


Figure 43 – Porosity ratio versus size value S for all samples examined in this study. Points in green indicate images that adhere to criteria for REV porosity and REV tortuosity defined in this study, while red points correspond to those images that do not adhere to these criteria.

Images exhibiting an REV fall in a region in the upper left portion of the graph in Figure 43. On the other hand, images with high size values ($S > 12$) contain relatively large pore diameters which tend not to fit entirely within small volume subdomains. Conversely, images with smaller average pore sizes are more readily contained within smaller subdomain volumes for REV. Of the subdomain volumes tested, the data for image S4 converge at the largest tested volume with a

fractional frequency of 0.87. However, due to its small size, the larger subdomain volumes can capture the low connectivity of its structure and accurately reflect its bulk transport properties. At the other extreme, image S6 contains the largest sized pores among those tested here, making it difficult for an REV to be determined using the criteria defined in this study. Sample C2 is an interesting case since it does not meet the REV criteria but has a smaller size factor than S7 which does meet the criteria. However, its percolating porosity is much lower than most of the other samples, suggesting that both parameters play a role.

In summary, this analysis reveals that images with low to moderate size values and a high porosity ratio are most likely to meet the REV criteria defined above and that small images with small pores can offset the effect of having low porosity ratios.

5. Tortuosity versus Image Resolution

The accuracy of tortuosity measurements is inherently tied to the resolution of the underlying image data. Since tortuosity describes the complexity of transport pathways through a porous medium, it is sensitive to the level of structural detail captured. For this reason, it is preferable to use high resolution images that preserve fine-scale pore features and connectivity, enabling more precise characterization. However, high resolution images require relatively small fields of view and are susceptible to failing REV tests. It is worth considering whether lower resolution images with larger fields of view could suffice to simulate tortuosity. Thus, we have investigated the relationship between image resolution and tortuosity by systematically reducing image fidelity and assessing how the resulting measurements deviate from those obtained at full resolution by zooming the original image. This is analogous to obtaining lower resolution images.

Figure 44 presents various selected downscaled versions of the same image, with a) representing the original image. As the resolution is reduced, the original structure remains but some of the fine details of the solid phase are lost or distorted.

Figure 45 a) depicts the calculated tortuosity of the resulting images at the various scales with missing datapoints since the resulting image is unable to percolate due to the zoom. The scale represents the percentage of the original resolution used for generating the zoomed image. Given that this downscale of the resolution has been conducted on a 2D image, it provides fewer paths for diffusion and yields a higher tortuosity than would be the case in the real 3D sample from which the image has been obtained. Figure 45 b) depicts the same information for a different 3D image sample.

In both cases, tortuosity is overestimated at the coarsest resolutions, but the values rapidly converge toward the true reference point as the zoom scale increases. Importantly, beyond a zoom scale of 0.2 – 0.3, the estimates stabilize and remain within about 5% of the true value, even when the image has been substantially downscaled. This suggests that such an analysis could be based on much larger images which do not necessarily capture the finer details of the void space but would still be useful for estimating tortuosity.

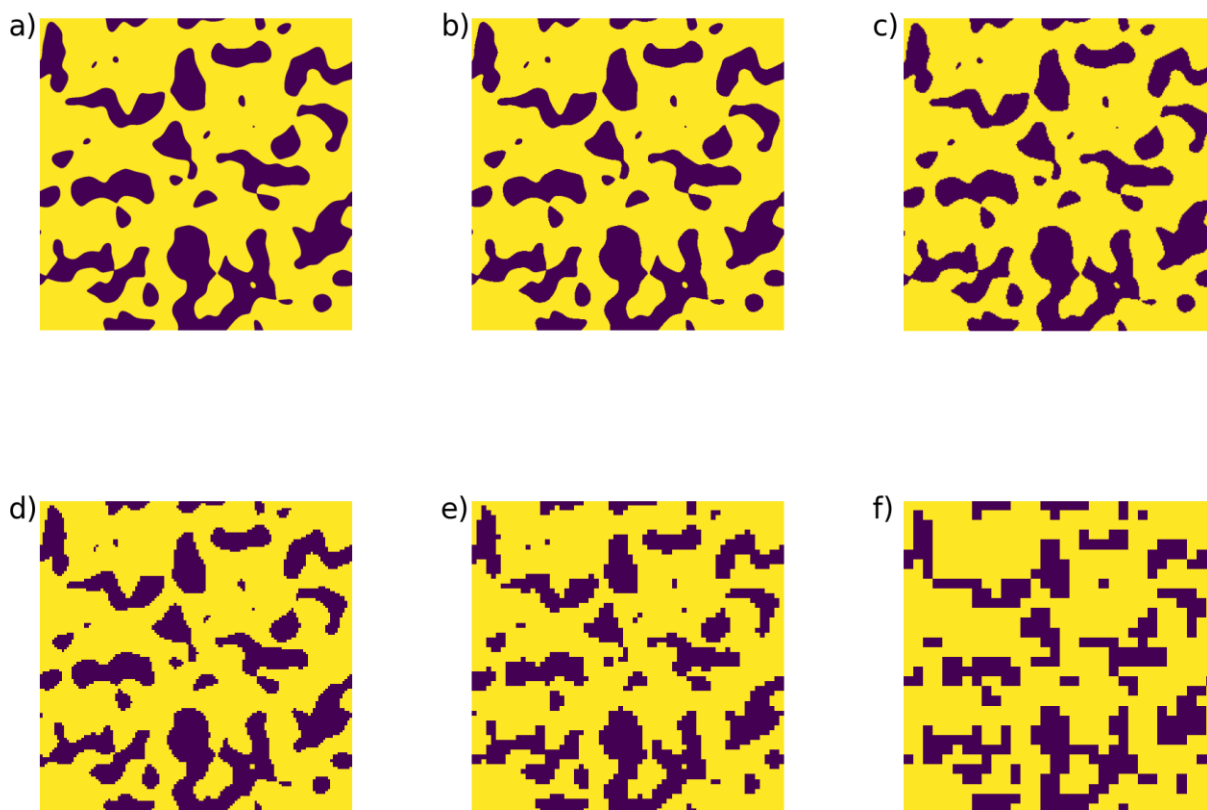


Figure 44 – Downscaling of the same base image at magnitudes of 1 (base image), $\frac{1}{2}$, $\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{16}$ and $\frac{1}{32}$ for a), b), c), d), e), and f) respectively.

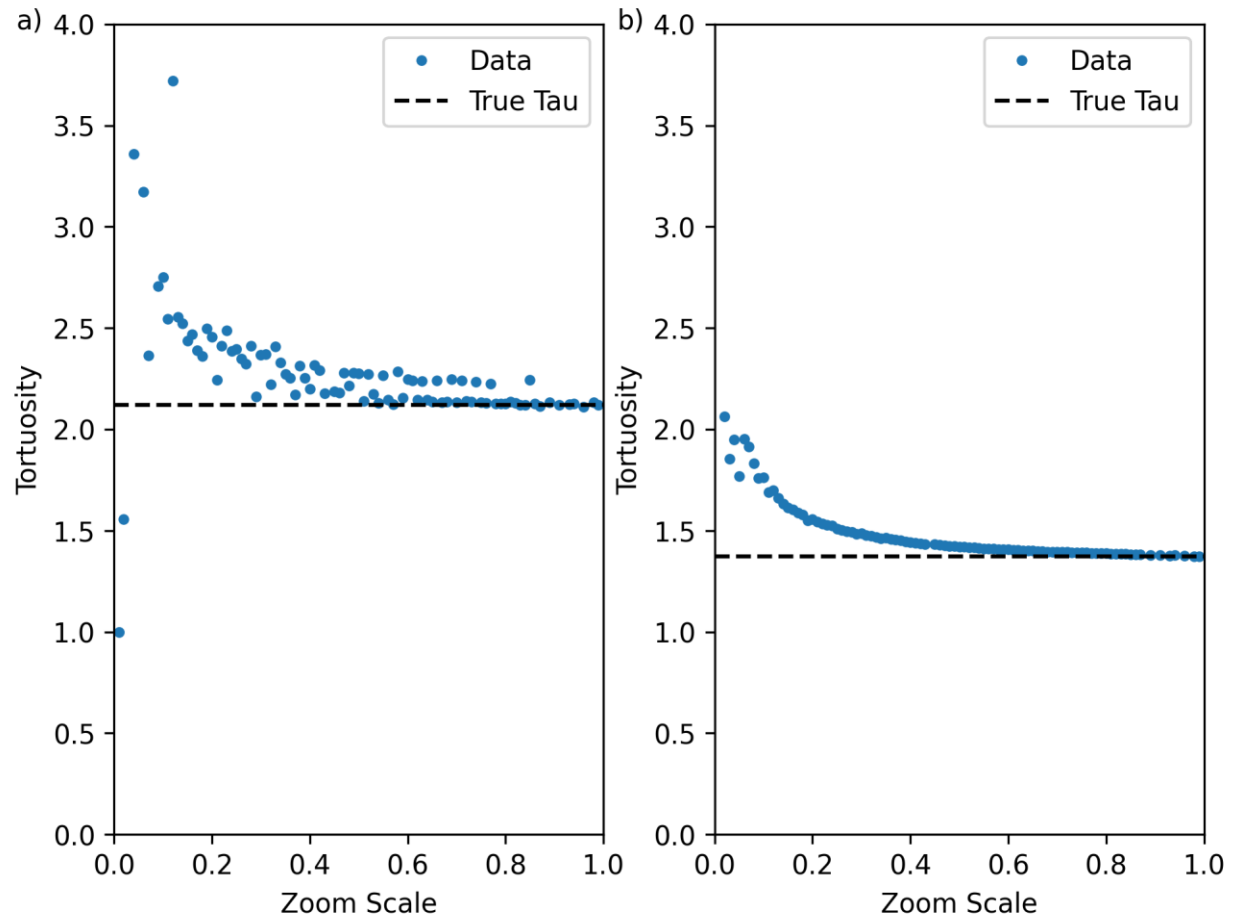


Figure 45 – Tortuosity of downscaled images versus the downscaling factor for a) 2D image and b) 3D image.

Another practical implication of this behavior is that tortuosity can be reliably obtained from moderately downscaled images, which reduces computational cost while maintaining accuracy. Only at the smallest zoom scales where excessive information of the material structure is lost, does the measure become unstable and inaccurate. It should be acknowledged that these findings are based on synthetic images and further testing on real porous media samples are required to confirm that the same stability holds in experimental datasets.

6. Predicting Tortuosity with REV Data

Figure 46 overlays the relation between tortuosity and porosity proposed by Tomadakis and Sotirchos, Equation (2.5), with the values obtained from the REV analysis of this study for different subdomain volumes [26].

$$\tau = \left(\frac{\varepsilon - \varepsilon_p}{1 - \varepsilon_p} \right)^{-\alpha} \quad (2.5)$$

Shown here are the results for image sample A1. The corresponding plots for the remaining samples can be found in Appendix F Tortuosity Prediction Plots. Since each subdomain results in a unique curve, the resulting curves can be compared, as shown in Figure 47.

Each data series in Figure 47 is plotted to determine which one predicts the ground truth value of tortuosity for A1 at the correct porosity. The analysis shows that the data series obtained from 33^3 voxels most closely predicts the true value at the correct porosity. Interestingly, the minimum volume which satisfies the REV criteria according to Figure 28 is 35^3 voxels for porosity and 44^3 for tortuosity. It is unlikely that the most accurate data series will always coincide with the minimum volume for REV as larger subdomains can incorporate more structural information from the whole sample. Using the coefficients obtained from the fit, the overall tortuosity of the whole image can be predicted with the original porosity. All coefficients found for the TS model can be found in Appendix G TS Model Coefficients. Figure 48 compares the predicted tortuosity value to the actual tortuosity for all real image samples. In all cases, the coefficient obtained from the data series corresponding to the largest subdomain is used for purposes of consistency. If all data points fall along the line $y = x$, this indicates a perfect agreement between predicted and actual values. The predicted values consistently overestimate the actual value and deviate more severely as the tortuosity increases, similar to the observations reported by Costanza-Robinson et al. [19]. The errors associated with these predictions value may be attributed to the image having a low porosity ratio or too high of a size value, as discussed in Section 4.3.

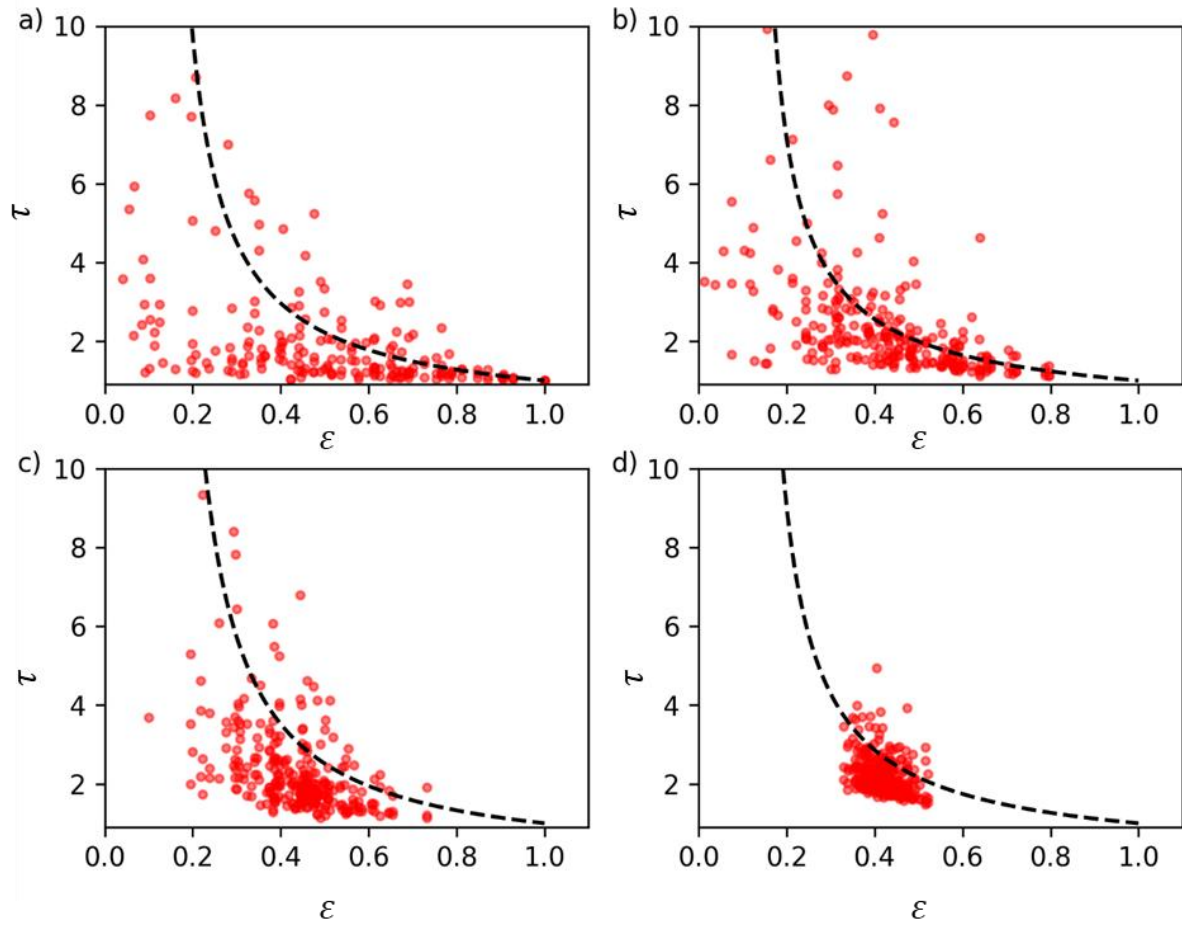


Figure 46 – Tortuosity versus porosity for image A1. The dotted black line represents the predicted tortuosity from the proposed correlation by Tomadakis and Sotirchos. Each plot corresponds to the values obtained in this study for different subdomain volumes of a) 10^3 , b) 20^3 , c) 25^3 and d) 50^3 .

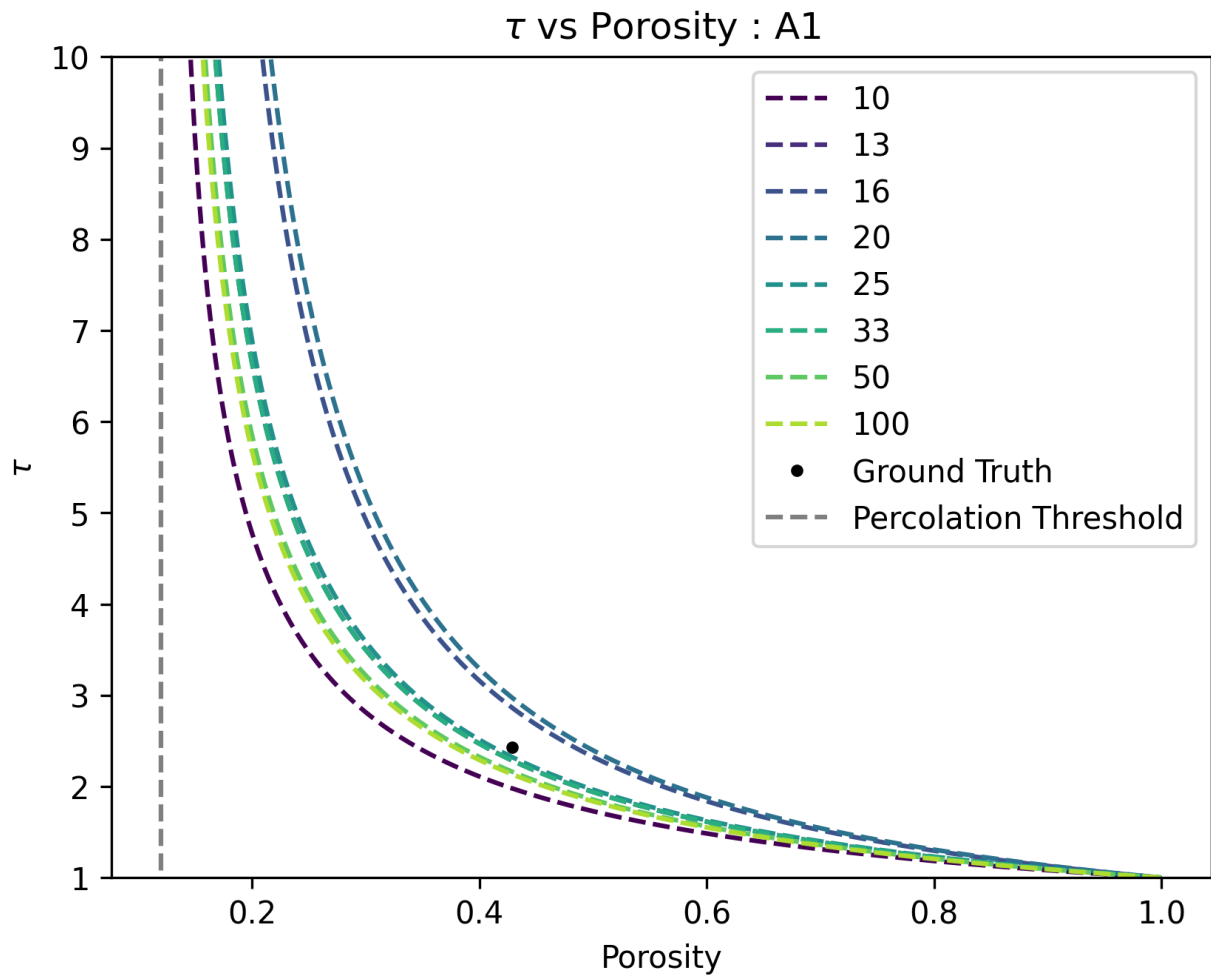


Figure 47 – Dependence of tortuosity on porosity, as generated from the correlation proposed by Tomadakis and Sotirchos.

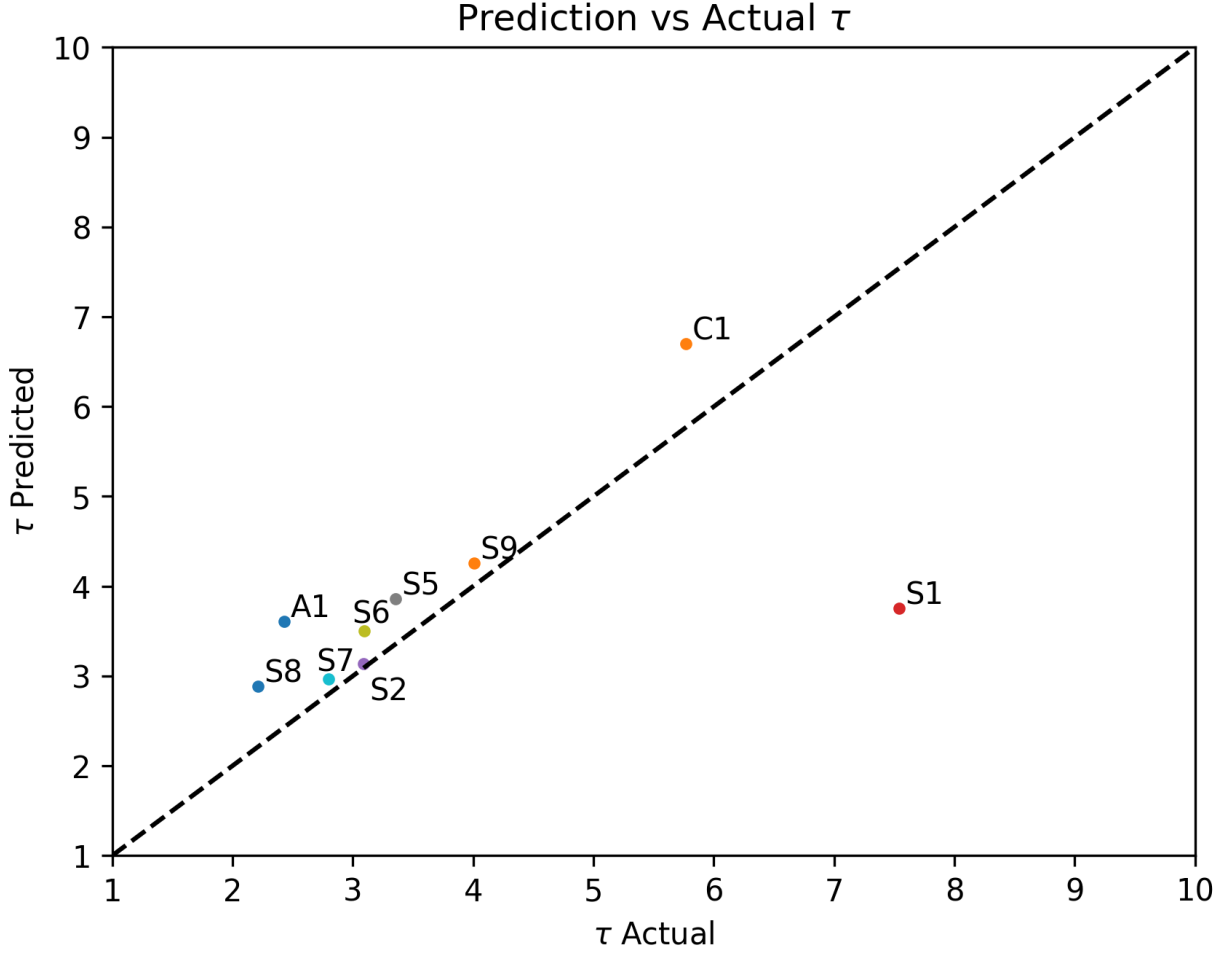


Figure 48 – Comparison of predicted tortuosity value from the proposed correlation by Tomadakis and Sotirchos to the actual tortuosity calculated through the finite difference method [2]. Missing from here are images C2, S3 and S4, as the calculated tortuosity resulted in $\tau \gg 20$. The colours are purely for data point distinction and have no meaning.

