UNIVERSIDADE DE SÃO PAULO
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Topological study of reservoir rocks and acidification processes using
complex networks methods

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Topological study of reservoir rocks and acidification processes using
complex networks methods

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To my beloved parents.

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“Somewhere, something incredible is waiting to be known.”
Carl Sagan

ABSTRACT

ANDREETA, M. B. **Topological study of reservoir rocks and acidification processes using complex networks methods.** 2017. 117 p. Thesis (Doctor in Science) - Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, 2017.

The X-Ray imaging technology opened a new branch of science in which the internal porous structure can be captured and the reconstructed volume can be used for fluid flow simulations and structural measurements. However, there is still the question of how the internal structure of the pore space impacts in the observed simulations. A way to characterize this internal structure is by simplifying it into well-defined elements and the interaction between them, describing it as a network. The interaction between elements are the edges of the network and elements are the nodes. This opens the possibility of applying complex network theory on the characterization of porous media which has proven to give powerful insights into how the structure of porous materials influences on the dynamics of the permeating fluid. The problem with this description is in definition of the basic elements that will compose the network, since there isn't a consensus on this definition. The purpose of this work is to provide a method to analyze μ CT data through networks in which the separation of the space is done in a semi-continuous method. The recovering of the pore's local geometry is captured through a network analysis method of centrality, instead of a geometrical definition. This way the intrinsic morphology of the samples is what governs the pore-space separation into different entities. The method developed is based on the network extraction method Max Spheres Algorithm (MSA). The volumetric data is recovered through a network composed by *sphere cells*. The output of this process are two distinct networks: the complete volume network and a network which represents the variation of the channel's diameter. These networks give unbiased real information on pore connectivity and can provide important data to better understand the morphology and topology of the samples. This method was successfully applied to samples of Berea sandstone, Estailades carbonate, and to characterize the morphology of *wormholes*. Wormhole is the denomination of the channel formed after the application of an acid treatment as a stimulation procedure of an oil reservoir, a method of EOR (Enhanced oil recovery). This treatment consists of a reactive fluid flow injected in the inner rock of the reservoir, which creates a preferential path (*wormhole*) that optimizes the extraction of the hydrocarbon fluids.

Keywords: Digital rock. Petrophysics. Pore networks. Complex networks. Wormhole.

RESUMO

ANDREETA, M. B. **Estudo topológico de rochas de reservatório e processos de acidificação por métodos de redes complexas**. 2017. 117 p. Tese (Doutorado em Ciências) - Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, 2017.

A microtomografia de raios-X permitiu a evolução de uma nova área da ciência aplicada a meios porosos: a Rocha Digital. Através desta técnica, todo o espaço poroso é recuperado, e é possível entender a dinâmica do fluido que o permeia através de simulações computacionais. No entanto, ainda há a questão de como a estrutura do meio influencia nos resultados observados. Entender questões como conectividade e clusterização de regiões podem dar informações valiosas sobre como a origem do meio poroso influencia na dinâmica do fluido que o permeia. Esta avaliação do meio é possível através da simplificação do mesmo em uma rede de conexão de elementos básicos e as interações entre estes. O problema com a descrição do meio poroso em uma rede de conexão é que não existe um consenso na definição destes elementos básicos. O propósito deste trabalho foi encontrar uma maneira de descrever o meio que fosse aplicável a qualquer litologia, e que se aproximasse ao máximo dos dados extraídos pela micro tomografia para a análise das topologias de diferentes rochas através de teoria de redes complexas. Para isso, utilizamos o algoritmo robusto de extração de redes de poros, *esferas máximas*, como base para dividir o espaço-poroso em células esféricas. Desta forma, todo o volume do espaço poroso observado através da micro tomografia é recuperado e descrito em uma rede de conexão. O resultado final do método aplicado é uma rede que descreve o meio completo e uma rede que descreve o eixo medial das interconexões entre poros. A geometria local dos poros é recuperada através de um critério de centralidade de rede, assim a separação é governada pela morfologia intrínseca das amostras, ao invés de fatores geométricos. Desta forma podemos analisar o efeito da tortuosidade real do meio, assim como a interconexão entre poros, com relação a permeabilidade do meio. O método se mostrou eficaz na análise de rochas com diferentes litologias: arenito (Berea) e carbonato (Estaihlades). O método também foi aplicado na avaliação da estrutura de canais formados pelo processo de acidificação de rochas (wormholes).