The obvious outlier among the cases shown in Figure 48 is S1, which has the following properties:

$$\varepsilon = 0.141$$

$$\varepsilon_p = 0.07$$

$$S = 7.5$$

As the correlation proposed by Tomadakis and Sotirchos cannot account for pore size distributions and only accounts for the porosity and percolation threshold, the tortuosity is underestimated by nearly a factor of 2, i.e., $\tau_{actual} = 7.54$ and $\tau_{pred} = 3.75$.

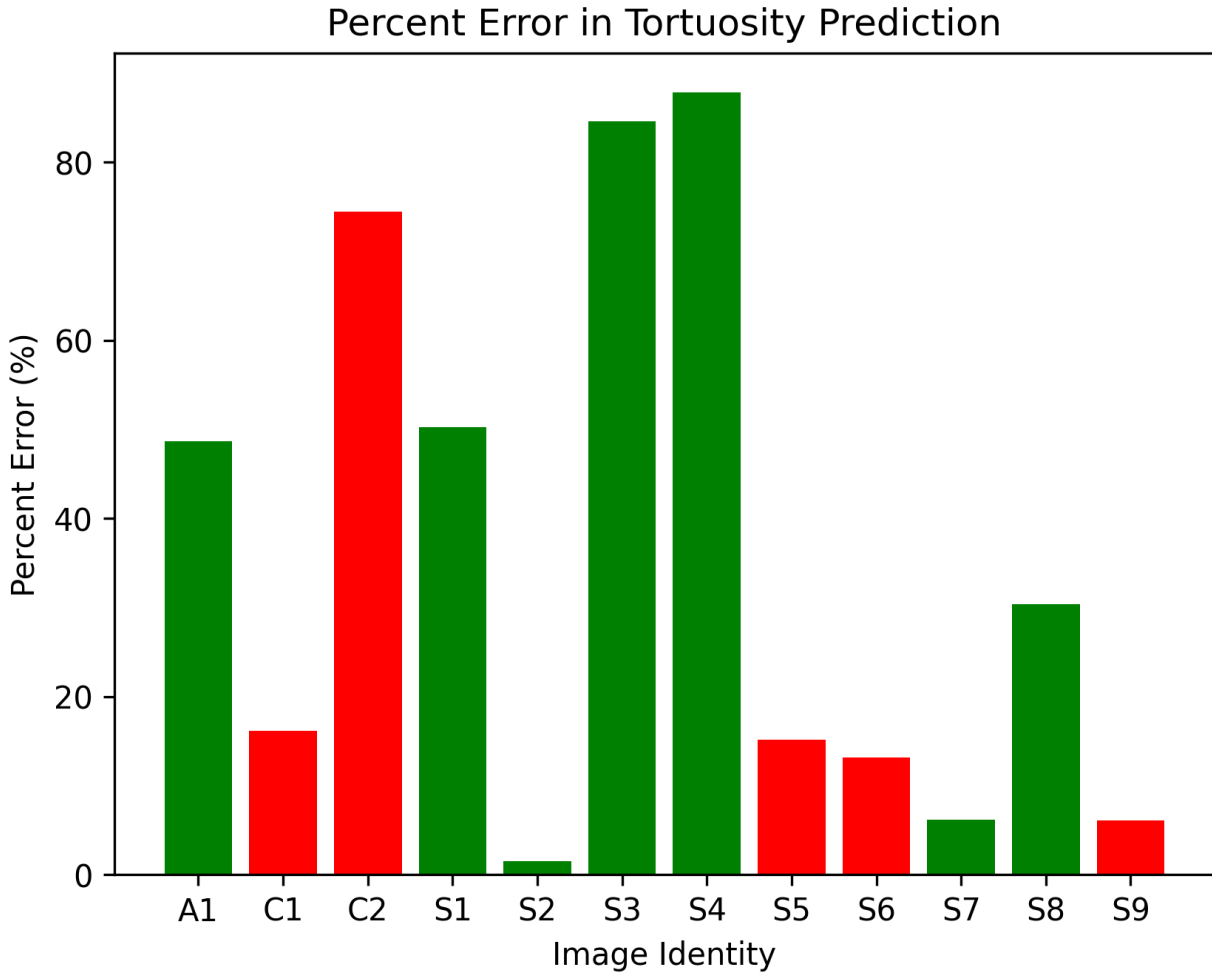


Figure 49 – Percent error in tortuosity prediction compared to the ground truth value. The green bars indicate cases where an REV is obtained, while the red ones indicate cases where no REV is found.

Figure 49 shows the percent error in prediction for tortuosity for the real image samples. No correlation appears to exist between the ability to accurately predict tortuosity and determine an REV for a given image. This seemingly paradoxical behaviour arises because the Tomadakis-Sotirchos correlation captures tortuosity through idealized structural assumptions that may not reflect the true complexity of the pore space, as alluded to above. As much of the work done by Tomadakis and Sotirchos is focused on fibers, it is also possible that their correlation cannot be applied to sandstone samples.

The results highlight a critical distinction between statistical representation and predictive accuracy. The presence of a REV ensures that subdomains capture bulk structural statistics, but it does not guarantee that tortuosity correlations, such as the one proposed by Tomadakis and Sotirchos, will provide reliable predictions. Conversely, the analysis of some images without a clearly established REV can still yield accurate predictions, suggesting that local structural features are coincidentally aligned with the assumptions made in developing a given correlation. These findings indicate that the reliability of correlation-based tortuosity models depends less on the existence of an REV and more on the compatibility between pore-scale geometry and the structural assumptions/simplifications inherent to the model.

7. Conclusions and Recommendations

The aim of this thesis was to establish criteria for identifying whether a given image was large enough to be considered a representative elementary volume of the sample from which it was taken. Criteria were defined such that an image satisfies the REV condition when at least 80% of 100 randomly selected subdomains yield porosity or tortuosity values within 20% of the overall average for that volume. These values of 20% and 80% can be adjusted to more or less stringent values on a case by case basis, but these values seemed appropriate for the 12 rock images studied here.

This methodology was applied to both synthetic datasets and real samples provided by Dong and Blunt, with subdomain volumes ranging from 10^3 to 100^3 voxels. Of the 12 real samples analyzed, 7 met the proposed criteria and REVs were successfully determined for both porosity and tortuosity. Samples that satisfied the criteria consistently exhibited a combination of low average pore sizes relative to the image size and higher porosity ratios, where the original porosity significantly exceeded the percolating porosity. Outliers were explained using additional insights from pore size distribution data.

To further assess the robustness of the proposed method, predicted tortuosity values obtained using the correlation proposed by Tomadakis and Sotirchos were compared against ground truth tortuosity values. This comparison allowed the self-consistency of subdomains within an image to be evaluated. It was found that the ground truth values of certain samples could not be accurately predicted, demonstrating that even when an image satisfies the criteria for REV, it may still lack internal self-consistency. At first glance, this may appear to contradict the concept of an REV since one might expect that representativeness implies accurate prediction of material behaviour. However, REV and self-consistency measure different aspects of porous media, the former addressing the stability of averaged properties across subdomains, while the latter tests the validity of predictive correlations. The discrepancy therefore does not negate the existence of an REV, but rather highlights that REV determination alone is insufficient for guaranteeing predictive accuracy.

The findings demonstrate that reliable REV determination is feasible at relatively small fractions of the total image volume, with tested subdomain volumes representing at most 3.7% of the full domain in some cases. This limitation highlights a constraint of the current methodology, but also suggests that expanding the tested subdomain volumes and refining threshold definitions could yield more comprehensive results in future work.

It was shown that obtaining a stable value for porosity or tortuosity as a function of size was insufficient to guarantee the existence of an REV. Instead, the distribution of porosity and tortuosity proved to be the better indicator. If the distribution of values is wider than what a random sample can be expected to present, this runs counter to the very definition of an REV. Therefore, we recommend that the distribution of values lie entirely within the desired threshold limits of the average. The size of the threshold is somewhat arbitrary, but we found that 80% of the samples lying within 20% of the mean provided a good starting point.

Beyond methodological considerations, these results carry important implications for real-world applications. By providing a robust framework for determining REV in both porosity and tortuosity, this work enables more reliable upscaling of pore-scale data to large-scale models. Such reliability is critical in fields where porous media play a central role, including hydrogeology, petroleum recovery, carbon sequestration, fuel cell design and filtration technologies. The establishment of consistent REV criteria reduces the risk of misrepresentation in material characterization and offers a practical balance between accuracy and computational efficiency.

To the best of our knowledge, this study is the first to explore explicit definitions of representative elementary volume for porosity and tortuosity. By establishing clear criteria for identifying REV in these contexts, this work not only addresses a gap in the existing literature but also provides a framework that can be applied in future experimental and computational studies.

In conclusion, this thesis contributes a systematic and flexible approach for identifying representative elementary volumes in porous media, demonstrated across both synthetic and real samples. While further refinement is needed, the criteria developed here lay a foundation for more efficient and trustworthy characterization of porosity and tortuosity, ultimately bridging the gap between microstructural imaging and predictive modeling in practical applications.

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9. Appendix A Image Generation Code

All relevant scripts and code are available on an external GitHub repository.

The following code is an example of how to generate an image and REV data for the image, as seen in Figure 2.

```
import porespy as ps
import numpy as np
import matplotlib.pyplot as plt

im = ps.generators.blobs([1000,1000], porosity=0.3)

s = ps.tools.get_slices_random(im, n=1000, lims=[10, 1000])
rev = ps.metrics.rev_porosity(im, slices=s)
fig, ax = plt.subplots(dpi=300, ncols=2, figsize=[8,4])
plt.tight_layout()

plt.sca(ax[0])
plt.imshow(im)
plt.axis(False)

plt.sca(ax[1])
plt.plot(rev.volume, rev.porosity, '.k', alpha=0.5)

mask = np.abs((rev.porosity - 0.3) / 0.3) < 0.2
plt.plot(rev.volume[mask], rev.porosity[mask], 'g', alpha=0.5)
plt.plot([0, 1e6], [0.3, 0.3], '-r')
plt.xlabel("Volume")
plt.ylabel("Porosity")
plt.title("REV Porosity")
```

10. Appendix B Image Analysis Code

The following code is used to generate REV data for real image samples, loaded from a file with the .h5 extension.

```
import porespy as ps
import h5py
import pandas as pd
import numpy as np
from tqdm import tqdm

f = "dummy_file.h5"

with h5py.File(f) as data:
    keys = [k for k in data if "image" in k]

    for k in tqdm(keys):
        all_data = []
        if "image" in k:
            print(k)
            im = np.array(data[k])

            for size in tqdm([10,13,16,20,25,33,50,100]):

                s = ps.tools.get_slices_random(im, n=100, lims=[size,size])

                df = ps.metrics.rev_tortuosity(im=im, slices=s)
                tmp = ps.tools.results_to_df(df)
                all_data.append(tmp)

    all_data_df = pd.concat(all_data)
    all_data_df.to_csv(f"output_file/{k}.csv")
```

The following code is used to analyze the results of the REV data and generate the appropriate plots as seen in section 4 and 12.

```
import h5py
from glob import glob
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import matplotlib.gridspec as gridspec
from matplotlib import cm
from matplotlib.colors import Normalize, LogNorm
import porespy as ps
from scipy.optimize import fmin
from sklearn.metrics import r2_score
from scipy.stats import chi2

# plt.rcParams['font.family'] = 'serif'
# plt.rcParams['font.serif'] = ['Times New Roman']
all_mask = True
cmap = cm.viridis
colours = ['C0', 'C1', 'C2', 'C3', ]

block_size_universal = [
    10,
    13,
    16,
    20,
    25,
    33,
    50,
    100,
]

def hex_plot(df, im_size, ep_thresh, fig=None, axes=None, bounds=None, actual_tau=None,):

    for unique_axis in np.unique(df['axis']):
        if axes != None:

            plt.sca(axes[unique_axis])

        else:
            fig, ax = plt.subplots(dpi=300)

            tmp = df[df['axis']==unique_axis]
```

```

mask1 = tmp['tau'] != 0
mask2 = tmp['tau'] != np.inf
mask3 = tmp['eps_perc'] < ep_thresh*1.1
mask4 = tmp['eps_perc'] > ep_thresh*0.9

tmp = tmp[np.logical_and(
    mask1,
    mask2,
    # mask3,
    # mask4,
)]

ny = 12
nx=int(np.sqrt(3) * ny)

vol_frac = np.log10(tmp['length']**3 / (im_size **3))

bin1 = plt.hexbin(
    vol_frac,
    1 / tmp['tau'],
    gridsize = [nx, ny],
    cmap='hot',
    mincnt=1,
    edgecolors='red',
    norm=LogNorm(vmin=1, vmax=1000)

)
plt.xlabel(fr"$\log_{10}(\phi)$")
plt.ylabel(fr"$1 / \tau$")
plt.title(fr'Tau Distribution - Axis {unique_axis}')
plt.ylim([0, 1])

if unique_axis == 2 and axes!=None:
    cb = plt.colorbar(bin1)
    cb.set_label(fr'Frequency of $\tau$')

else:
    cb = plt.colorbar(bin1)
    cb.set_label(fr'Frequency of $\tau$')

if bounds and type(actual_tau) == np.ndarray:
    # plt.plot(vol_frac, np.array(mean_vals) * 1.2, '--k', alpha=0.5)
    # plt.plot(vol_frac, np.array(mean_vals) * 0.8, '--k', alpha=0.5)
    plt.plot([min(vol_frac), max(vol_frac)], [(1 / actual_tau[unique_axis]) * 1.2] * 2, '--k', alpha=0.5)
    plt.plot([min(vol_frac), max(vol_frac)], [(1 / actual_tau[unique_axis]) * 0.8] * 2, '--k', alpha=0.5)

```

```

if axes != None and len(axes) == 4:
    axes[3].clear()
    plt.sca(axes[3])

else:
    fig, ax = plt.subplots(dpi=300)
bin2 = plt.hexbin(
    np.log10(tmp['length']**3 / (im_size **3)),
    tmp['eps_perc'],
    gridsize = [nx, ny],
    cmap='viridis',
    mincnt=1,
    edgecolors='red',
    norm=LogNorm(vmin=1, vmax=1000)

)
plt.xlabel(fr"$\log_{10}(\phi)$")
plt.ylabel(fr"$\varepsilon$")
plt.title(fr'Porosity Distribution')
plt.ylim([0, 1])

cb = plt.colorbar(bin2)
cb.set_label(fr'Frequency of $\varepsilon$')

plt.show()

def rev_plot(df, size, im_n, title="", ep_thresh=0.5, figs=None, axes=None, bounds=False, actual_tau=None):
    plot_size = 4

    valid_tau_values = {}

    if figs == None or axes == None:
        # figs, axes = plt.subplots(ncols=3, figsize=[4*3, 4])
        f1, ax1 = plt.subplots(dpi=300)
        f2, ax2 = plt.subplots(dpi=300)
        f3, ax3 = plt.subplots(dpi=300)
        figs = [f1,f2,f3]
        axes = [ax1,ax2,ax3]

    for i, axis in enumerate(np.unique(df['axis'])):
        tmp = df[df['axis']==axis]

        log_tau = []

```

```

vol_frac = []
mean_vals = []
st_dev = []

tmp_dict = {}

# for vol in np.unique(tmp['volume']):
for uu in range(1,5):
    tmp_valid = []
    for vol in np.array(block_size_universal)**3:
        tmp2 = tmp[tmp['volume']==vol]["tau"]
        taus = np.copy(tmp2)
        # eps = tmp[tmp['volume']==vol]['porosity_perc']
        eps = tmp[tmp['volume']==vol]['porosity_perc']
        # second_largest = np.unique(tmp2)[-2]
        # taus[tmp2==np.inf] = second_largest
        taus = 1/taus
        mask = taus!=0
        mask2 = eps < ep_thresh * (1 + uu * 0.05)
        mask3 = eps > ep_thresh * (1 - uu * 0.05)

        if all_mask and uu == 4:
            log_tau.append(taus[mask * mask2 * mask3])
            mean_vals.append(np.mean(taus[mask * mask2 * mask3]))
            st_dev.append(np.std(tmp2[mask*mask2*mask3]))

        elif uu==4:
            log_tau.append(taus[mask])
            mean_vals.append(np.mean(taus[mask]))
            st_dev.append(np.std(tmp2[mask]))

        if uu==4:
            vol_frac.append(np.log10(vol / (size**3)))

        if all_mask:
            tmp_valid.append(len(taus[mask * mask2 * mask3]) / len(taus))

        else:
            tmp_valid.append(len(taus[mask]) / len(taus))

    tmp_dict[uu] = tmp_valid

valid_tau_values[i] = tmp_dict

```

```

plt.sca(axes[i])

norm = Normalize(vmin=0, vmax=len(log_tau)-1)
parts = plt.violinplot(log_tau, vol_frac, widths=0.1)
for item in ['cbars', 'cmins', 'cmaxes']:
    parts[item].set_color('k')

for qq in range(1,5):

    plt.plot([min(vol_frac), max(vol_frac)], [(1 / actual_tau[i]) * (1 + qq*0.05)] * 2, f'--{colours[qq-1]}')
    plt.plot([min(vol_frac), max(vol_frac)], [(1 / actual_tau[i]) * (1 - qq*0.05)] * 2, f'--{colours[qq-1]}')

for j, body in enumerate(parts['bodies']):
    color = cmap(norm(j))
    body.set_facecolor(color)
    body.set_edgecolor(color)
    body.set_alpha(0.7)
    m = np.mean(body.get_paths()[0].vertices[:, 0]) # middle position
    verts = body.get_paths()[0].vertices
    verts[:, 0] = np.clip(verts[:, 0], m, np.inf)

plt.plot(vol_frac, mean_vals, 'k')
plt.title(f"REV: Axis {axis} : {title}")
plt.xlabel(r"$\log_{10} \left( \frac{V_B}{V_T} \right)$")
plt.ylabel(r"$\frac{1}{\tau}$")
plt.tight_layout()
plt.savefig(fr"Figures/rev_tau_{im_n}_{axis}.png")

return figs, axes, mean_vals, st_dev, log_tau, valid_tau_values

def analyze_rev_poro(poro_df, p_compare, ax, im_n, im_size, ep_thresh=None):
    plt.sca(ax)

    poro_check = {}
    valid_frac = {}
    # =====POROSITY CHECK=====

    all_porosity = []

    for vol in np.unique(poro_df['volume']):
        all_porosity.append(poro_df['porosity'][poro_df['volume']==vol])

    plt.plot(np.log10(poro_df['volume'] / im_size), poro_df['porosity'], '.k', alpha=0.5)

```

```

# plt.violinplot(all_porosity, np.log10(np.unique(poro_df['volume']) / im_size))

for ii in range(1,5):
    upper_bound = p_compare * (1 + ii * 0.05)
    lower_bound = p_compare * (1 - ii * 0.05)

    plt.plot([np.log10(min(poro_df['volume']) / im_size), np.log10(max(poro_df['volume']) / im_size)],
             [lower_bound]*2,
             f'--{colours[ii-1]}',
             label=fr"$\pm${ii*0.05:.2f}")

    plt.plot([np.log10(min(poro_df['volume']) / im_size), np.log10(max(poro_df['volume']) / im_size)],
             [upper_bound]*2,
             f'--{colours[ii-1]}')

    tmp1 = []
    tmp2 = []
    for vol in np.unique(poro_df['volume']):
        porosity_info = poro_df[poro_df["volume"]==vol]['porosity']

        valid_poro = np.logical_and(porosity_info >= lower_bound,\
                                    porosity_info <= upper_bound)

        tmp_check = (np.sum(valid_poro) / len(porosity_info))

        tmp1.append(tmp_check >= 0.95)
        tmp2.append(tmp_check)

    poro_check[ii] = tmp1
    valid_frac[ii] = tmp2

# plt.plot([min(poro_df['volume']), max(poro_df['volume'])], [ep0, ep0], '--k', alpha=0.5)
plt.xlabel(r"$\log_{10} (\frac{V_B}{V_T})$")
plt.ylabel("Porosity")
plt.title(f"REV Porosity : {im_n}")
plt.legend()

if ep_thresh != None:
    plt.plot([np.log10(min(poro_df['volume']) / im_size), np.log10(max(poro_df['volume']) / im_size)],
             [ep_thresh] * 2,
             '--C6',
             label="Percolation Threshold")

plt.savefig(f"Figures/REV_Poro_image {im_n[-2:]}.png")