Palavras-chave: Rocha digital. Petrofísica. Rede de poros. Redes complexas. Acidificação.

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1 INTRODUCTION

The structure of porous materials is of interest in several areas, from the extraction of oil and gas¹ to agriculture, construction and health. For instance, porous ceramics are used for water filtration,² a concern for health issues. Bone is a porous structure, and osteoporosis is also a major health concern.³ Porous materials are also used to dispose of radioactive waste.⁴ Soil is a porous medium, its structure govern water transport, important in agriculture;⁵ finally, the porous properties of cement is an important area of research on construction.⁶

The range of approaches to understand the porous structure is proportional to the range of applications. Two main characteristics are of interest of most areas: porosity and permeability. Porosity is the bulk volume of the porous space and governs the medium's storage capacity. Permeability is a quantification of the ability of a fluid to go through the porous medium.

There are many experimental techniques for the quantification of these properties. Our group focuses in two: nuclear magnetic resonance (NMR) and digital rock. We have applied NMR relaxometry on the characterization of siliciclastic rocks,⁷ cement⁸ and collaboration with work of osteoporosis evaluation.⁹ A technique for the synthesis of ceramics with controlled porosity was also developed¹⁰ and there is continuous research on the development of the NMR techniques to observe molecular dynamics inside porous media.¹¹

The Digital Rock front acts as a powerful complementary technique to understand the characteristics of porous materials. The acquisition of the pore space with high resolution made possible the development of a realistic simulation of the interactions of the fluid molecules with the pore space. Through techniques of statistical physics, an algorithm for the simulation of NMR relaxometry has been developed in our laboratory as well, with great results.¹²

One of the questions that remained unanswered, however, is how the interconnection of the pore space influences the experimental results seen in NMR and other techniques. In order to answer this question, we propose a statistical analysis of the pore space through the data acquired through μ CT imaging, with the application of complex networks theory.

There have been successful applications of network theory to understand the complexity of the interconnecting porous space of soils.¹³ The work of *Valentini et al.* observed the small

world property of fracture networks.¹⁴ Other works have compared the fluid flow properties with the statistical characteristics of fracture networks.^{15–19} Network models were also used to understand the dynamics of bacterial leaching through soil.²⁰ Other works focused on the granular structure of porous media.^{21–22} Networks have also been applied in the study of bone structure.^{23–26} More recently, the work of *van der Linden and A. Narsilio* were able to correlate the measurement of the closeness centrality of pores in pore-throat networks to the permeability of the samples.²⁷

Even though the reduction of the volumetric data from μ CT imaging to a network can be a powerful technique to acquire the main features of the porous structure, there is the question of what algorithm of network extraction should be used. There are many techniques that have been developed over the years.^{23,28–39} Each technique aims at acquiring different features of the pore space, relevant for the application proposed.

Since our proposal is to understand topological features of the pore space for any porous media, we needed a general method that was robust and allowed the acquisition of the pore space morphology with minimum loss of all of its features. For that reason, we developed a “*intermediate*” network extraction method in which the pore-space is separated into sphere cells. This method is based on the well-established maximum spheres algorithm,^{28,30–31} and works as an intermediate reduction of the pore-space between the commonly used pore-throat network and the volumetric data. Through this method we were able to apply network theory on the networks extracted from samples with very different topologies: sandstone, carbonate and wormhole formations.

Wormhole is the denomination of a pathway formed after the application of an acid treatment as a stimulation procedure for the reservoir, a method of EOR (Enhanced oil recovery). This treatment consists of a reactive fluid flow injected in the inner rock of the reservoir, which creates a preferential path (*wormhole*) that optimizes the extraction of the hydrocarbon fluids.^{40,41} Therefore, the characterization of the wormhole’s structure is of vital importance to assess the efficiency of the stimulation procedure.