```

```

return poro_check, valid_frac

def analyze_rev_tau(tau_df, ax, actual_tau=None, actual_p=None, ep_thresh=None):
    percents = []
    coeffs = []
    sigma_sqs = []
    p_vals = []
    rsquare = []

    for block_size in np.array(block_size_universal)**3:
    # for block_size in np.unique(tau_df["volume"]):
        data_rev = tau_df[tau_df["volume"]==block_size]

        x_in = np.array(data_rev['porosity_perc'])
        y_in = data_rev['tau']

        mask = data_rev['tau']!=np.inf
        mask2 = x_in < poro_avg * 1.1
        mask3 = x_in > poro_avg * 0.9

        valid = sum(mask2 * mask3)
        percent = valid / x_in.size * 100
        percents.append(percent)

    if all_mask:
        x_in = x_in[mask * mask2 * mask3]
        y_in = y_in[mask * mask2 * mask3]

    else:
        x_in = x_in[mask]
        y_in = y_in[mask]

    def loss(params):
        # tomadachis - sotirchos, eqn13
        # https://sci-hub.se/https://aiche.onlinelibrary.wiley.com/doi/10.1002/aic.690390304
        b = params
        y_pred = func(x_in, b)
        # y_pred = ((1 - a) / (x_in - a)) ** b

        return np.mean((y_in - y_pred)**2)

    guess = fmin(loss, [0.872], disp=False)
    b = guess
    y_pred = func(x_in, b)

```

```

clear_nan = np.array(~np.isnan(y_pred))

xrange = np.linspace(ep0,1,1000)
# xrange = np.unique(x_in)
y_line = func(xrange, b)

# r2 = r2_score(y_in[clear_nan], y_pred[clear_nan])
residuals = y_in - y_pred
sigma_sq = np.sum(residuals ** 2) / (len(y_in) - 2)

chi2_stat = np.sum(residuals**2) / sigma_sq
ddof = len(y_in) - 2 #2 parameters
p_value = 1 - chi2.cdf(chi2_stat, ddof)

sigma_sqs.append(sigma_sq)
coeffs.append(guess)
p_vals.append(p_value)
# rsquare.append(r2)

x_vals = np.linspace(ep0, 1, 1000)
t_s_colors = [cmap(i / len(coeffs)) for i in range(len(coeffs))]

plt.sca(ax)

for ind, (b, size) in enumerate(zip(coeffs, np.unique(tau_df["volume"]))):
    # print(b[0])
    y_vals = func(x_vals, b)
    # print(y_vals)
    plt.plot(x_vals, y_vals, '--', color=t_s_colors[ind], label=f"{round(size**(1/3))}")

    plt.xlabel("Porosity")
    plt.ylabel(r"$\tau$")
    plt.title(fr"$\tau$ vs Porosity : {im_n[-2:]}")

    plt.ylim([1, 10])

if actual_p != None and actual_tau != None:
    plt.plot(actual_p, actual_tau, '.k', label="Ground Truth")

if ep_thresh != None:
    plt.plot([ep_thresh] * 2, [0, 10], '--k', alpha=0.5, label="Percolation Threshold")

plt.legend()

```

```

return percents, coeffs, sigma_sqs, p_vals

all_coeffs = {}
all_sigma_sq = {}
all_p_vals = {}
all_rsquare = {}
all_sizes = {}
all_poro_check = {}
all_tau_check = {}
all_TS_check = {}
all_tau_comparison = {}
all_vol_fracs = {}
all_unique_vol = {}
all_tau_fracs = {}
all_rev_vols = {}
all_im_size = {}
all_tau_valid = {}

image_names = glob("Blunt_REV_set_blocks/*.csv")

image_names = [f[-12:-4] for f in image_names]
image_names.sort()

files = glob("Blunt/rev*.xlsx")
files.sort()

# change this to modify which images to process
for im_n in image_names[:]:
    print(im_n)
    with h5py.File("Blunt_images.h5") as f:
        im = np.array(f[f"{im_n}"])
        p = im.sum() / im.size
        temp = np.array([np.array(f["tortuosity_x"][f"{im_n}"]),
                        np.array(f["tortuosity_y"][f"{im_n}"]),
                        np.array(f["tortuosity_z"][f"{im_n}"])]).flatten()

    rev_data = pd.read_csv(f"Blunt/csv_files/rev_{im_n[-2:]}_raw.csv")
    data_ep = pd.read_csv(f"porosity_threshold_Blunt/{im_n[-12:]}_csv")
    set_blocks_data = pd.read_csv(f"Blunt_REV_all_same_blocks/{im_n}.csv")
    # tau_data = pd.read_csv(f"Blunt/csv_files/rev_{im_n[-2:]}_raw.csv")
    tau_data = pd.read_csv(f"Blunt_REV_all_same_blocks/{im_n}.csv")
    porosity_data = pd.read_csv(f"Blunt_REV_porosity/{im_n}.csv")
    ep0 = np.array(data_ep[data_ep['axis']==0]['eps_thresh'])[0]
    tmp_taus = pd.read_csv(f"tmp.csv")

```

```

actual_tau = np.array(tmp_taus[tmp_taus["name"]==im_n]).flatten()[2:]

def func(x_in, b):
    return ((1 - ep0) / (x_in - ep0)) ** b

# PLOTTING
macrofig = plt.figure(dpi=300, figsize=[10,7])
# plt.tight_layout(pad=2.0)
gs = gridspec.GridSpec(2,6, height_ratios=[1, 1])
ax1 = macrofig.add_subplot(gs[0,0:3])
ax2 = macrofig.add_subplot(gs[0,3:6])
ax3 = macrofig.add_subplot(gs[1,0:2])
ax4 = macrofig.add_subplot(gs[1,2:4])
ax5 = macrofig.add_subplot(gs[1,4:6])

plt.subplots_adjust(hspace=0.4)
plt.subplots_adjust(wspace=1)

# REV POROSITY GRAPH
std = np.std(porosity_data['porosity'])
poro_avg = np.mean(porosity_data['porosity'])

# poro_fig, poro_ax = plt.subplots(dpi=300)

poro_check, valid_frac = analyze_rev_poro(porosity_data,
                                          p_compare=p,
                                          im_n=im_n[-2:],
                                          im_size=im.size,
                                          ax=ax1,
                                          ep_thresh=ep0)

# CALCULATIONS FOR T-S GRAPHS

# fig_ts, ax_ts = plt.subplots(dpi=300)
percents, coeffs, sigma_sqs, p_vals, = analyze_rev_tau(set_blocks_data, ax2,
                                                         actual_tau=actual_tau[0],
                                                         actual_p=p,
                                                         ep_thresh=ep0)

all_coeffs[im_n] = coeffs
all_sigma_sq[im_n] = sigma_sqs
all_p_vals[im_n] = p_vals
all_sizes[im_n] = np.unique(tau_data["volume"])
all_poro_check[im_n] = poro_check

```

```

all_vol_fracs[im_n] = valid_frac
all_unique_vol[im_n] = np.unique(porosity_data['volume'])
# all_rsquare[im_n] = r_sq

# =====TS CHECK=====
predicted_tau = func(p,all_coeffs[im_n])

ts_check = 1 - (actual_tau[1] - predicted_tau) / actual_tau[1]
all_TS_check[im_n] = ts_check

# =====TAU CHECK=====
# filtering data to only include valid points, between +-5, 10, 15, 20% of actual tau

tau_check = {}
tau_fracs = {}
for jj in range(1,5):
    upper_bound = p * (1 + jj * 0.05)
    lower_bound = p * (1 - jj * 0.05)

    tmp1 = []
    tmp2 = []

    for vol in np.unique(tau_data['volume']):
        porosity_info = tau_data[tau_data['volume']==vol]['porosity_perc']
        poro_mask = np.logical_and(porosity_info >= lower_bound,\
                                   porosity_info <= upper_bound)

        tau_info = 1 / np.array((tau_data[tau_data['volume']==vol]['tau']))[poro_mask]
        # average_tau = np.mean(tau_info)
        average_tau = 1 / actual_tau[1]

        # boundaries based on average tau within specific bin
        upper_bound_tau = average_tau * (1 + jj * 0.05)
        lower_bound_tau = average_tau * (1 - jj * 0.05)

        valid_tau = np.logical_and(tau_info >= lower_bound_tau,\
                                   tau_info <= upper_bound_tau)

        tmp_check = (np.sum(valid_tau) / len(tau_info))

        tmp1.append(tmp_check > 0.95)
        tmp2.append(tmp_check)

    tau_check[jj] = tmp1

```

```

tau_fracs[jj] = tmp2

all_tau_check[im_n] = tau_check
all_tau_fracs[im_n] = tau_fracs
all_rev_vols[im_n] = np.unique(tau_data['volume'])
all_im_size[im_n] = np.prod(im.shape)

# VIOLIN PLOTS
try:
    fig_t, plots, mean_taus, standard_devs, tau_inv, valid_tau_values = rev_plot(
        tau_data,
        # rev_data,
        im_n=im_n[-2:],
        size=im.shape[0],
        title=im_n[-2:],
        ep_thresh=poro_avg,
        figs=macrofig,
        axes=[ax3,ax4,ax5,ax1],
        bounds=True,
        actual_tau=actual_tau)

except:
    fig_t, plots, mean_taus, standard_devs, tau_inv, valid_tau_values = rev_plot(
        # set_blocks_data,
        rev_data,
        im_n=im_n[-2:],
        size=im.shape[0],
        title=im_n[-2:],
        ep_thresh=poro_avg,
        figs=macrofig,
        axes=[ax3,ax4,ax5,ax1],
        bounds=True,
        actual_tau=actual_tau)

all_tau_valid[im_n] = valid_tau_values

plt.savefig(f"Figures/Macro_Final_{im_n}.png")

```

The following code is used to generate the plots seen in section 4.2.

```

tmp = []

PLOT_A = False
PLOT_B = False

t_s_colors = [cmap(i / len(all_coeffs[im_n])) for i in range(len(all_coeffs[im_n]))]

# all_vol_fracs[]

for i, k in enumerate(all_coeffs.keys()):

    # fig, ax = plt.subplots(dpi=300)
    # plt.sca(ax)
    # plt.plot(np.log10(all_sizes[k]), all_coeffs[k], '-.')
    # plt.ylim([0,1.5])
    # plt.title(f"Coeffs vs Block Size : {k}")
    tmp.append({
        "im_name" : k,
        # "porosity_check" : True in (np.array([all_vol_fracs[k][spread] for spread in all_vol_fracs[k].keys()]).flatten() >
0.95),
        # "tau_check" : True in (np.round(np.array([all_tau_fracs[k][spread] for spread in
all_tau_fracs[k].keys()]).flatten(), 5) > 0.8),
        # "ts_check" : True in (all_TS_check[k] <= 0.1),
        "porosity_check_value" : max(np.round(np.array([all_vol_fracs[k][spread] for spread in
all_vol_fracs[k].keys()]).flatten(), 5)),
        "tau_check_value" : max(np.round(np.array([all_tau_fracs[k][spread] for spread in
all_tau_fracs[k].keys()]).flatten(), 5)),
        "ts_check_value" : [0 if (i>=1.5 or i<=0) else i for i in np.round((np.array(all_TS_check[k]).flatten()), 4) ],
    })

subplot_size = 4
if PLOT_A and PLOT_B:
    fig, ax = plt.subplots(ncols=2, dpi=300, figsize=(2 * subplot_size, subplot_size))
    plt.subplots_adjust(hspace=1)

    plt.sca(ax[0])
    # ax[0].set_aspect('equal', adjustable='box')
    for spread in all_vol_fracs[k].keys():
        plt.plot(np.log10(all_unique_vol[k] / all_im_size[k]), all_vol_fracs[k][spread], '.',
label=rf"$\pm$\{spread*0.05:.2f}$")
        plt.plot([-5, -1.3], [0.8, 0.8], '--k', alpha=0.5)
    plt.xlabel(r"$\log_{10}(\frac{V_B}{V_T})$")

```

```

plt.ylabel("f")
plt.xlim([-5, -1.3])
plt.ylim([-0.1, 1.1])
plt.title(f"Valid Porosity Fraction vs Volume : {k[-2:]}")
plt.legend()
# plt.savefig(fr"Figures/Volume_fraction {k[-2:]}")

plt.sca(ax[1])
# ax[1].set_aspect('equal', adjustable='box')

# for spread in all_tau_fracs[k].keys():
for spread in all_tau_valid[k][0].keys():
    plt.plot(np.log10(all_rev_vols[k] / all_im_size[k]), all_tau_valid[k][0][spread], '.',
label=rf"$\pm${spread*0.05:.2f}")
    plt.plot([-5, -1.3], [0.8, 0.8], '--k', alpha=0.5)
    plt.xlabel(r"$\log_{10}(\frac{V_{\{B\}}}{V_{\{T\}}})$")
    plt.ylabel("f")
    plt.xlim([-5, -1.3])
    plt.ylim([-0.1, 1.1])
    plt.title(f"Valid Tau Fraction vs Volume : {k[-2:]}")
    plt.legend()

plt.tight_layout()
plt.savefig(fr"Figures/Macro_Fraction_image {k[-2:]}")

elif PLOT_A:
    fig, ax = plt.subplots(dpi=300)

    for spread in all_vol_fracs[k].keys():
        plt.plot(all_unique_vol[k], all_vol_fracs[k][spread], '.', label=rf"$\pm${spread*0.05:.2f}")
        plt.xlabel(r"$\log_{10}(V_{\{B\}})$")
        plt.ylabel("f")
        plt.ylim([0, 1.1])
        plt.title(f"Valid Porosity Fraction vs Volume : {k[-2:]}")
        plt.legend()
        plt.savefig(fr"Figures/Volume_fraction {k[-2:]}")

elif PLOT_B:
    fig, ax = plt.subplots(dpi=300)

    for spread in all_tau_fracs[k].keys():
        plt.plot(all_rev_vols[k], all_tau_fracs[k][spread], '.', label=rf"$\pm${spread*0.05:.2f}")
        plt.xlabel(r"$\log_{10}(V_{\{B\}})$")
        plt.ylabel("f")
        plt.ylim([0, 1.1])

```

```

plt.title(f"Valid Tau Fraction vs Volume : {k[-2:]}")
plt.legend()
plt.savefig(fr"Figures/Tau_fraction_average_tau {k[-2:]}")

fig_tau_compare, ax_tau_compare = plt.subplots(dpi=300)

def func(x_in, b, ep0):
    return ((1 - ep0) / (x_in - ep0)) ** b

for i, k in enumerate(all_coeffs.keys()):
    b = all_coeffs[k][-1]
    with h5py.File("Blunt_images.h5") as f:
        im = np.array(f[f"{im_n}"])
        p = im.sum() / im.size

    data_ep = pd.read_csv(fr"porosity_threshold_Blunt/{im_n[-12:]}.csv")
    ep0 = np.array(data_ep[data_ep['axis']==0]['eps_thresh'])[0]
    actual_tau = np.array(tmp_taus[tmp_taus["name"]==k]).flatten()[2:][0]
    pred_tau = func(x_in=p, b=b, ep0=ep0)

    if "S2" in k:
        plt.text(actual_tau+0.05, pred_tau-0.4, k[-2:])

    elif "S6" in k or "S7" in k:
        plt.text(actual_tau-0.1, pred_tau+0.09, k[-2:])

    elif actual_tau<=10 and pred_tau<=10:
        plt.text(actual_tau+0.05, pred_tau+0.05, k[-2:])

plt.plot(actual_tau, pred_tau, '.')

plt.plot([1,10], [1,10], '--k')
plt.ylim([1,10])
plt.xlim([1,10])
plt.xlabel(r"$\tau$ Actual")
plt.ylabel(r"$\tau$ Predicted")
plt.title(r"Prediction vs Actual $\tau$")
# plt.legend()
tmp2 = pd.DataFrame(tmp)
tmp2

fig_tau_error, ax_tau_error = plt.subplots(dpi=300)

error_val = []

```

```

shortened_names = [f[-2:] for f in image_names]
for i, k in enumerate(all_coeffs.keys()):
    ts_check_value = [0 if (i>=1.5 or i<=0) else i for i in np.round((np.array(all_TS_check[k]).flatten()), 4) ]
    print(ts_check_value)
    error_val.append(ts_check_value[-1])

plt.bar(np.arange(len(all_coeffs.keys())), np.abs(np.array(error_val)-1) * 100)
plt.xticks(np.arange(len(all_coeffs.keys())), shortened_names)
plt.xlabel("Image Identity")
plt.ylabel("Percent Error (%)")
plt.title("Percent Error in Tortuosity Prediction")

```


11. Appendix C Tables

Table V – Various calculated properties of each slab in image appearing in Figure 4b

Slice Number	Original Porosity	Percolating Porosity	Diffusive Conductance (m^2/m)	Tortuosity
1	0.7061	0.6647	4.1402	1.6216
2	0.7608	0.7110	5.2770	1.3609
3	0.8226	0.7338	6.4469	1.1497
4	0.9405	0.9405	9.0914	1.0450
5	0.7123	0.7123	5.7320	1.2552
6	0.5229	0.4621	3.3376	1.3985
7	0.6294	0.5887	4.3348	1.3718
8	0.5916	0.5667	4.6960	1.2189
9	0.5812	0.5685	3.9344	1.4596
10	0.7327	0.6946	4.5888	1.5291

Table VI – Various calculated properties of each slab in image appearing in Figure 4c

Slice Number	Original Porosity	Percolating Porosity	Diffusive Conductance (m^2/m)	Tortuosity
1	0.7334	0.6592	1.5252	2.1718
2	0.8815	0.8815	3.3043	1.3406
3	0.6176	0.5882	1.8342	1.6115
4	0.6105	0.5777	2.0948	1.3858
5	0.6569	0.6442	1.5319	2.1132

Table VII – Complete table of pore structure properties of extracted AB Networks on image samples from Dong and Blunt [32] [33].

Samples	A1	C1	C2	S1	S2	S3	S4	S5	S6	S7	S8	S9
Resolution (μm)	3.85	2.85	5.35	8.68	4.96	9.1	8.96	4	5.1	4.8	4.89	3.4
Size	300 ³	400 ³	400 ³	300 ³	300 ³	300 ³	300 ³	300 ³	300 ³	300 ³	300 ³	300 ³
Porosity (%)	42.9	23.3	16.8	14.1	24.6	16.9	17.1	21.1	24	25	34	22.2
Network porosity (%)**	42.9	21.3	14.1	14.1	24.6	16.6	16.5	21.1	24	25	34	22.1
No. of pores**	4065	2957	4600	1857	2249	8571	8433	577	708	1293	1603	610
No. of throats**	10059	4938	7093	2725	4608	12911	11057	899	1219	2717	3820	992
ACN**	4.95	3.34	3.08	2.93	4.1	3.01	2.62	3.12	3.44	4.2	4.77	3.25
APR**	14.83	9.78	16.26	30.12	18.83	21.38	21.84	18.18	20.89	20.03	21.91	18.3
ATR**	9.03	5.85	9.16	16.83	10.63	11.41	11.97	11.09	12.25	11.68	12.89	10.04
AAR**	2.7	3.44	2.93	2.75	2.86	2.51	2.41	3.74	3.88	3.25	3.1	3.8
APV**	1.28	0.94	2.64	11.44	2.9	3.35	3.31	5.48	10.64	4.78	5.36	3.27
ATV**	1.39	0.75	2.29	13.24	3.37	3.9	3.74	5.3	8.72	4.84	5.61	3.52
ATL**	99.2	82.8	115.6	211.3	132.6	141.9	135.6	161.3	190.6	158.2	162.2	139.4
V_{pore}/V_{space} (%)**	78.84	88.27	88.22	85.49	80.8	85.07	87.08	86.9	87.63	82.44	80.02	85.09
K_x (mD)**	6,773	1,289	136	2,138	4,198	744	439	6,847	13,175	7,915	14,999	2,283
K_y (mD)**	9,232	2,282	289	2,597	4,883	1,200	596	6,396	13,976	9,254	15,666	2,790
K_z (mD)**	9,664	1,138	139	2,816	5,174	733	587	6,202	14,660	9,271	14,897	3,506
K_{avg} (mD)**	8,556	1569	188	2,517	4,751	892	541	6,481	13,937	8,813	15,187	2,860
F_x**	5.58	27.94	281.8	50.41	12.52	62.4	104.2	15.74	13.34	10.58	6.42	17.69
F_y**	4.4	21.46	136.2	38.07	11.03	39.19	67.78	14.4	11.78	9.48	6.05	20.22

F_z^{**}	4.29	35.88	214	36.37	10.88	50.23	69.6	14.17	11.52	9.41	6.21	15.74
F_{avg}^{**}	4.69	27.21	192.8	40.76	11.43	48.82	77.49	14.74	12.17	9.79	6.22	17.7

*ACN, APR, ATR, AAR, APV, ATV, ATL are the averages of coordination number, pore radius, throat radius, aspect ratio, pore volume, throat volume, and throat length respectively. V_{pore} and V_{space} are the total pore volume and pore space volume respectively. K_x , K_y , K_z , and K_{avg} are the directional absolute permeability in the x , y , and z directions, respectively. F_x , F_y , and F_z are the formation factors in the x , y , and z directions respectively. F_{avg} is the harmonic mean of formation factors of the three directions.

**Each metric corresponding to a network was determined from the extracted AB network [1]

12. Appendix D Excluded Image Montages

The following plots were excluded from 4.2 as the features were similar to that of other images and were already discussed.