Knowing that the permeability of rock cores is governed by the number of interconnections between the pores through pore throats, the developed method is able to distinguish the regions considered as throats from the regions considered as pores. Instead of simply based on geometrical properties of the pore-space, the method uses the centrality of nodes to make this separation.

1.1 OBJECTIVES

The main objective of this work is the development of a network extraction method that could retain and model properties such as tortuosity of the samples and flux through porous media. Another requirement is that the network extraction should be able to work independently of the lithology of the samples. To verify this, the method is applied to a sandstone sample, a carbonate sample, and a glass sphere packing sample. Then the final networks properties are compared to results from direct simulations on the volumetric data. Finally, we use network theory to understand how the topology of the samples influences on the expected permeability and flow.

1.2 THESIS ORGANIZATION

The thesis is organized as follows: On chapter 2 we make a summary of complex networks theory applied in this work. Chapter 3 presents the samples used and the basis of the μ CT imaging and the simulations on the volumetric data. In Chapter 4 we discuss the different methods for network extraction and the basis of the developed software. Finally, chapters 5 and 6 present the results and conclusions of this work respectively.

2 COMPLEX NETWORKS

The mapping of complex systems into networks is proving to be a good alternative for the characterization of their complexity, and the reason behind it is that recent studies of real life networks are presenting evidences that there is a set of laws which are common to all of them.

With the development of technology, scientists were able to acquire information from larger samples of real networks, and very interesting characteristics of these networks started to emerge. The study of the topology of the Web,⁴²⁻⁴³ showed that it has properties that separates it from random graphs, such as the scale free degree distribution, and small world effect. What was more impressive is that those properties appear to be part of other complex systems.

As we have discussed before, the application of network theory on porous media has given promising results into characterizing their structure. In this chapter we will make a short summary of the basis of graph theory and the measurements applied in this work.⁴³⁻⁴⁴

2.1 GRAPH THEORY

An *undirected* graph G is defined by a pair of sets $G = (V, E)$ where V is set of *node* elements $v_i \in V, i = 1, \dots, N$, and E is the set of *edges* or links that connects a pair of different *nodes* $i, j \in V$. The nodes that are connected by the *edge* (i, j) are said to be *adjacent*, or *neighbors*. The mathematical representation of these connections can be done through what is called the *adjacency matrix* $\mathbf{A} = \{a_{ij}\}$. This is a $N \times N$ matrix defined such that:

$$a_{ij} = \begin{cases} 1, & \text{if } (i, j) \in E \\ 0, & \text{if } (i, j) \notin E \end{cases} \quad (2.1)$$

A property of this structure is that, for undirected graphs, $a_{ij} = a_{ji}$, resulting in a symmetric matrix. Another important characteristic is that, if there are no *self-loops*, meaning, no node connected to itself, the main diagonal of the matrix is zero.

Figure 1 - Example of EDT applied to a 2D slice of a Berea sandstone. (a) the binary original image (b) the resulting EDT. The color scale represents the calculated distance of each pixel to the wall.

Source: By the author

Usually it is useful to assign to the edge a real value, called *weight*, that represents the strength of the connection. This value is modelled according to the problem being tackled. For instance, if the network represents the connection between computers composing the internet, the edge's weight can represent the bandwidth of data that can flow between computers. In this case of weighted networks, the adjacency matrix is not binary, but instead the position (i,j) represents the weight of the connection of nodes i and j.