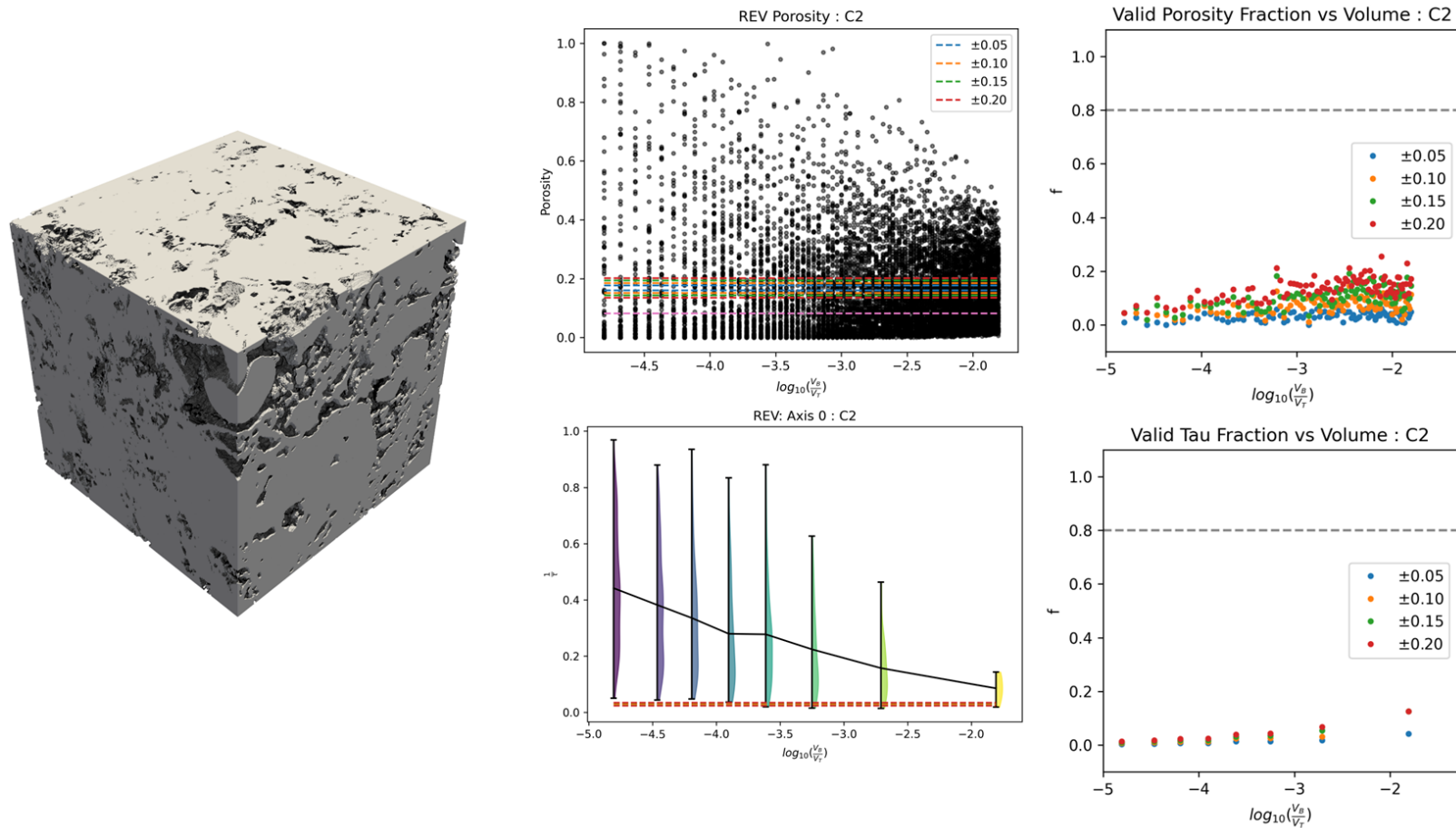


Figure 50 – A montage of the relevant plots for image C2.

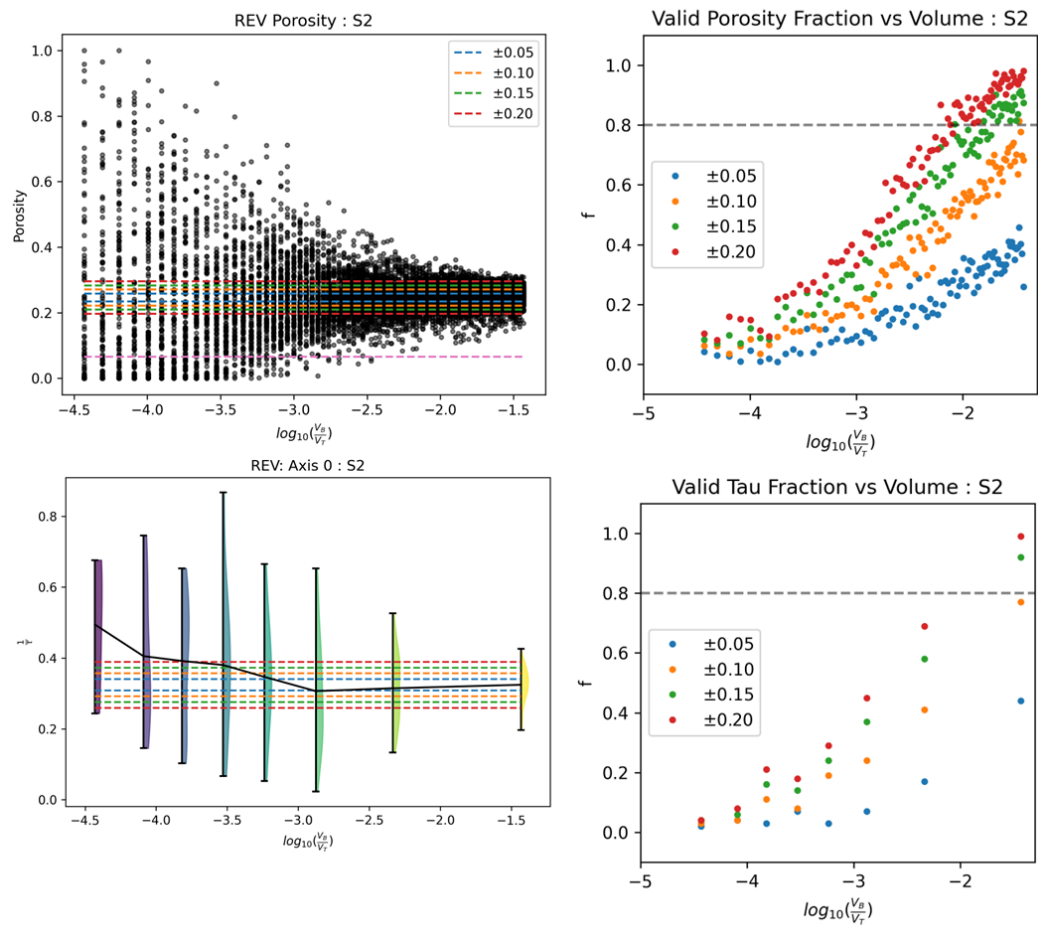
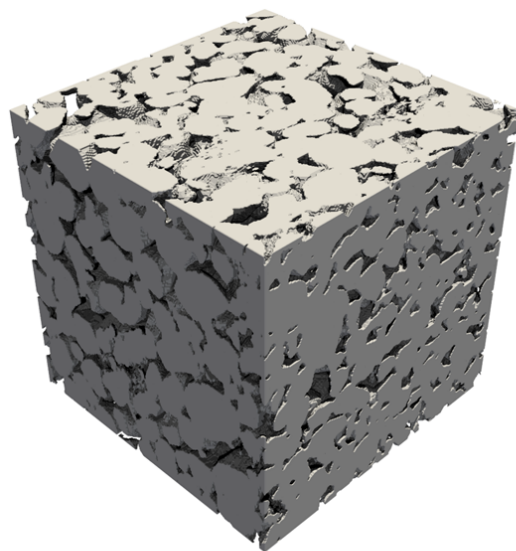


Figure 51 – A montage of the relevant plots for image S2.

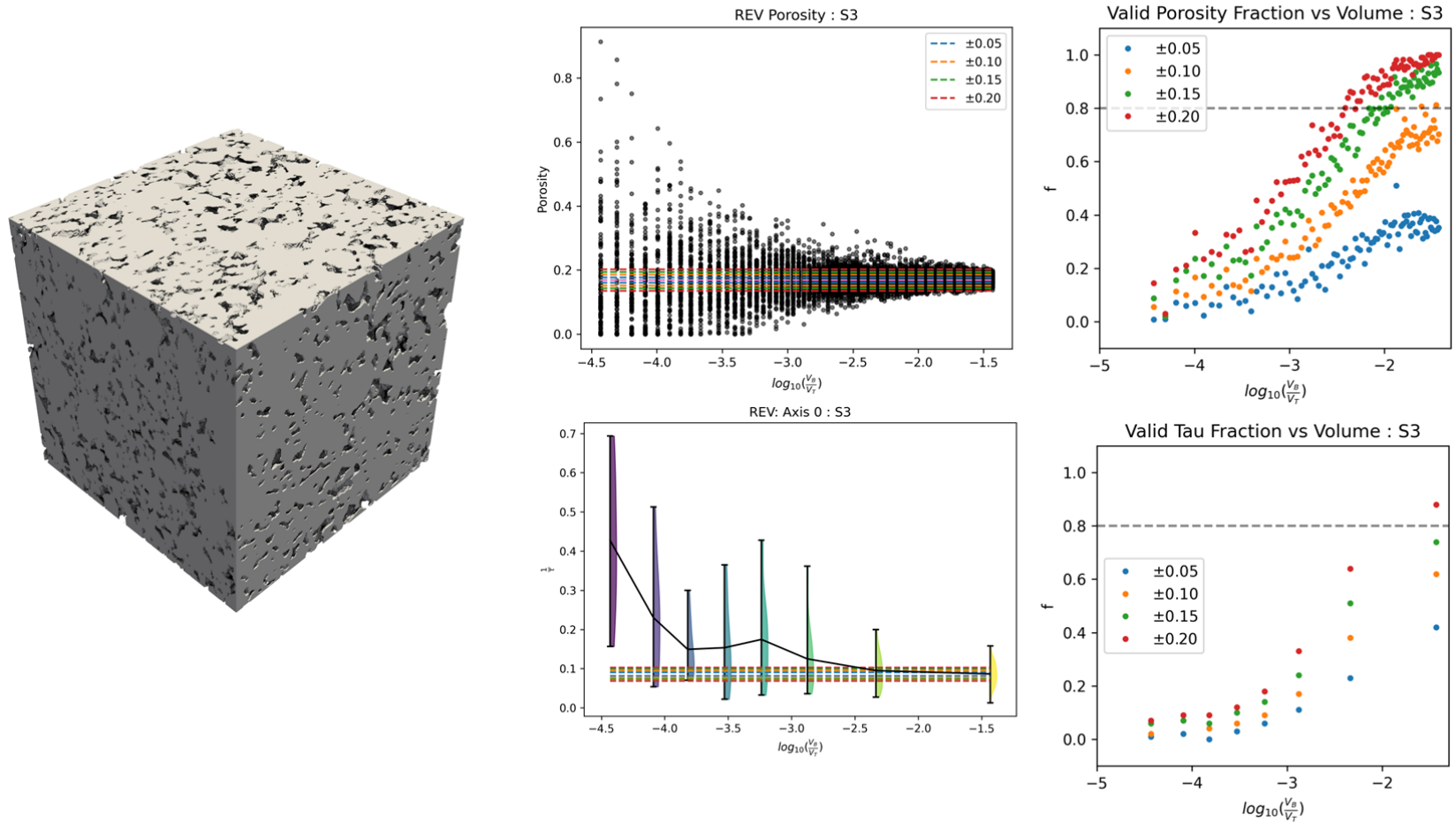


Figure 52 – A montage of the relevant plots for image S3.

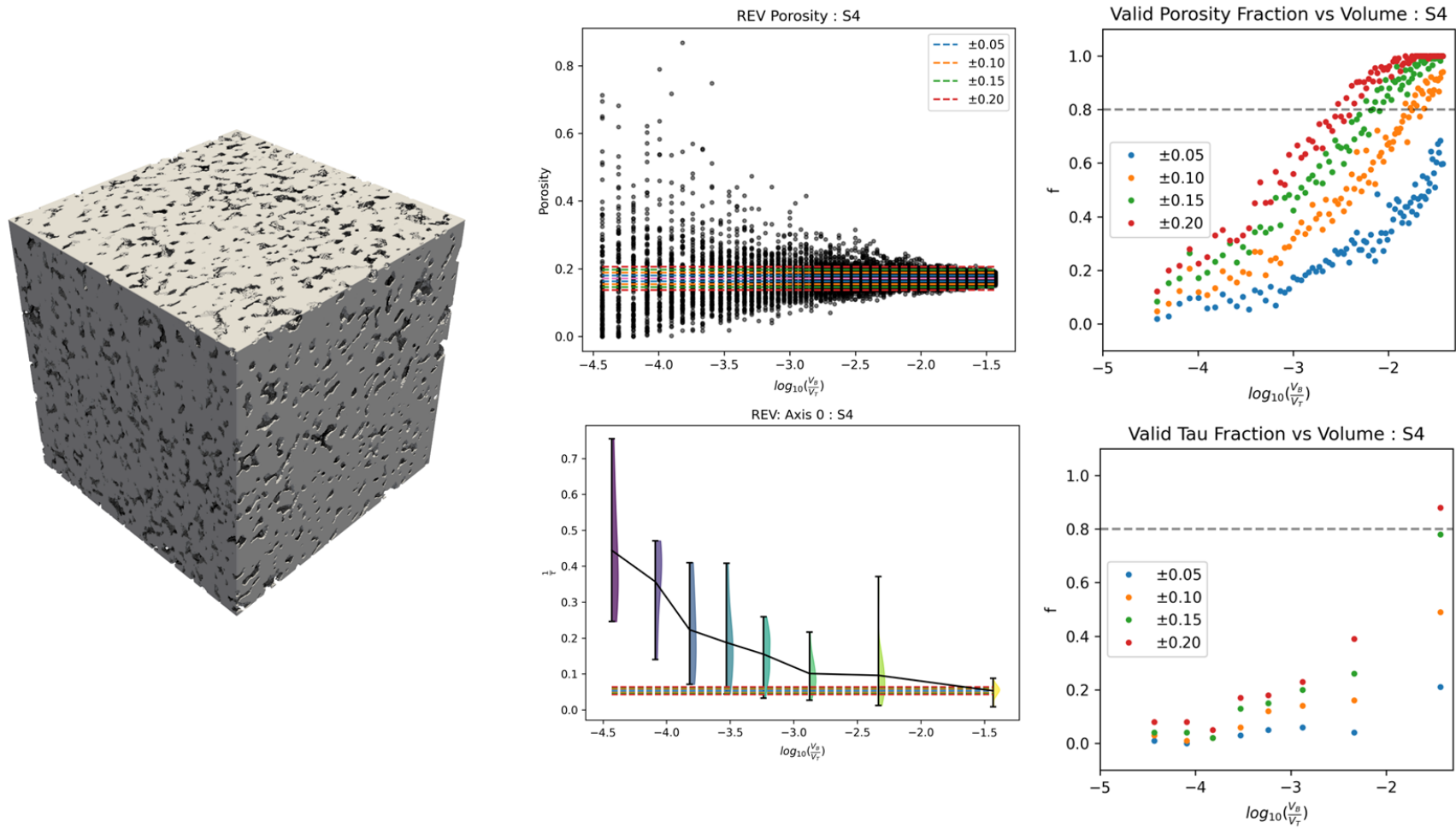


Figure 53 – A montage of the relevant plots for image S4.

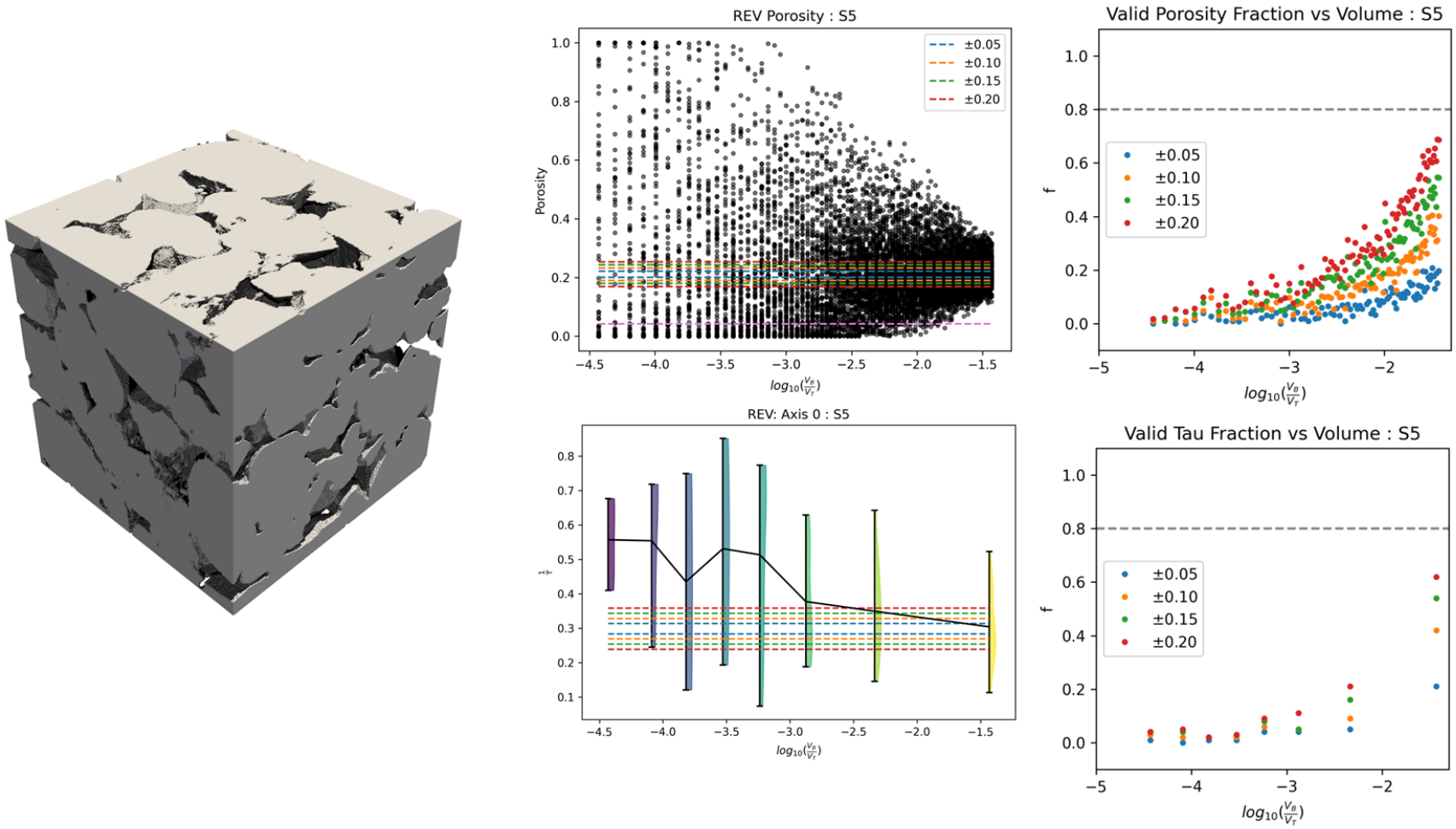


Figure 54 – A montage of the relevant plots for image S5.

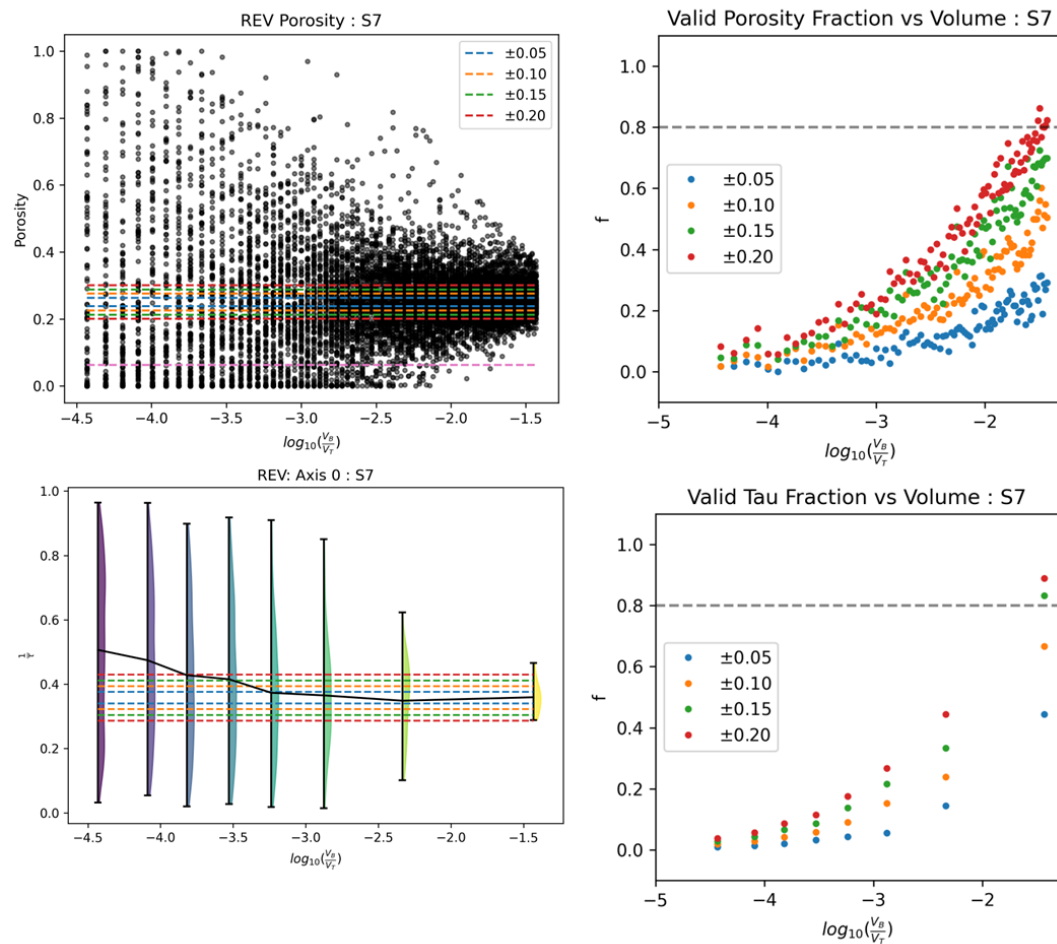
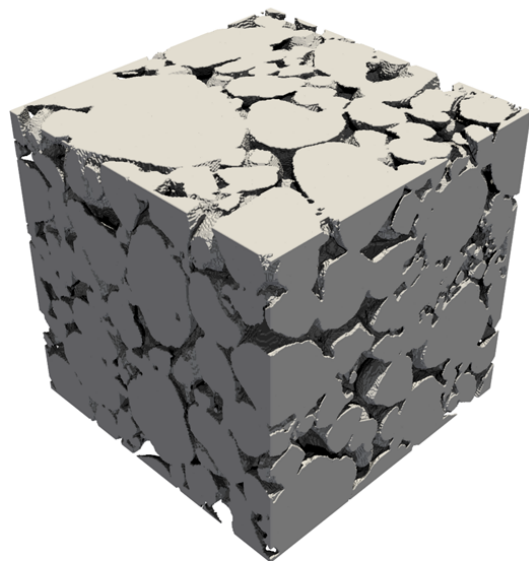


Figure 55 – A montage of the relevant plots for image S7.