Closely related to the adjacency matrix, we have the definition of the *graph's Laplacian*. The definition of the graph Laplacian matrix is given by the diffusion processes in networks. If we have a substance on the nodes of the network, the node i with the amount Ψ_i , the rate at which the substance Ψ_i changes overtime, given it can move along the edges of the graph, is described as:

$$\frac{d\Psi_i}{dt} = C \sum_j a_{ij} (\Psi_j - \Psi_i) \quad (2.2)$$

where C is the *diffusion constant*. So, the equation (2.2) states that the substance will move along the nodes which are connected, this information given by the adjacency matrix elements. We can rewrite equation (2.2), splitting into two terms:

$$\frac{d\Psi_i}{dt} = C \sum_j a_{ij} \Psi_j - C \Psi_i \sum_j a_{ij} \quad (2.3)$$

We can make use of the notion of *node degree*, which is the number of connections the node has. In an undirected graph, the node's degree is simply defined as:

$$k_i = \sum_j a_{ij} \quad (2.4)$$

Making use of the result in equation (2.4) on equation (2.3), we can write:

$$\frac{d\psi_i}{dt} = C \sum_j (a_{ij} - \delta_{ij}k_i)\psi_j \quad (2.5)$$

δ_{ij} is the Kronecker delta. We can easily see that equation (2.5) can be rewritten in matrix form:

$$\frac{d\boldsymbol{\psi}}{dt} = C(\mathbf{A} - \mathbf{D})\boldsymbol{\psi} \quad (2.6)$$

where $\boldsymbol{\psi}$ is the vector whose components are the quantities ψ_i of each node i , $\mathbf{A}$ is the adjacency matrix, and $\mathbf{D}$ is the diagonal of the nodes degree:

$$D = \begin{pmatrix} k_1 & 0 & \dots \\ 0 & k_2 & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \quad (2.7)$$

Combining the two matrices, we have a new matrix such as:

$$\mathbf{L} = \mathbf{D} - \mathbf{A} \quad (2.8)$$

And we see that equation (2.6) becomes:

$$\frac{d\boldsymbol{\psi}}{dt} + C\mathbf{L}\boldsymbol{\psi} = 0, \quad (2.9)$$

The new matrix $\mathbf{L}$ is called the *graph's Laplacian*, since (2.9) is the same form as the diffusion equation for a gas, except that the Laplacian operator ∇^2 has been replaced by the matrix $\mathbf{L}$. Using the definition on equation (2.8), the elements of the matrix $\mathbf{L}$ are defined by:

$$L_{i,j} = \begin{cases} k_i, & \text{if } i = j, \\ -1, & \text{if } i \neq j, (i,j) \in E, \text{ and } i \text{ connected to } j \\ 0, & \text{otherwise,} \end{cases} \quad (2.10)$$

The *graph's Laplacian* is a symmetric real valued matrix. In the context of diffusion, the spectrum decomposition of $\mathbf{L}$ can be used to solve equation (2.9). We can write the vector Ψ as a linear combination of the Laplacian eigenvectors $\mathbf{v}_i$:

$$\mathbf{L}\mathbf{v}_i = \lambda_i\mathbf{v}_i, \quad (2.11)$$

$$\psi(t) = \sum_i \phi_i(t)\mathbf{v}_i, \quad (2.12)$$

with the coefficient for the i^{th} node $\phi_i(t)$ changing over time and λ_i the eigenvalue corresponding to the $\mathbf{v}_i$ eigenvector. Substituting into (2.9), we get:

$$\sum_i \left(\frac{d\phi_i(t)}{dt} + C\lambda_i\phi_i(t) \right) \mathbf{v}_i = 0, \quad (2.13)$$

from which we get:

$$\frac{d\phi_i(t)}{dt} + C\lambda_i\phi_i(t) = 0, \quad (2.14)$$

and finally, we can get the variation over time of the coefficients for each node:

$$\phi_i(t) = \phi_i(0)e^{-C\lambda_it}, \quad (2.15)$$

So, given the initial condition of the coefficients and knowing the spectrum of $\mathbf{L}$, we can solve for the state at any later time. The graph's Laplacian gives insight on how the topology of the graph influences in the dynamic of the system.

2.2 CENTRALITY MEASURES

The reach of the diffusion processes in the network will be correlated with the *paths* between nodes. A path is defined as a sequence of nodes such that every pair of consecutive nodes in that sequence is connected by an edge.

$$p(u_i) = \{u_i, u_{i+1}, u_{i+2}, \dots, u_n\}, (i, i+1) \in E \quad (2.16)$$

Usually, two nodes will be connected by many *paths*. However, the number of *independent or disjoint* paths between two nodes is considerably smaller. Two paths are said to be independent if they connect the same two nodes but don't share any edges. The number of independent paths is a measure of how strongly connected the two nodes are. A highly connected network is said to be robust, since it is necessary that many nodes or edges are removed to disrupt the flow of information on this network.

This is easily visualized if we take the internet as an example of a robust network. If just the connection (edge) to one computer (node) is removed, it is highly unlikely that the flow of information will stop. However, this will depend on how *important* this node is. If the node removed is a computer acting as an internet hub, this will affect the flow of information, disconnecting other nodes. So, this computer will have a *higher centrality* on the network.

Moreover, two nodes may not become disconnected even if a large group of edges are removed. An important measure of connectivity is the *minimum cut set*, or the minimum number of edges that, if removed, will disconnect a pair of nodes. If each edge's weight represents the maximum flow capacity between this pair of nodes, the *maximum flow* between this pair of nodes will be the sum of the weights of the edges of the *minimum cut set* between this pair.

The *maximum-flow: minimum cut* correlation takes in consideration the constraints that must be followed so the maximum flow can be calculated correctly. If we consider a flow network $G(s, t, c)$, such that two of its nodes are selected to be the source s and the sink t of

flow and each edge (u,v) has a capacity $c(u,v) > 0$ associated to it, we would have the following constraints:

- (a) The flow along an edge cannot exceed its capacity: $f(u,v) < c(u,v)$;

So, for each edge e there will be a **residual capacity** associated to it, given a flow f such as $r(e) = c(e) - f(e)$. This will originate a new network called the residual network $G_r(s,t,r(e))$ that models the amount of available capacity on the original network G .

- (b) The net flow from u to v must be the opposite of the net flow from v to u : $f(u,v) = -f(v,u)$;

- (c) Flow conservation: the sum of incoming flow to a node must be equal to the amount of flow going out:

$$\forall u \in G, \sum_{u \neq v}^{ne} f(u,v) = 0, ne = \text{number of neighbors of } v.$$

- (d) The total flow originated in s must be equal to the flow arriving in t .

The residual network $G_r(s,t,r(e))$ is the basis of the **Edmonds-Karp** algorithm that finds the maximum flow. The idea of the algorithm is that, while there is a path on the residual network, such as $t \in p(u_i)$ and $r(u_i, u_{i+1}) > 0$, the maximum flow isn't yet reached. The paths $p(u_i)$ are called **augmenting paths**.

Applying **Edmonds-Karp** algorithm to pore-networks can provide the path of maximum flow of that sample, given a source point and a sink. However, the question remains of how we can measure the impact of each pore in the path chain. As it was stated before, the impact of the removal of a hub in a computer network is much larger than removing an ordinary computer. There are different ways we can score a node's centrality on a network, we will discuss in the next session the metrics chosen for this work.

2.2.1 Geodesic paths and the betweenness/closeness centrality

As it was discussed before, the concept of a path is the basis of the definition of distance between two nodes. Considering an undirected unweighted graph, this distance is simply a measure of the number of *steps* one needs to take after departing of the node u to reach node v . In geographical networks, such as the pore-network, each node has a real position on tridimensional space. So, instead of simply taking the number of steps between two nodes, we can measure the real distance that a particle starting from u had to transverse to reach v .

However, as we have seen before, there can be many possible paths between nodes u and v . The shortest path l_{ij} between all possible ones is called *geodesic path* between two nodes.

The *typical diameter* of a network is defined as the maximum length between all possible *geodesic paths*:

$$d = \max_{i,j}(l_{i,j}) \quad (2.17)$$

Through the shortest paths, we can characterize the local influence of the nodes on the information distribution through the network, namely the *nodes' centrality*. One direct measure of centrality is the node *closeness centrality*:

$$g_i = \frac{1}{\sum_{i \neq j} l_{i,j}} \quad (2.18)$$

This measure gives larger centrality to nodes that have small shortest path distance to all others.