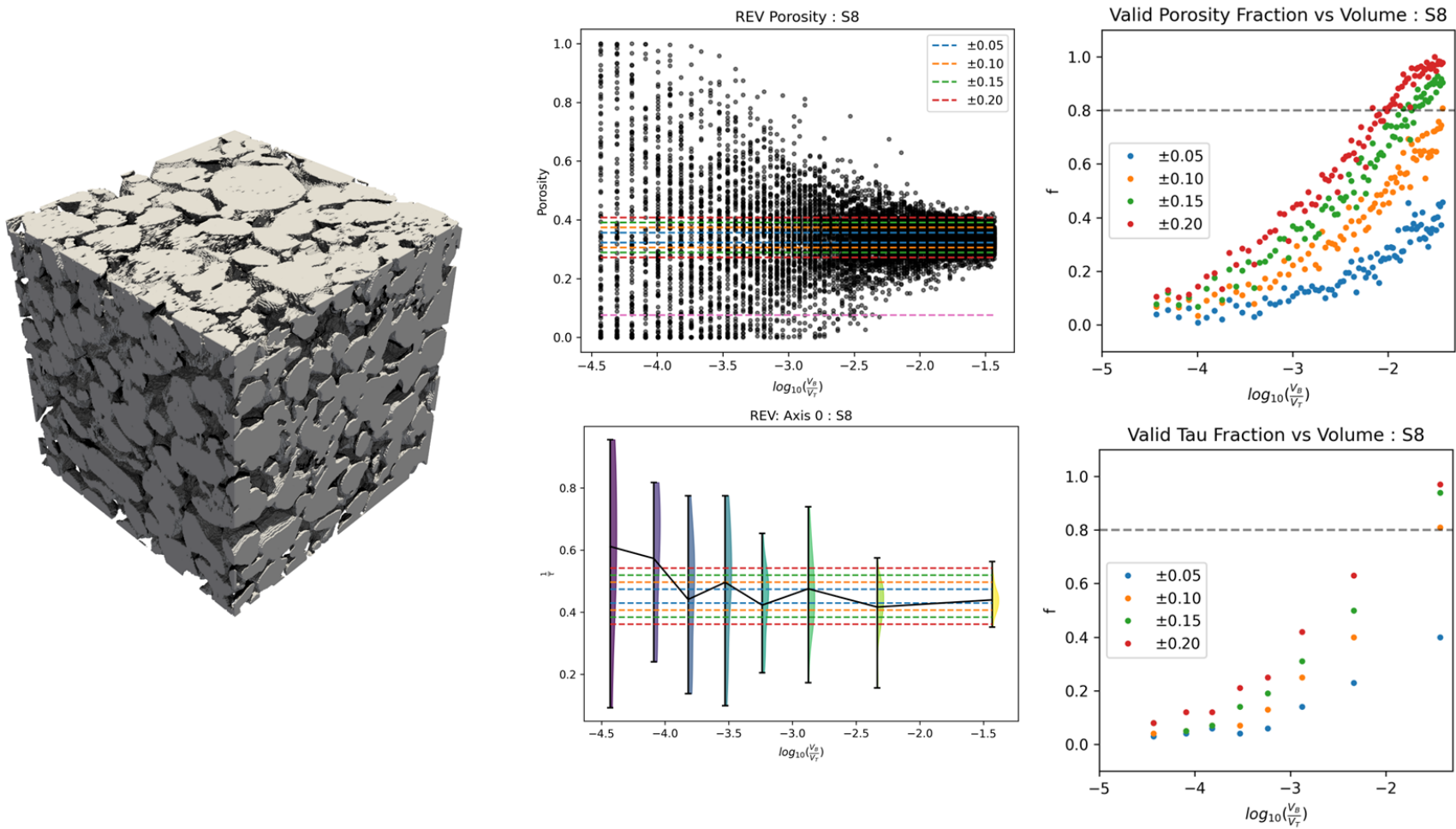


Figure 56 – A montage of the relevant plots for image S8.

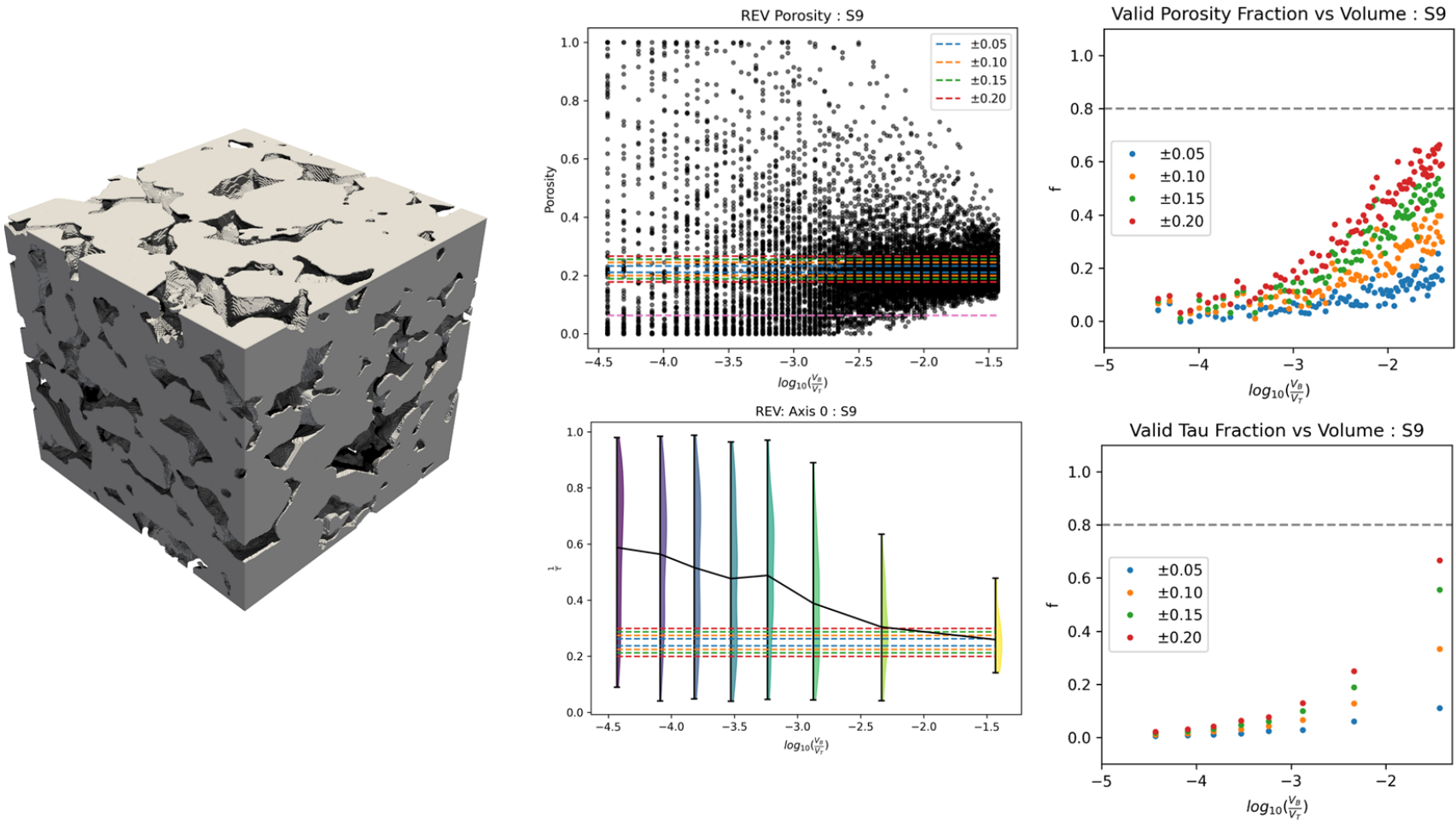


Figure 57 – A montage of the relevant plots for image S9

13. Appendix E Macro Image Montages

The following plots contain the excluded information for axis 1 and axis 2 from section 4.2, as well as the plots for the Tomadakis-Sotirchos correlation.

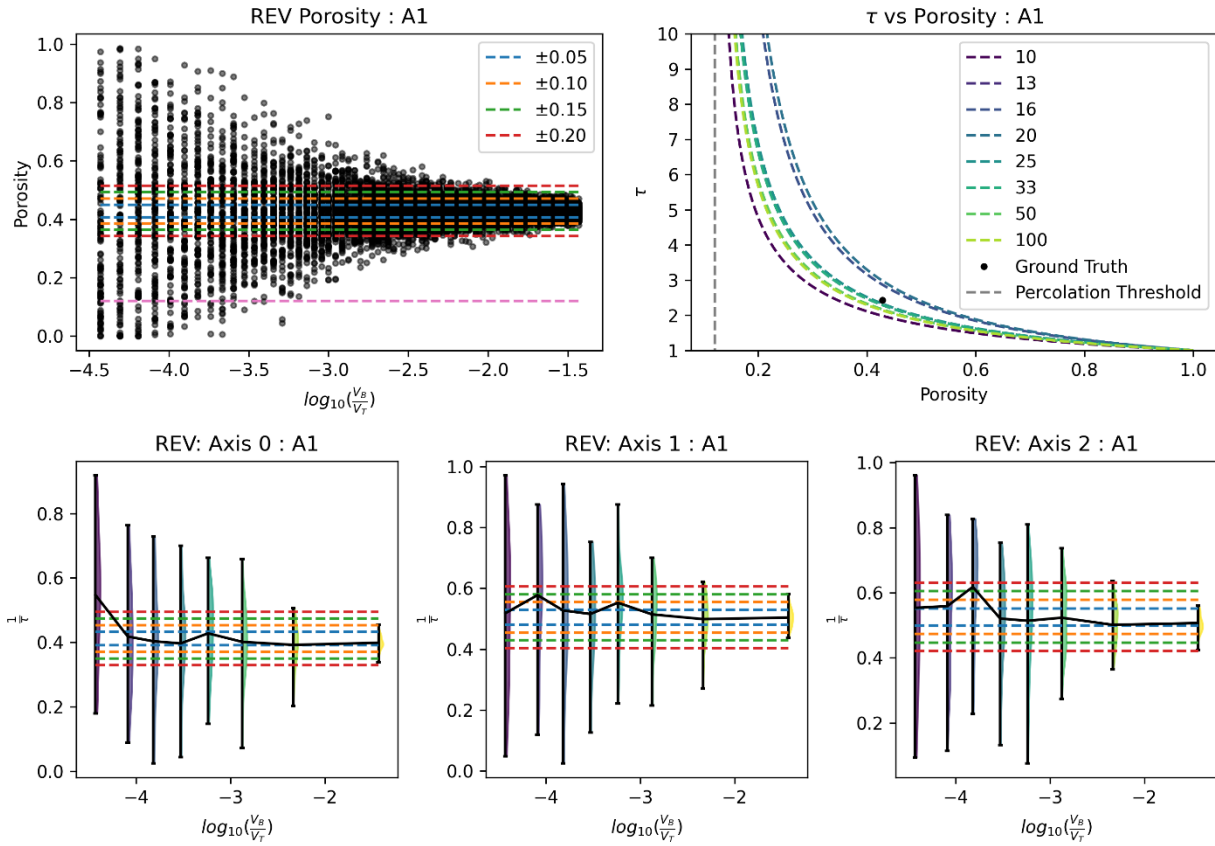


Figure 58 – Macro plot for A1.

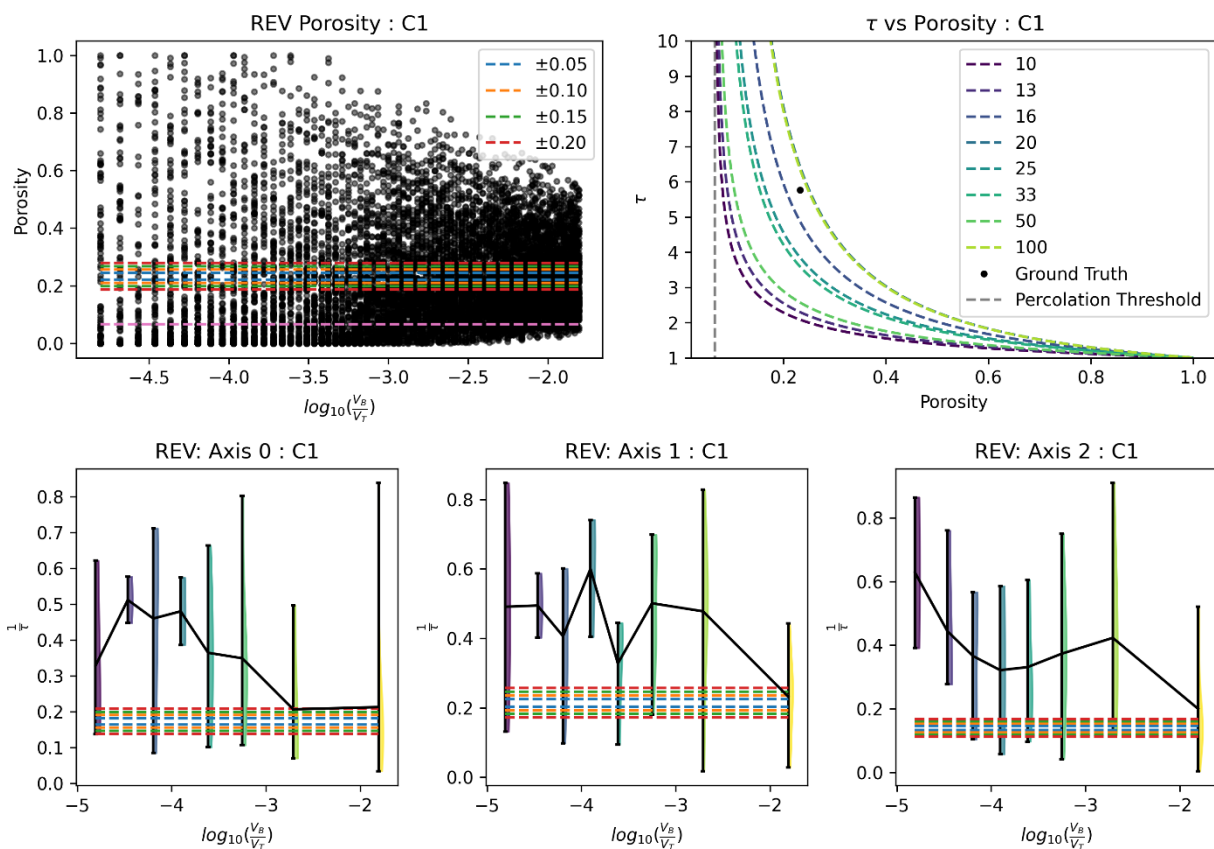


Figure 59 – Macro plot for C1.

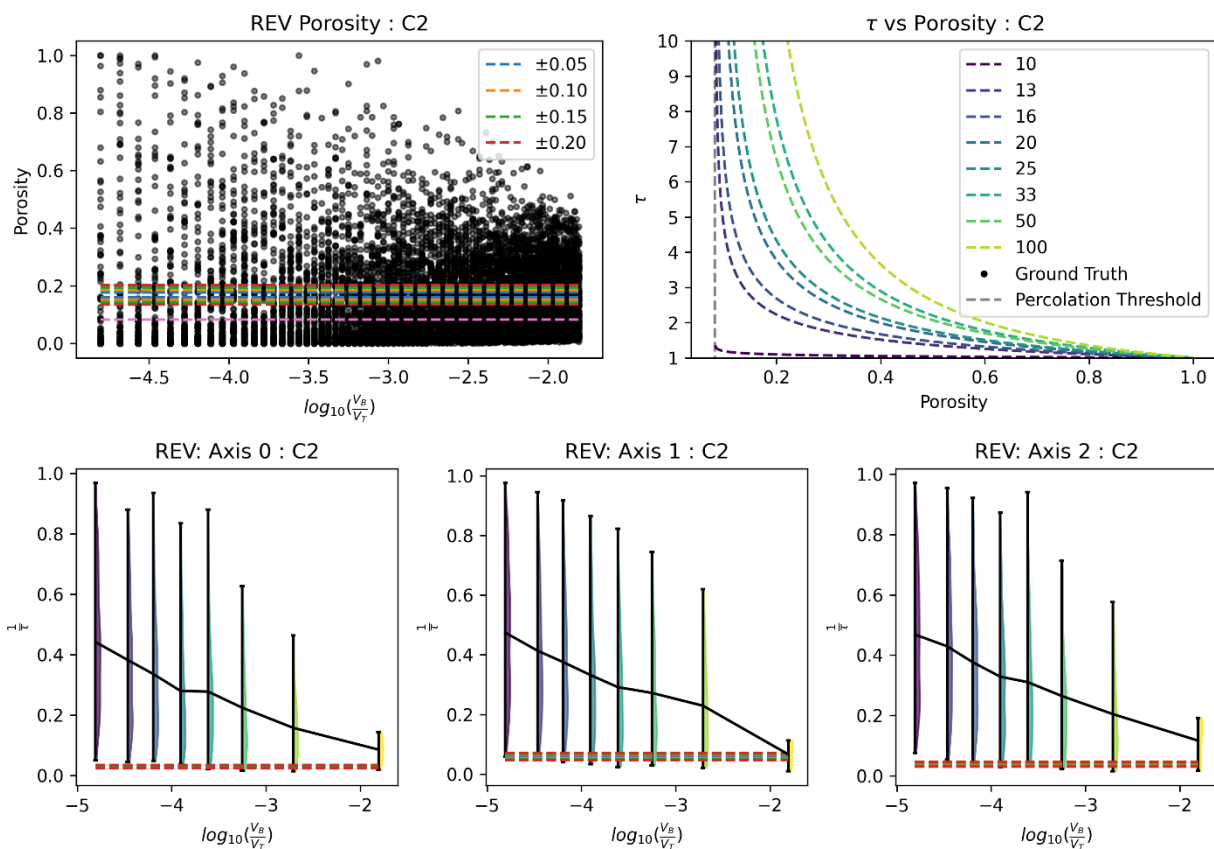


Figure 60 – Macro plot for C2.

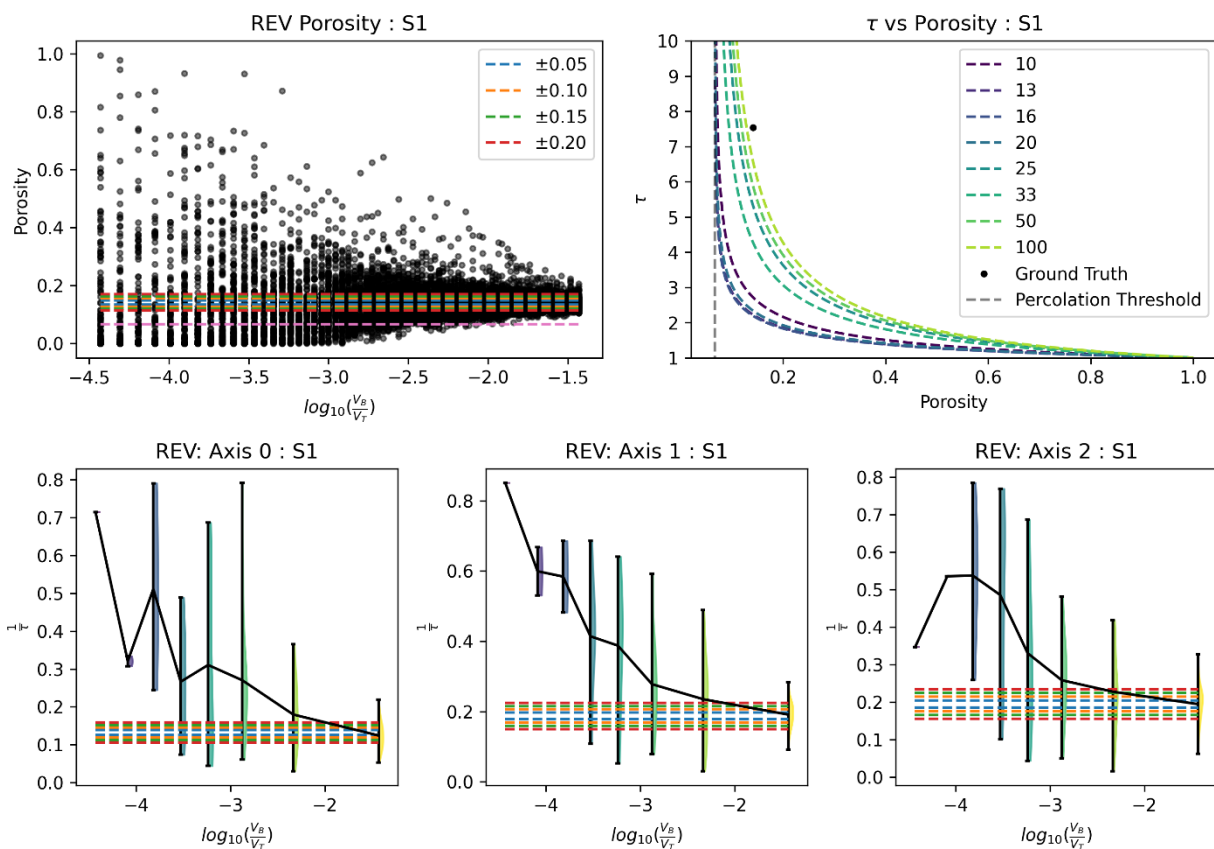


Figure 61 – Macro plot for S1.