Another very relevant measure is how often a node appears in the shortest paths between other nodes. This measurement is given by the *betweenness centrality*:

$$b_i = \sum_{k \neq j \neq i} \frac{\sigma_{k,j}(i)}{\sigma_{k,j}} \quad (2.19)$$

where $\sigma_{k,j}$ is the total number of shortest paths that starts from node k and ends in node j and $\sigma_{k,j}(i)$ is the number of these shortest paths that go through node i . This measure is called betweenness centrality because usually nodes with high b will be nodes that act as bridges between groups of other nodes. Since information, in most cases, passes through shortest paths, these nodes play an important role on information spread.

Even though the betweenness centrality and closeness centrality already provide important information on the topology of the networks, we concentrated our efforts into two more centrality measures. We will explain them further in the next sections.

2.2.2 Current flow betweenness centrality

The previous discussed methods of assessing centrality are limited, since they consider only geodesic paths. This is problematic, since if a path is just slightly longer than the geodesic path it is disregarded and the number of shortest paths that is premediated by each node is not taken into consideration at all. Another criticism is that information is not able to *split* between paths. A solution to account for this information was the development of a *centrality based on current flow*.

An electrical network is a graph with positive edge weights indicating either the *conductance* or the *resistance* to the passage of current, note that the conductance and resistance are related: $c(e) = 1/r(e)$ for all $e \in E$. Here, we consider a network of **resistors**, in which the nodes are the junctions between the resistors.

The Kirchhoff's law applied to this network, with V_i the voltage at node i , measured relative to a convenient reference potential,

$$\sum_j a_{ij} \frac{V_j - V_i}{r(i,j)} + b(v) = 0, \quad (2.20)$$

The current $b(v)$ represents the external current flowing through node v , due to the reference nodes s and t that being connected to an external voltage. The node v in which $c > 0$ it is called a *source*, if $b(v) \neq 0$ it is called an *outlet*, and the node v in which $b(v) < 0$ is called a *sink*. We will consider the case that a unit current enters the network at a single source s and leaves it at a single sink t , i.e:

$$b_{st}(v) = \begin{cases} 1, v = s \\ -1, v = t \\ 0, otherwise \end{cases} \quad (2.21)$$

Here, the graph's Laplacian again dictates the topology's influence on the total current flow. Rewriting equation (2.20) we get:

$$\sum_j (\delta_{i,j} k_i - a_{ij}) V_j = Rb(v), \quad (2.22)$$

Or in matrix form:

$$\mathbf{LV} = \mathbf{rb} \quad (2.23)$$

The centrality of each node by using this model of electrical network, needs to be unique for each node. In other words, the currents that passes in each edge must be unique. This only happens if we have *absolute potentials*, such as $p(i,j) = p(j) - p(i)$ for all node pairs in G . However, one of the properties of the Laplacian is that at least one of its eigenvalues is zero, making it a not inversible matrix. This implies that we can add any multiple of the eigenvector $(1,1,1..)$ to the solution and get another valid solution. In order to obtain a restricted system, we fix one of the potentials on a selected node as zero (removing the correspondent column and row from the Laplacian matrix).

Solving (2.23) for the current b of each node, we can define the current flow betweenness centrality as the sum of the current passing in each edge connecting to its neighbors. We know that the total throughput in a node i will be:

$$T_i = \frac{1}{2} \left(-|b(v)| + \sum_j |b(i,j)| \right) \quad (2.24)$$

And, accordingly, the measure of centrality, averaged for all node pairs, will be:

$$CF_i = \frac{1}{(n-1)(n-2)} \sum_{s,t \in V} T_i^{st} \quad (2.25)$$

2.2.3 Eigenvector centrality

The eigenvector centrality is a variation of the node centrality based on the node's degree. The node's degree is an important measure of centrality since a well-connected node will most probably belong to most paths of communication of the network. Moreover, when

we are analyzing pore networks, the measure of number of connections of a pore is correlated to how permeable the medium is.

The downside of the degree's centrality is that it doesn't differentiate between neighbors. The node's centrality score is only based on the number of neighbors, but a more accurate would be to award a node a centrality proportional to the sum of the centralities of its neighbors, such as:

$$x_i = \sum_j a_{ij} x_j, \quad (2.26)$$

If we apply equation (2.26) iteratively throughout the network, assuming as an initial condition that $x_i = 1$ for all i , after n steps, the centralities of each node, in matrix form, are:

$$\mathbf{x}(n) = \mathbf{A}^n \mathbf{x}(0) \quad (2.27)$$

Similarly, as done before, the vector $\mathbf{x}(0)$ can be rewritten as a linear combination of the eigenvector of the adjacency matrix $\mathbf{A}$, $\mathbf{x}(0) = \sum_i c_i \mathbf{v}_i$, and knowing that $\mathbf{A} \mathbf{v}_i = \lambda_i \mathbf{v}_i$,

$$\mathbf{x}(n) = \sum_i c_i \lambda_i^n \mathbf{v}_i \quad (2.28)$$

There are multiple eigenvectors, in general, that can be applied to (2.28) to get the centrality score for the node. However, the idea is to ensure that all indices $\mathbf{v}_i$ be *positive*. As the adjacency matrix for an undirected graph will always be a real positive square matrix, the Perron-Frobenius theorem states that the matrix spectrum has a unique positive largest eigenvalue that the correspondent eigenvector can be chosen to have strictly positive components. Since $\lambda_1 > \lambda_i, i > 1$ we get from (2.28):

$$\mathbf{x}(n) = \lambda_1^n \sum_i c_i \left(\frac{\lambda_i}{\lambda_1} \right)^n \mathbf{v}_i \quad (2.29)$$

As $n \rightarrow \infty$, we get that the centrality $x(n) \rightarrow c_1 \lambda_1^n \mathbf{v}_1$, the limiting vector of the centralities will be the vector corresponding to the largest eigenvalue of $\mathbf{A}$.

A well-discussed problem of the eigenvector centrality is that it only works well if the graph is strongly connected. If the nodes have few connections to other, it's centrality will rapidly become **null** in this measure. However, the case of real *undirected* networks usually, the largest component is of size proportional to the networks' size, with nodes well-connected.

2.2.4 Other local measures

Two other important local measures applied in this work are the *clustering score* and the *local entropy*. The clustering score, although it is a local measurement of a node, it describes a global feature of the graph, measuring local group cohesiveness. The clustering score of node i is defined by the ratio between the connectiveness of the nodes adjacent to i to the total number nodes pairs:

$$c_i = \frac{e_i}{k_i(k_i - 1)/2} \quad (2.30)$$

where e_i is the number of connection between nodes adjacent to i and k_i is i degree, given that $k_i > 1$.

Since we are dealing with weighted graphs in this work, a relevant local measure of the heterogeneity of the edges' weights is the *local entropy*:

$$f_i = -\frac{1}{\ln(k_i)} \sum_{j \in V_i} \frac{w_{i,j}}{s_i} \ln\left(\frac{w_{i,j}}{s_i}\right) \quad (2.31)$$

where V_i is the group of nodes adjacent to i , k_i is the node's degree, $w_{i,j}$ is the edge's weight between node i and j and s_i is the node's total strength. The strength of a node is defined as the sum of all edge's weights connected to it. The local entropy will be 0 if the

node's strength is concentrated in one edge and 1 for a homogeneous distribution between edges.

3 SAMPLES AND METHODS

3.1 X-RAY COMPUTED μ TOMOGRAPHY

The X-Ray computed micro-tomography has been used in the characterization of porous materials since the evolution of the technology permitted the acquisition of information of the pore space, that is, in the order of micrometers of resolution.^{45–48} The process is based on the interaction of the X-Ray beams with the sample's material. Depending on the sample's composition, the degree in which X-Ray beams will penetrate the material will vary. This will be either by absorption of the photon, by photoelectric effect or by Compton scattering.