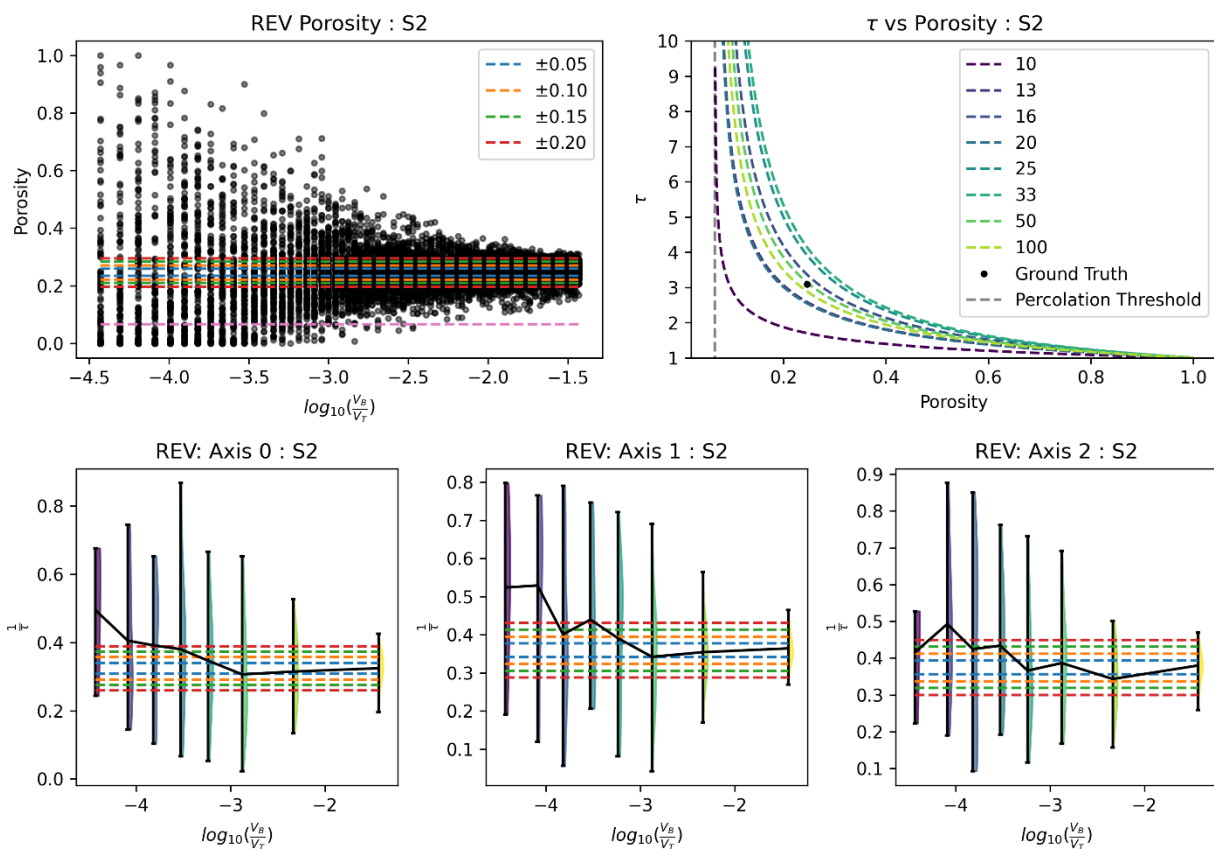


Figure 62 – Macro plot for S2.

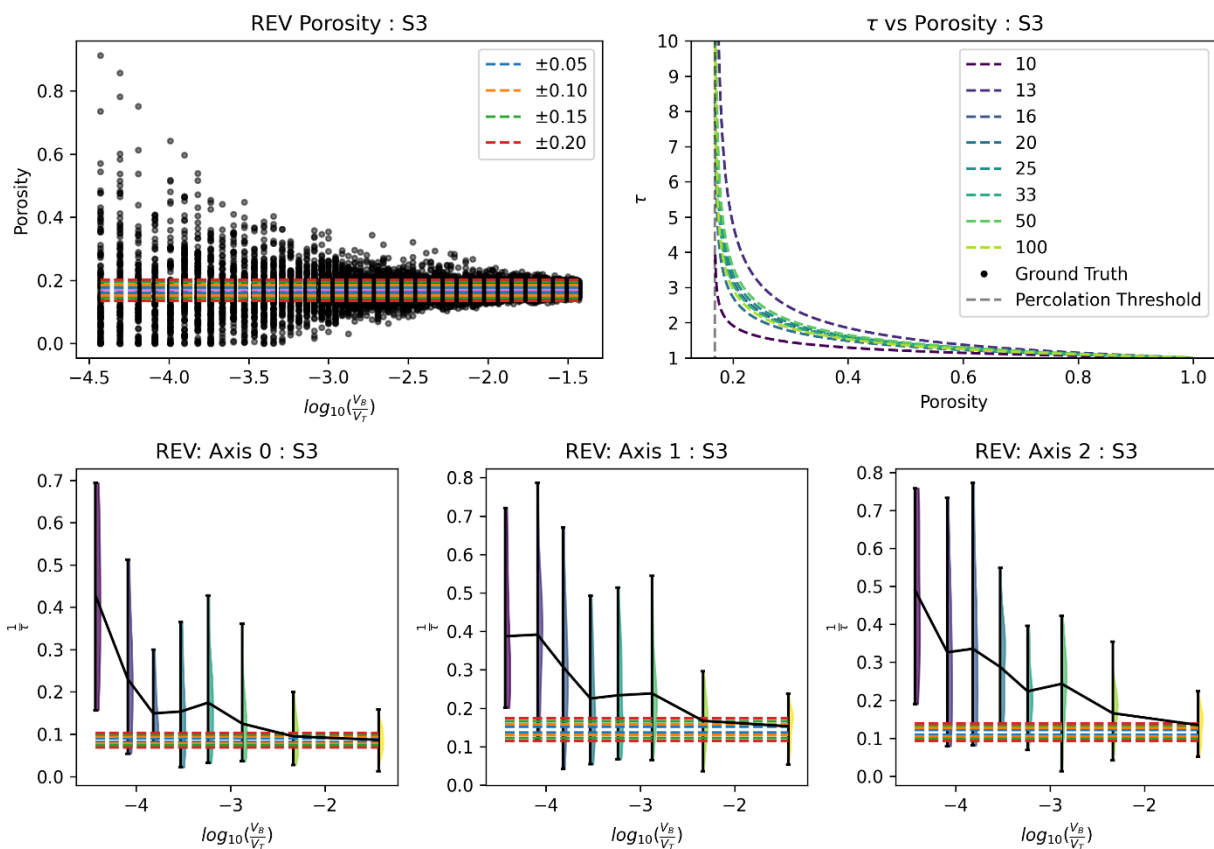


Figure 63 – Macro plot for S3.

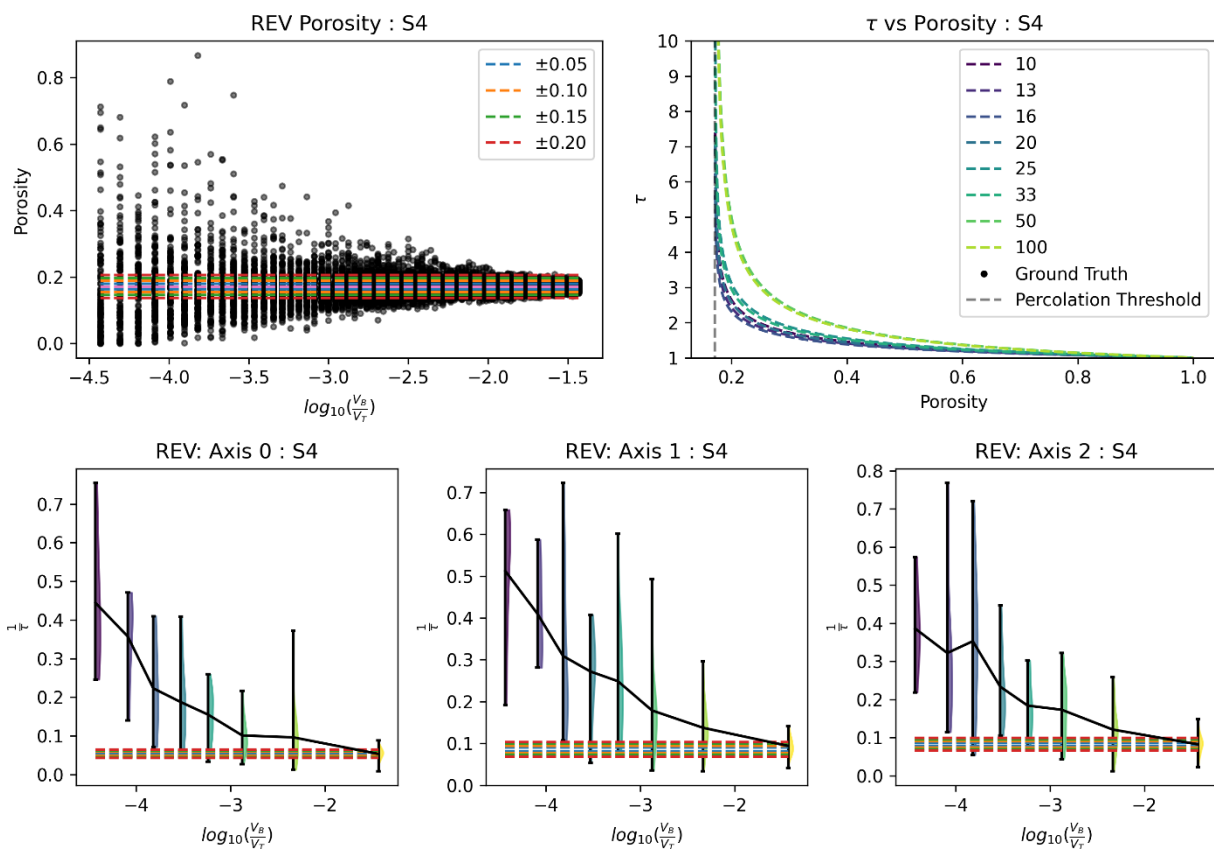


Figure 64 – Macro plot for S4.

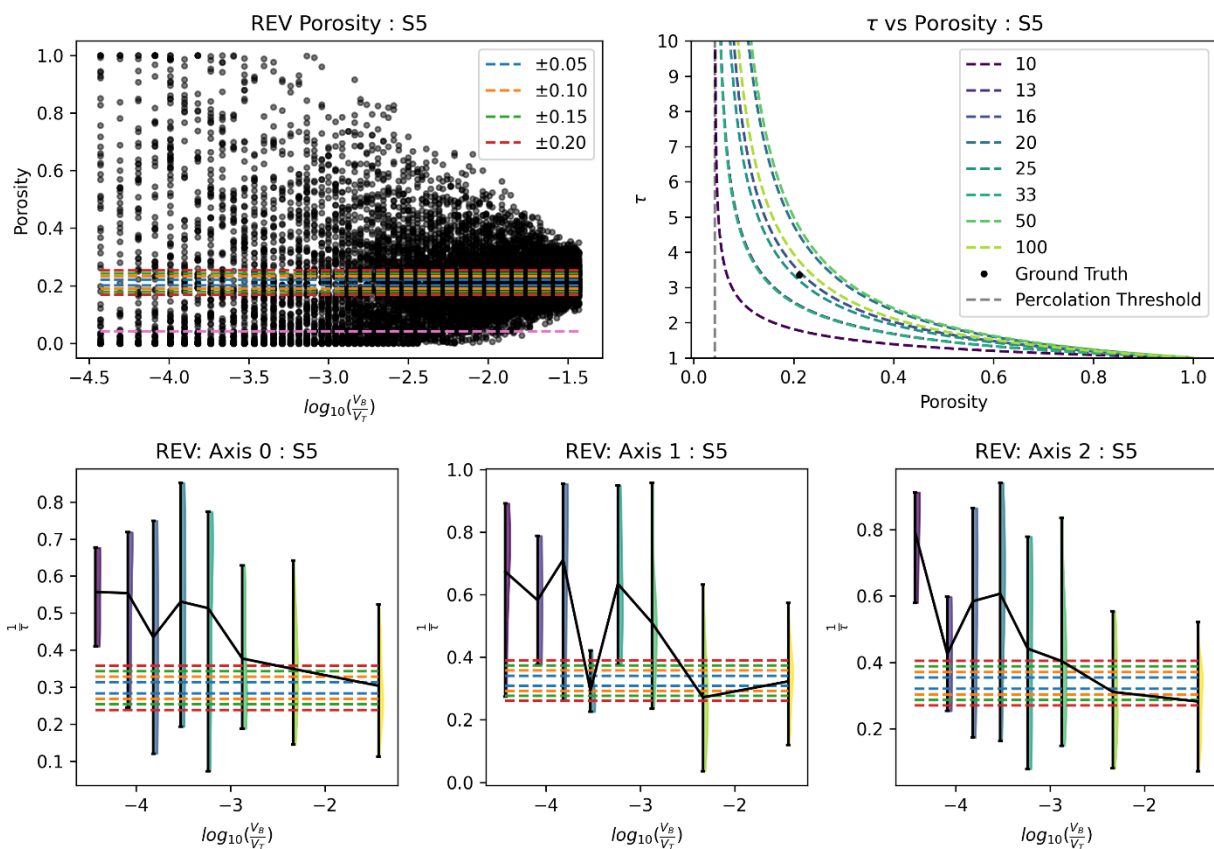


Figure 65 – Macro plot for S5.

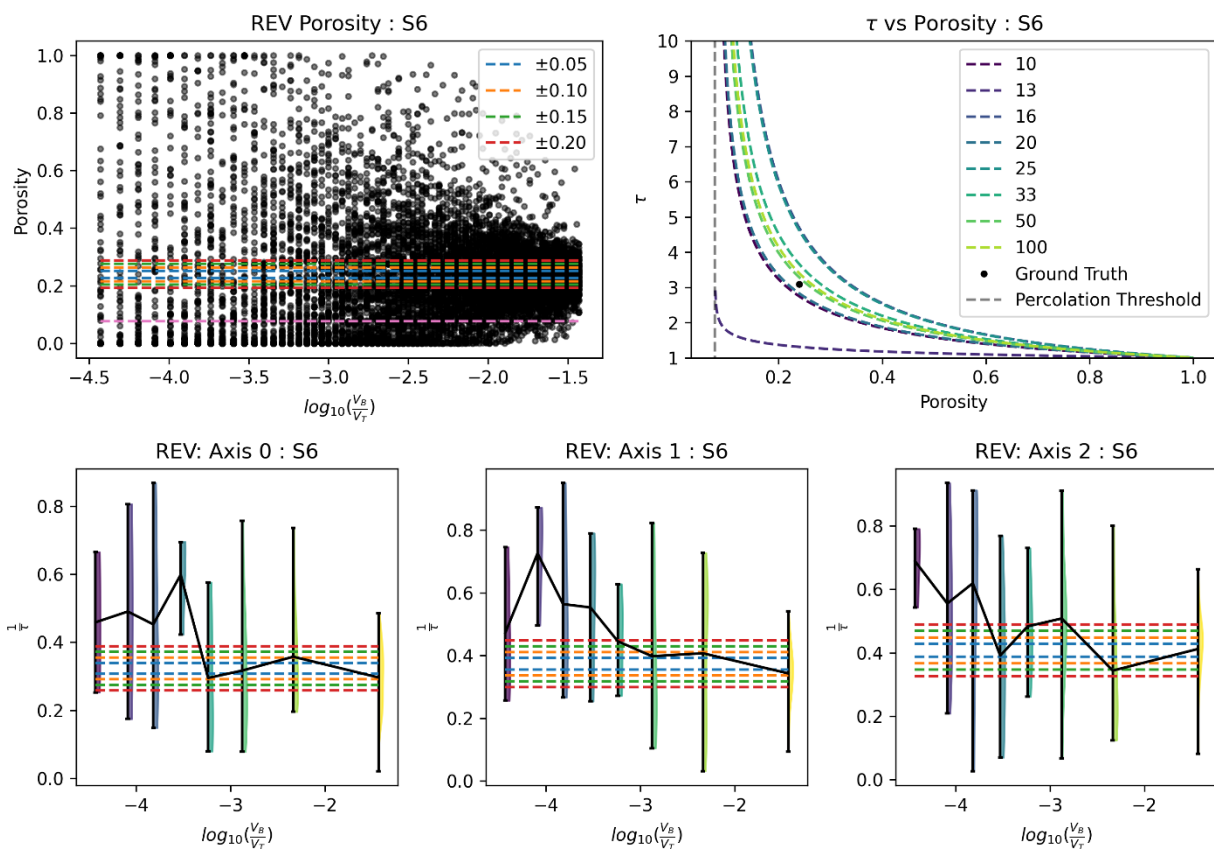


Figure 66 – Macro plot for S6.

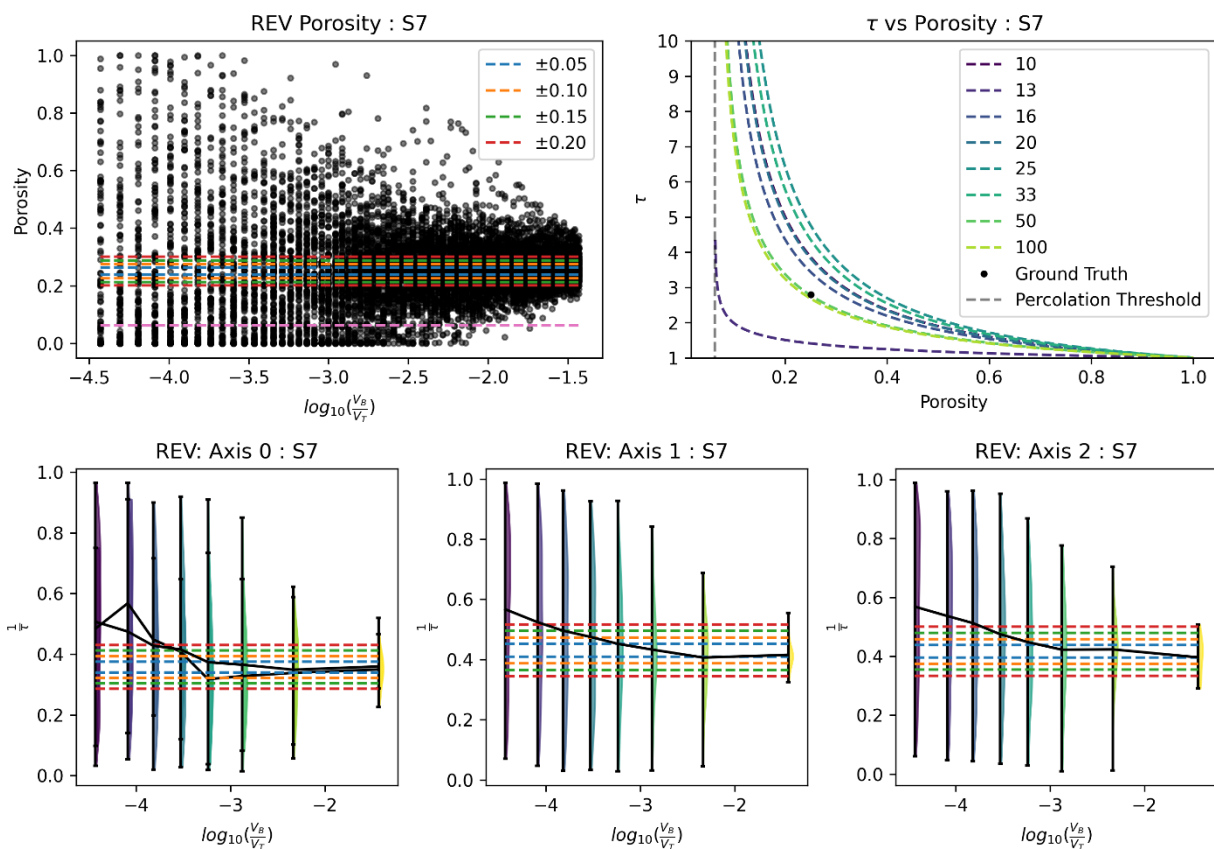


Figure 67 – Macro plot for S7

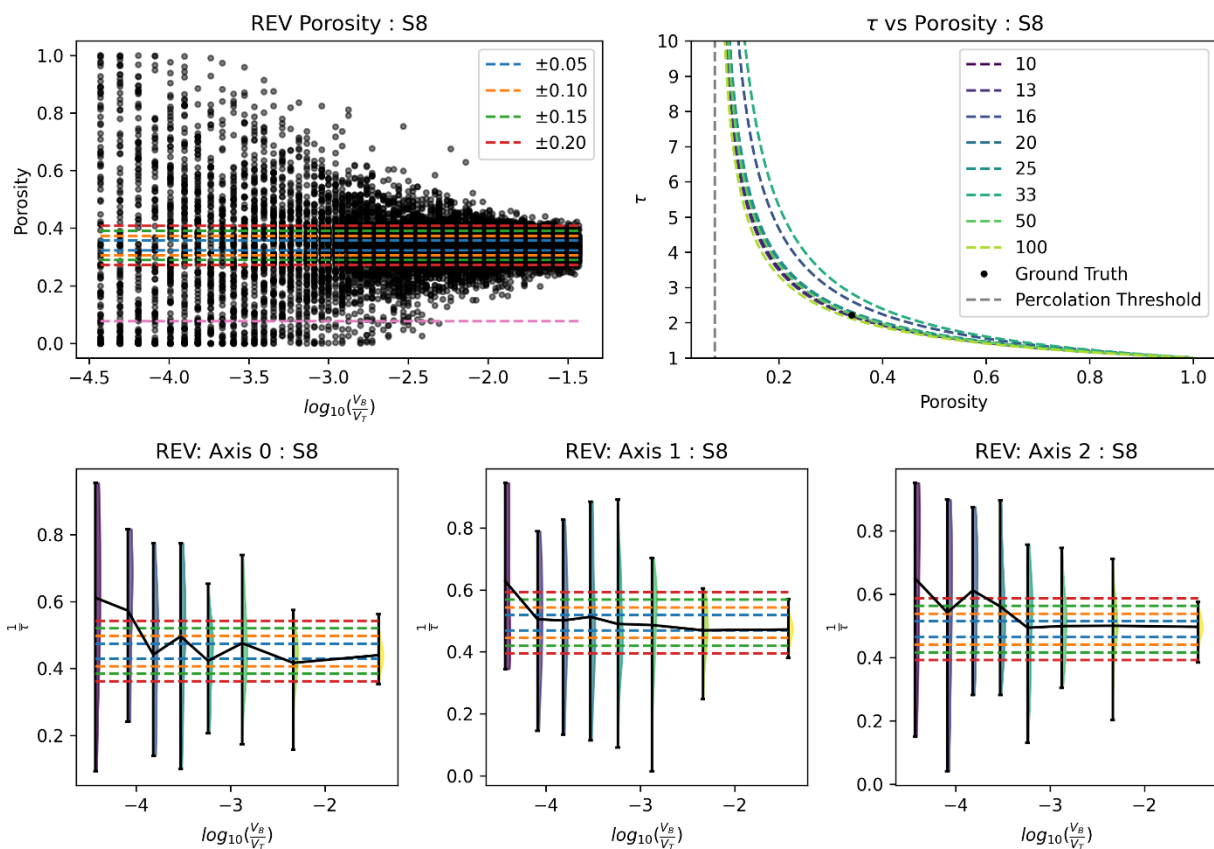


Figure 68 – Macro plot for S8.

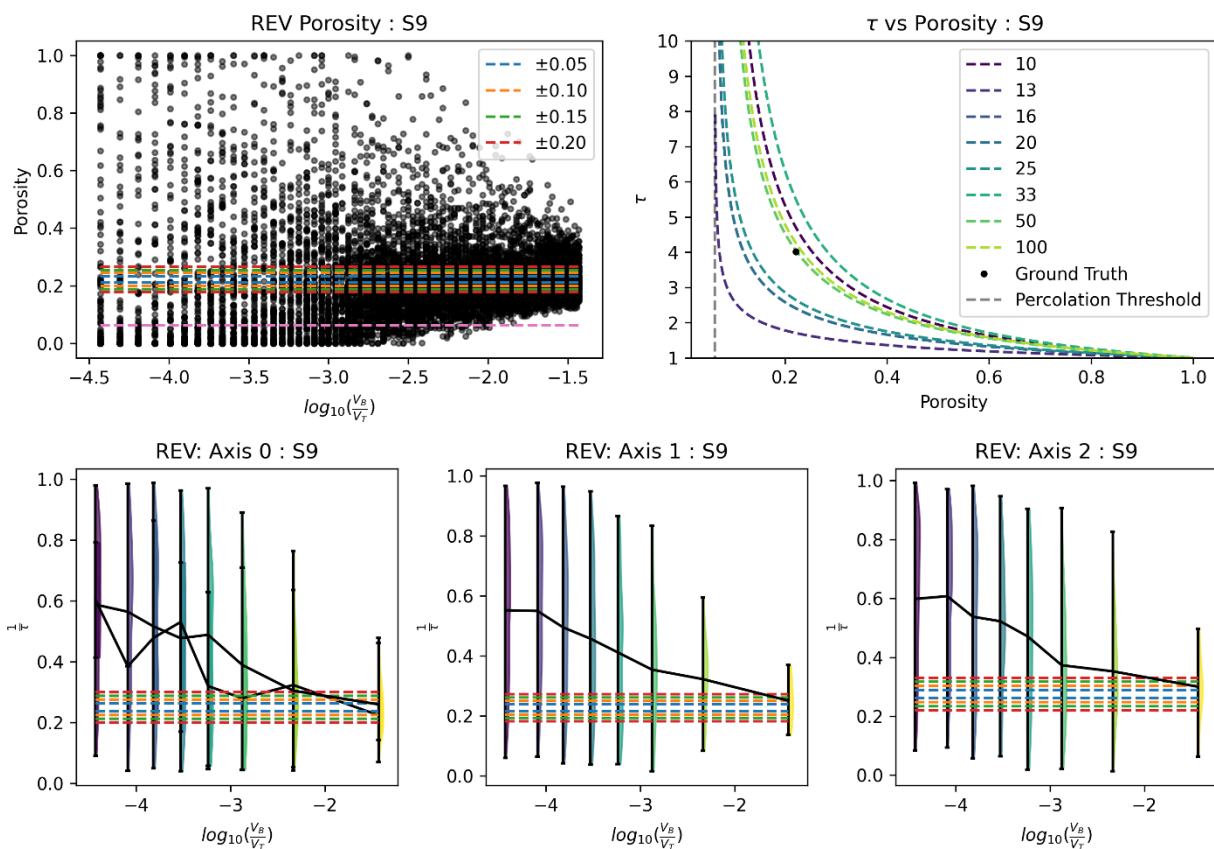


Figure 69 – Macro plot for S9.

14. Appendix F Tortuosity Prediction Plots

The following plots contain the excluded information for the tortuosity prediction plots found in section 6.

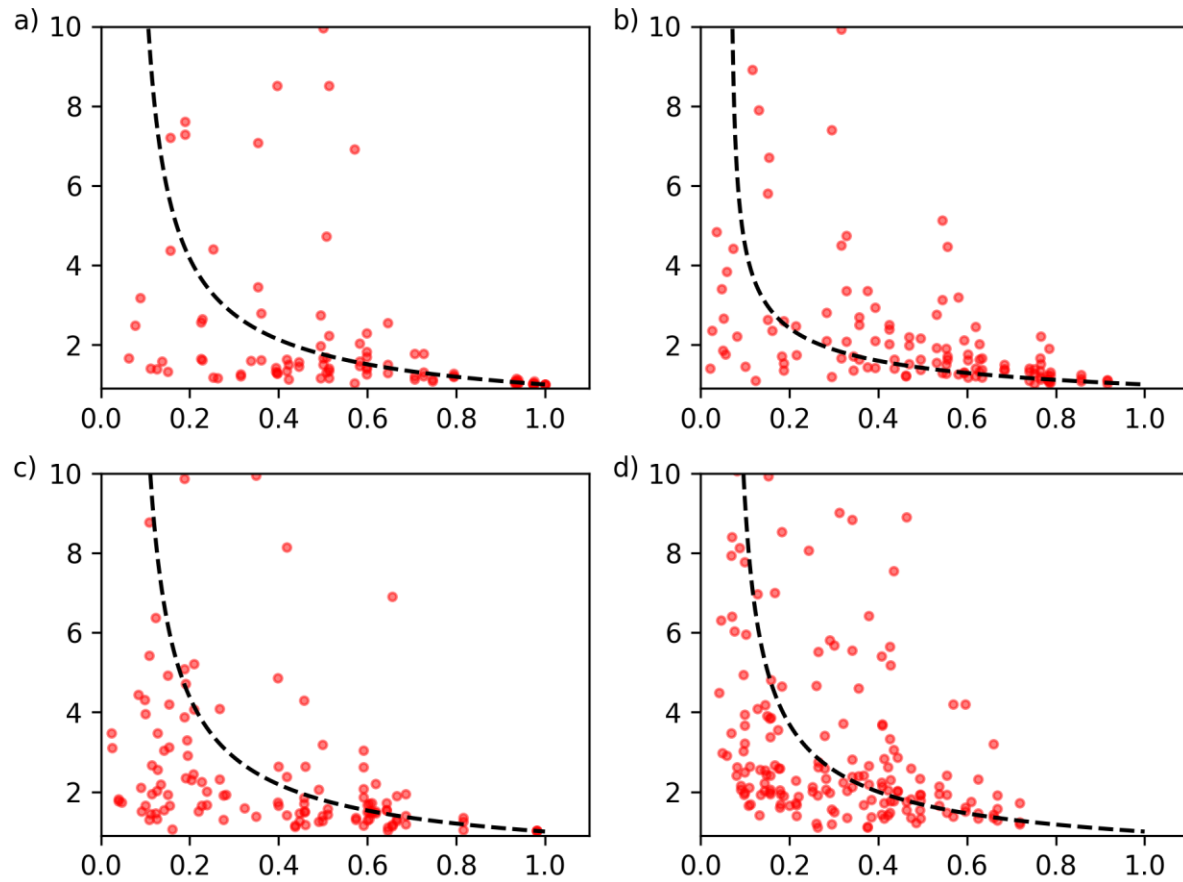


Figure 70 – Tortuosity vs porosity data for C1.

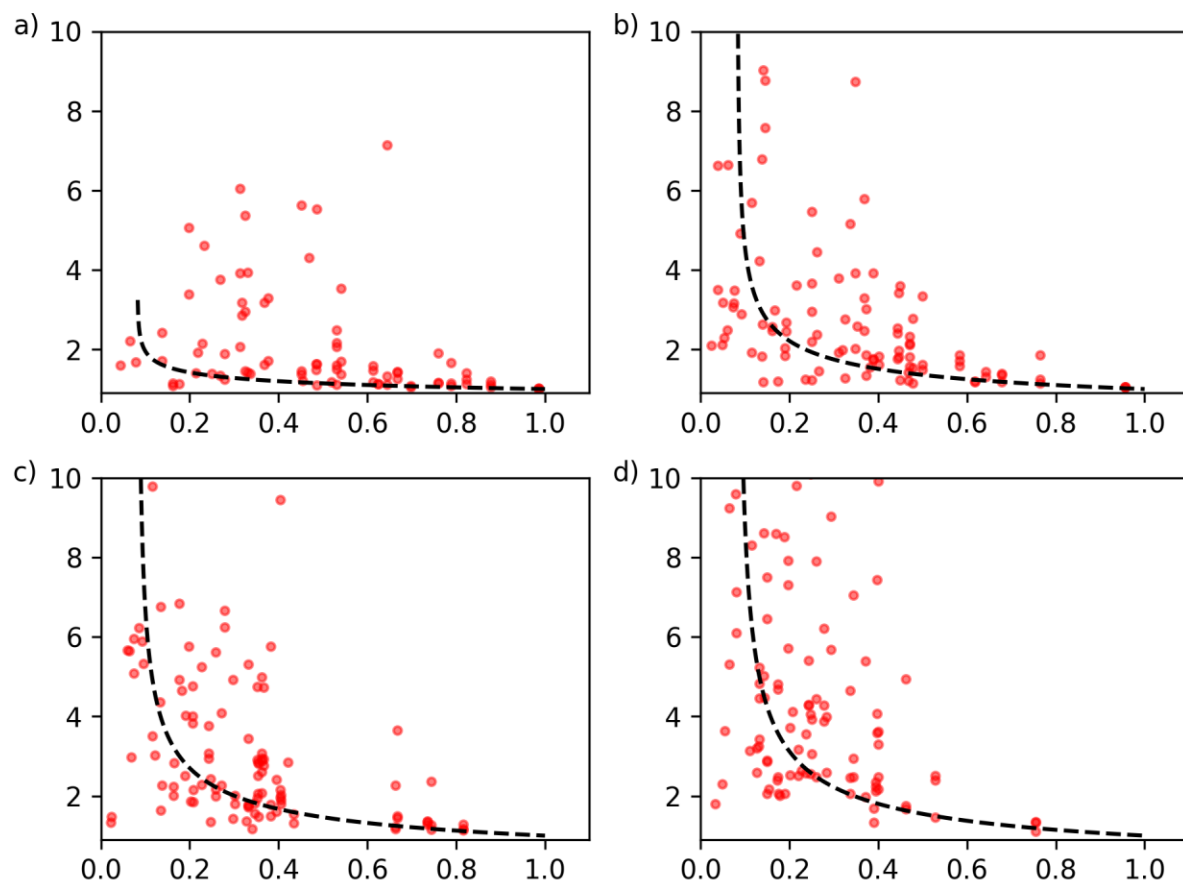


Figure 71 – Tortuosity vs porosity data for C2.

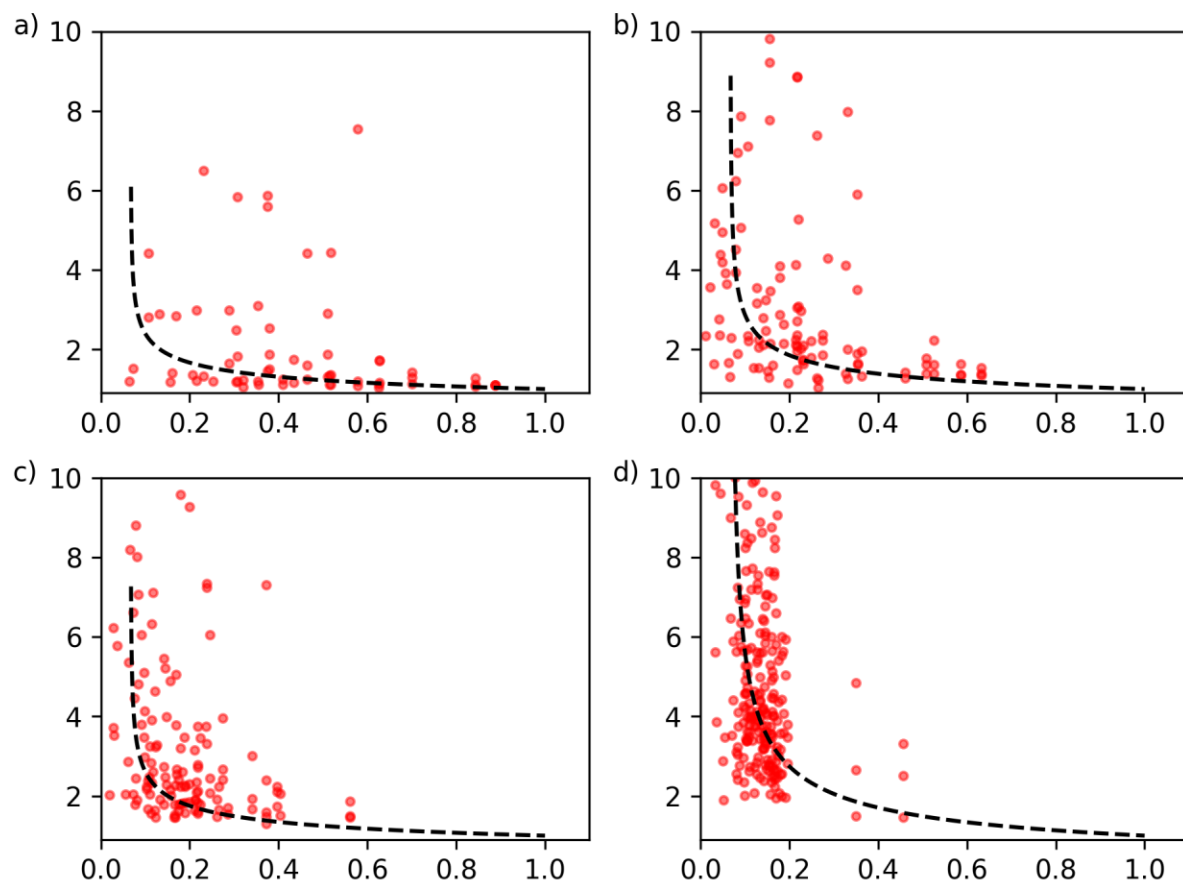


Figure 72 – Tortuosity vs porosity data for S1.

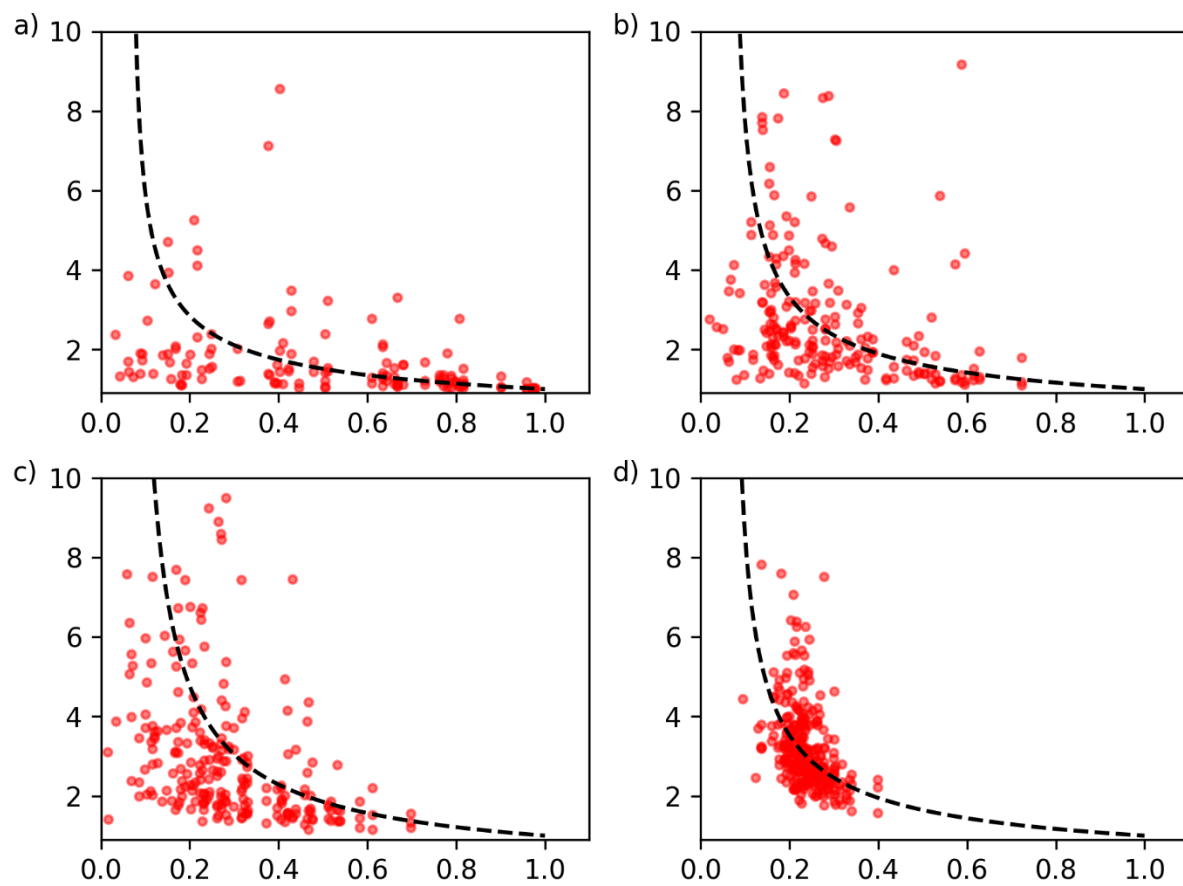


Figure 73 – Tortuosity vs porosity data for S2.

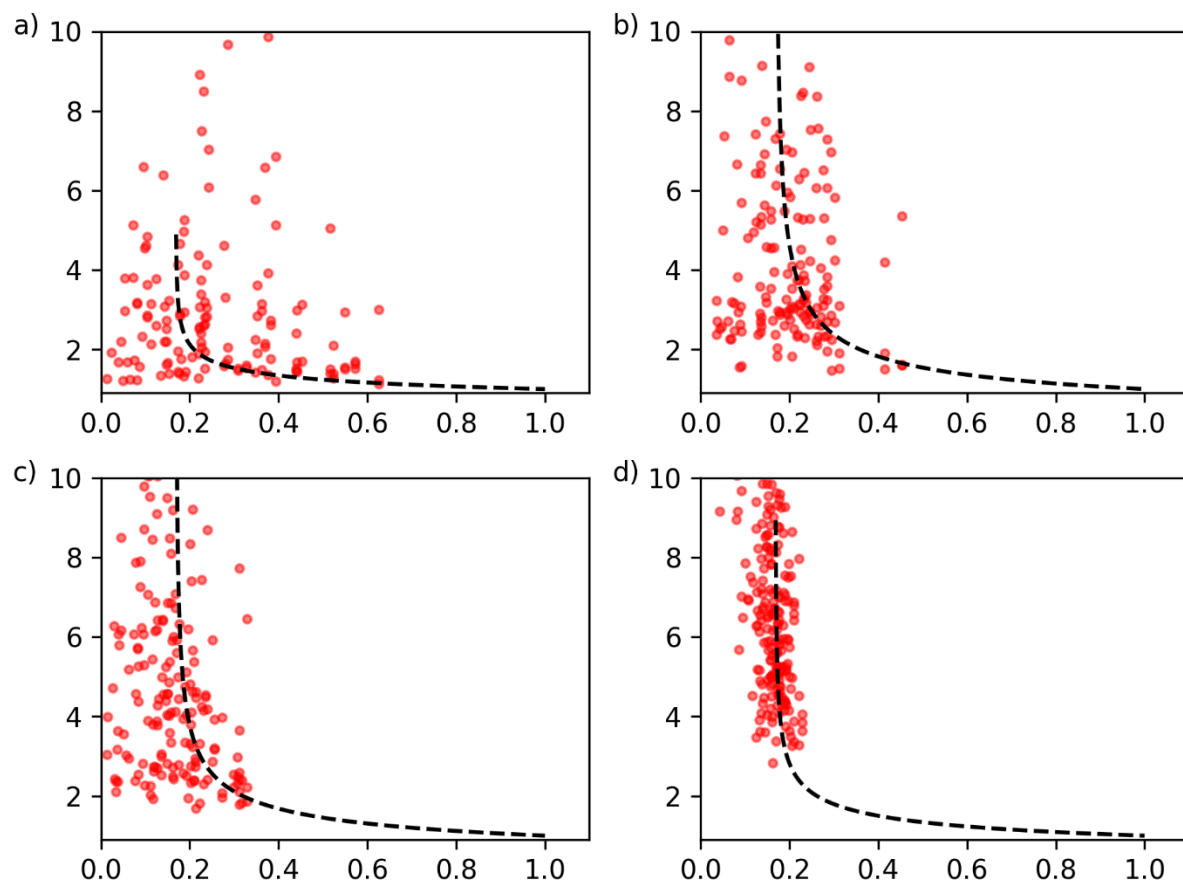


Figure 74 – Tortuosity vs porosity data for S3.

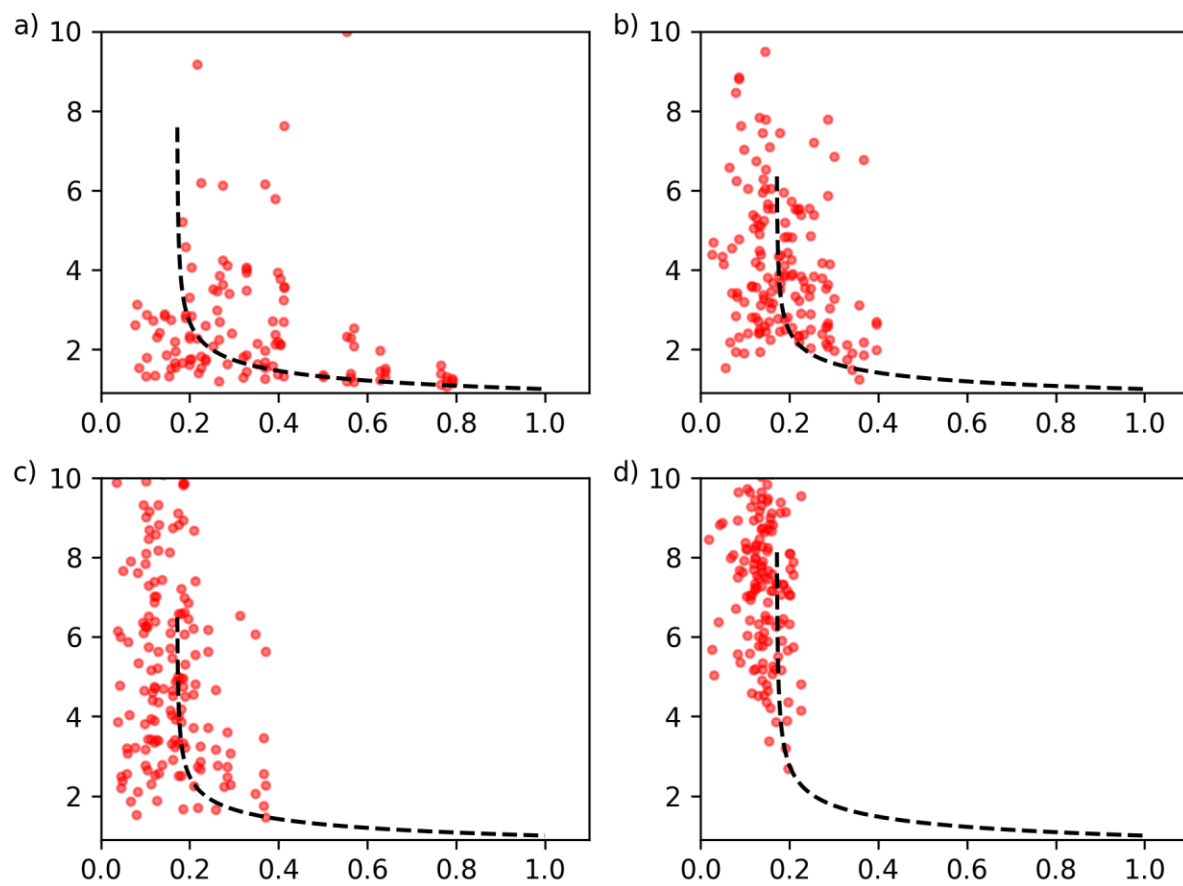


Figure 75 – Tortuosity vs porosity data for S4.

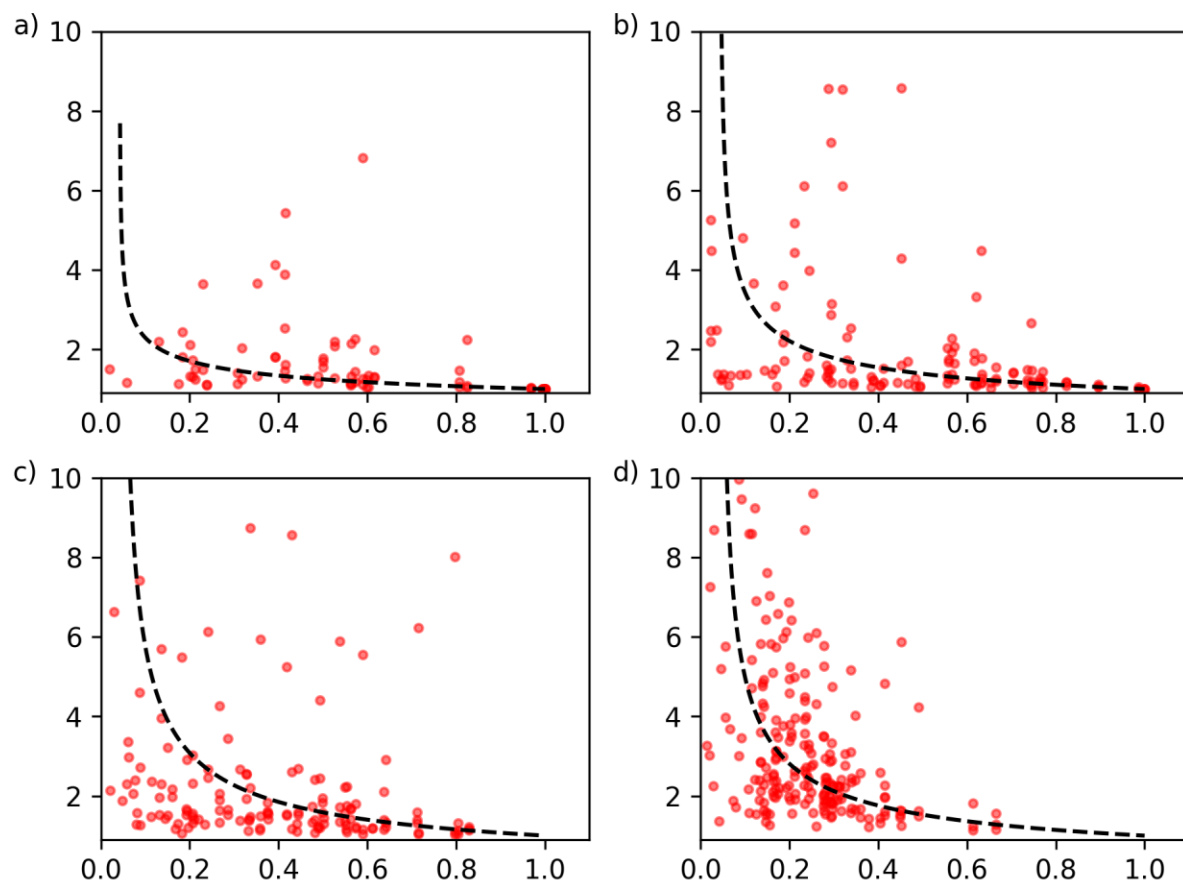


Figure 76 – Tortuosity vs porosity data for S5.

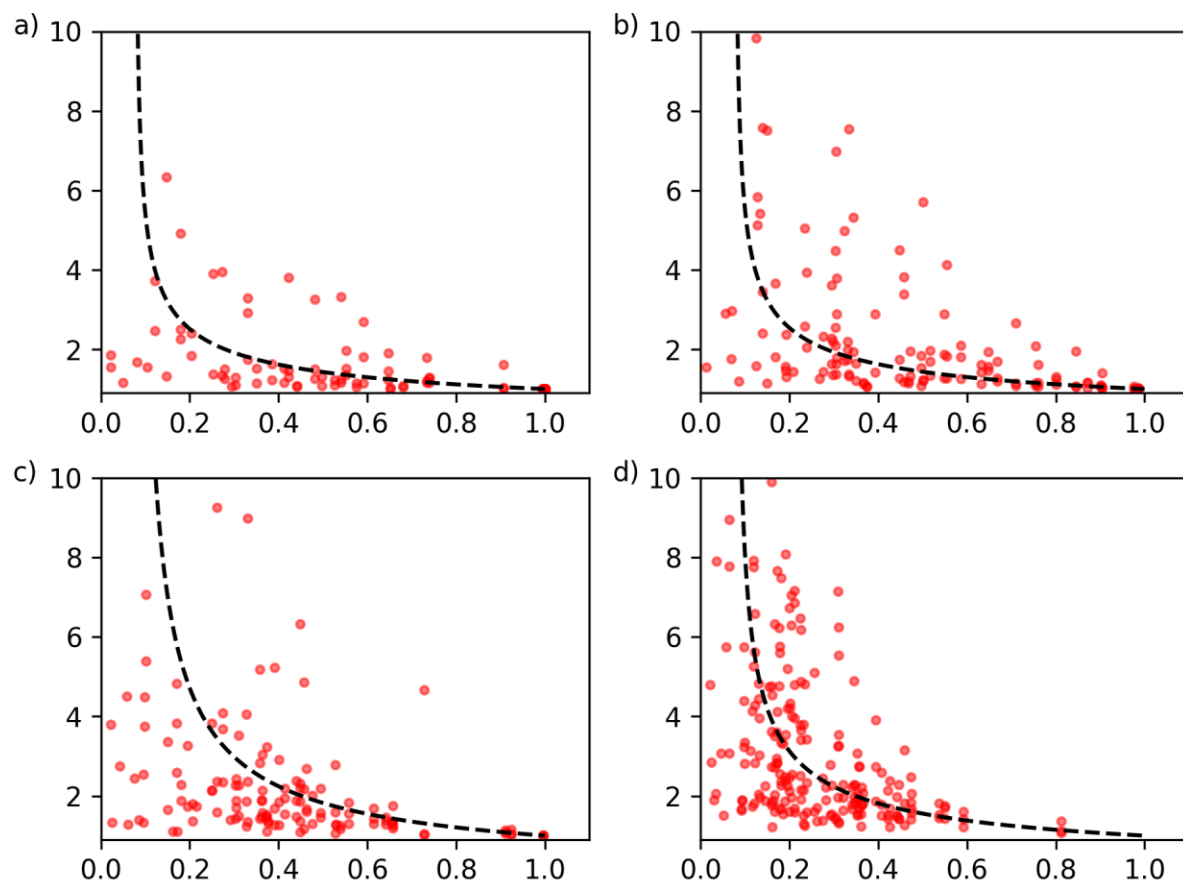


Figure 77 – Tortuosity vs porosity data for S6.

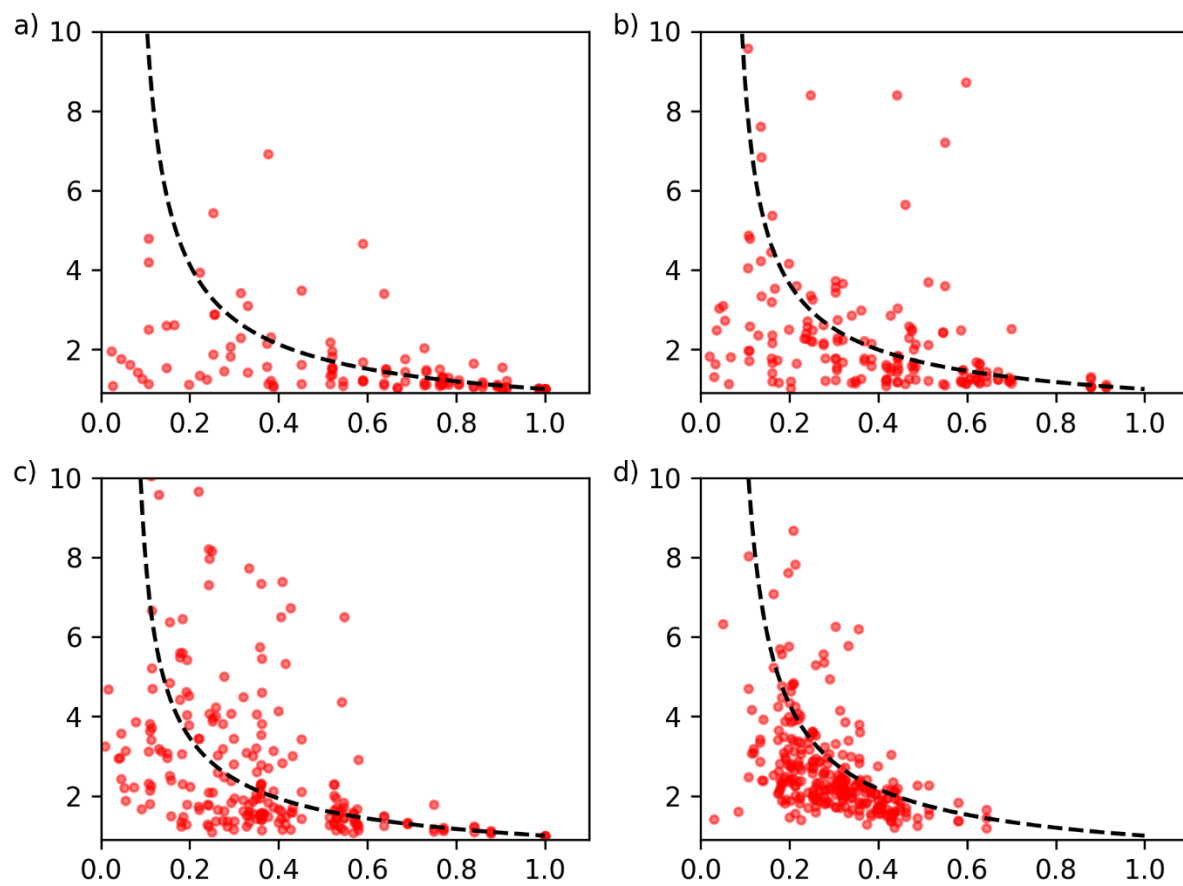


Figure 78 – Tortuosity vs porosity data for S7.

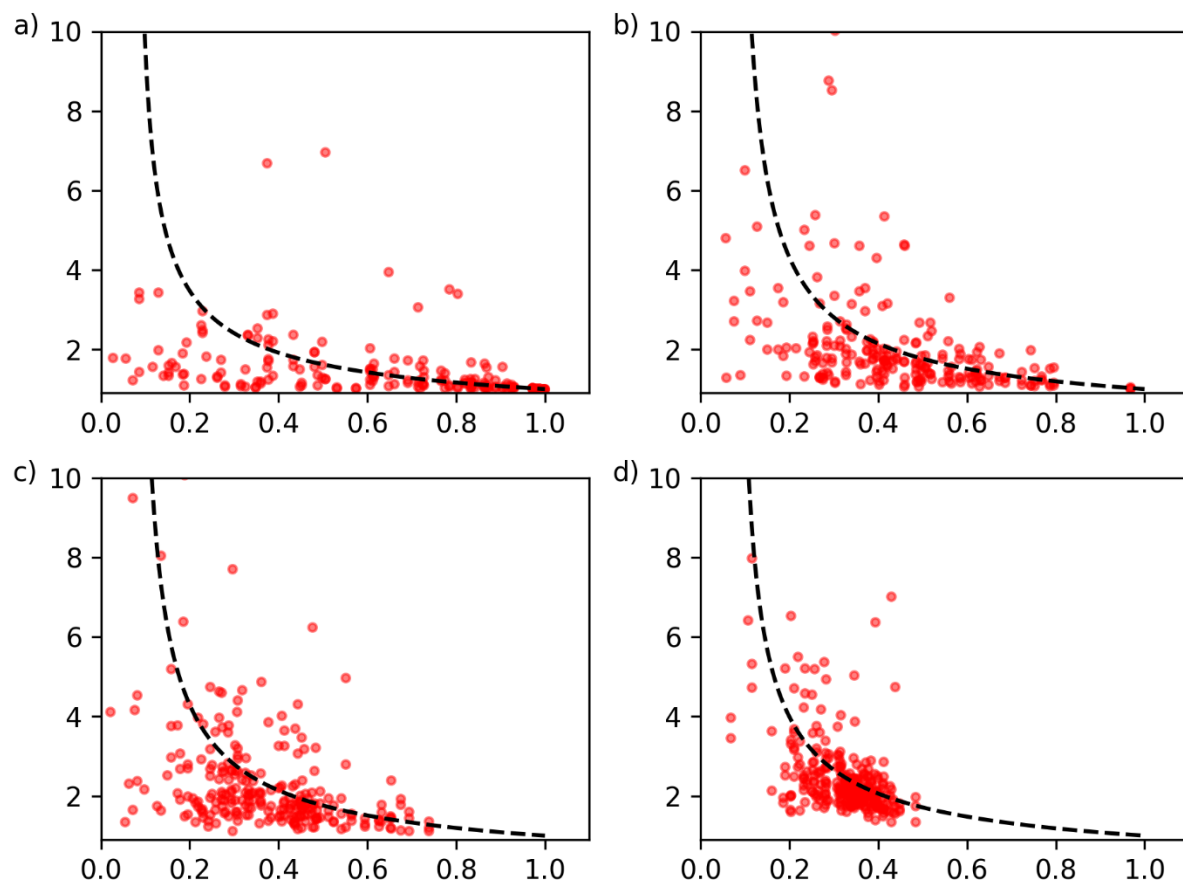


Figure 79 – Tortuosity vs porosity data for S8.

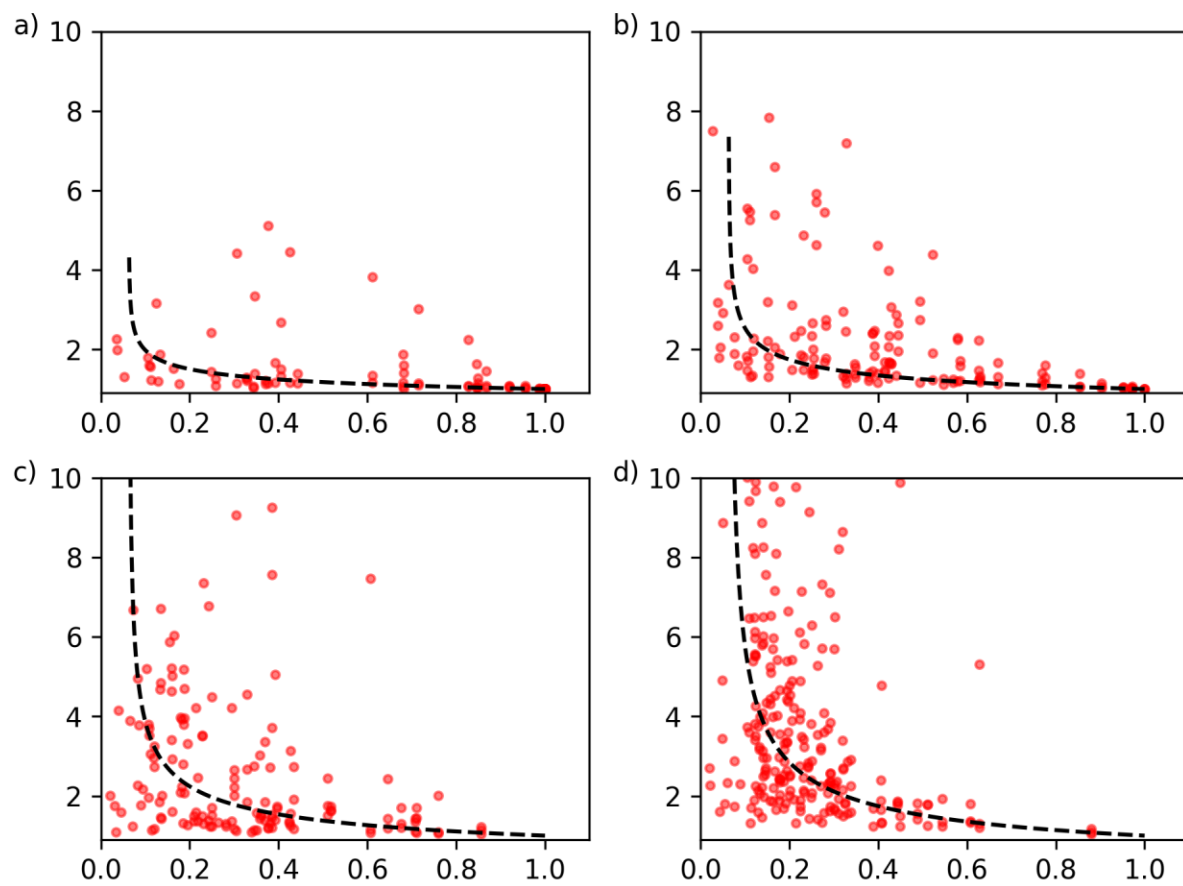


Figure 80 – Tortuosity vs porosity data for S9.

15. Appendix G TS Model Coefficients

Table VIII details the coefficient values for all subdomain sizes.

Table VIII – All coefficient values solved for using numerical methods.

	Image Name											
Subdomain Size	A1	C1	C2	S1	S2	S3	S4	S5	S6	S7	S8	S9
10³	0.9480	0.7347	0.1702	0.2616	0.5377	0.2298	0.2934	0.2953	0.4570	0.7383	0.6196	0.2116
13³	0.8195	0.4549	0.3870	0.3163	0.6187	0.4690	0.2676	0.4403	0.4627	0.6739	0.7283	0.2888
16³	1.0983	0.7599	0.4839	0.2872	0.8042	0.4056	0.2709	0.6239	0.7690	0.6466	0.7254	0.4197
20³	0.9172	0.6737	0.5550	0.5182	0.6497	0.3170	0.3034	0.5734	0.5659	0.7605	0.6896	0.5442
25³	0.8309	0.7695	0.6024	0.6304	0.7833	0.3986	0.3826	0.6538	0.6987	0.8896	0.6841	0.6204
33³	0.7766	0.7069	0.7874	0.6213	0.8138	0.3734	0.3394	0.5762	0.7574	0.9942	0.7757	0.8548
50³	0.7355	1.0006	0.8830	0.7690	0.6847	0.4019	0.5068	0.8591	0.7676	0.6984	0.6553	0.7889
100³	0.7239	1.3249	1.1851	0.7241	0.6457	0.3365	0.4647	0.7614	0.6775	0.6171	0.5918	0.7968