The photoelectric effect is the transmission of energy from a high energetic photon to an electron in the material, that absorbs this energy and disconnects from the atoms to which it was bounded. The Compton effect is the interaction of the X-Ray photon to a weakly bounded electron that changes the original wavelength of light due to loss of energy from the photon because of the interaction. The variation of the intensity of the x-ray beam due to these phenomena are described by the Lambert-Beer equation⁴⁹:

$$I = I_0 e^{-\int \mu(s) ds} \quad (3.1)$$

where I_0 is the incident beam, and $\mu(s)$ describes the attenuation due to the interaction with the material along the beam path. The exponential decay correlation with the attenuation variation is easily understood if we think of the following experiment: let N be the number of monochromatic (same energy) photons that are able to cross a homogeneous plate with width Δx . If ΔN is the number of photons that aren't able to cross by either effect described before, the rate of energy loss, due to interaction with the plate will respect the equation:

$$\frac{\Delta N}{N} = -\mu \Delta x \quad (3.2)$$

Equation (3.2) basically tells us that the rate of energy loss will be proportional to the material length Δx and the attenuation constant μ . This case μ is constant because we considered a homogeneous plate.

Now, if we consider that the width of the plate is infinitesimal, equation (3.2) becomes:

$$\frac{dN}{N} = -\mu dx \quad (3.3)$$

Considering that we have an intensity I_0 correspondent to the number $N=N_0$ of incident photons incident, we can integrate equation (3.3) which leads to:

$$\begin{aligned} \ln(I) - \ln(I_0) &= -\mu x \\ I &= I_0 e^{-\mu x} \end{aligned} \quad (3.4)$$

If the material is not homogeneous, the attenuation constant will vary along the sample. In this case, equation (3.4) becomes (3.1). This difference in attenuation according to the material type is what allows the identification of different regions on the sample. The attenuation of the beam will be correlated with the density of the material.

Figure 2 - Schematic of a X-ray tomography. The sample is placed between the X-ray source and the detector (usually an CCD screen). The beam passes through the sample and the attenuated X-Ray is captured by the screen. This information is stored and the sample is rotated, so the information can be captured in all directions.

Source: By the author

Usually, the experimental apparatus for lab-based microtomography equipment follows the schematic of Figure 2. The sample is placed between the X-ray source and the detector (CCD screen). The generated X-ray beam is in conical form, making geometrical magnification possible by changing the relative position between the sample and the source, the limitation being the focal point size and the detector resolution.

The sample is rotated so there can be enough projections to capture the information from the whole volume. Each projection is stored, and then a reconstruction algorithm uses this information to create a set of image slices, each slice representing a region (tomo) of the sample's volume.

Figure 3 - Example of the output of an image slice after the reconstruction stage. The lighter regions are the highly attenuated due to the material density. The dark regions are the low density regions, in this case air inside the pore space.

Source: By the author

The final output after the reconstruction procedure are images such as on the example shown on Figure 3. This is an image slice of an Indiana limestone rock sample that was acquired at voxel resolution of $35\mu\text{m}$. The grayscale coloring represents the density of different materials of the sample. The higher the density, lighter will be the color assigned to the voxel. The bright spots on the image are regions with high density materials. The grains

that are represented by voxels in various intensity of grey and the porous region are represented by the darker regions, the least dense regions of the sample.

After the images are acquired, before the identification of the pore space and image segmentation, the images undergo a pre-processing filtering stage to remove high frequency noise that can be residual from the image acquisition procedure. Even though the reconstruction procedure already provides a smoothing and artifact removal process, there can be still residual noise in the final images.

In this work, the pre-processing step and the segmentation of the pore space was applied with the commercial software **PERGEOS-FEI** (PerGeos)⁵⁰ (Figure 4).

Figure 4 - Usage example of the commercial software PERGEOS. Application of *Non-Local Means Filter* to eliminate high frequency noise.

Source: Adapted from PERGEOS⁵⁰

There are several possible image-processing noise removal filters, such as median and gaussian filters. The advantage of these filters is that they are fast to apply and the noise removal is efficient for most cases. However, the application of these filters results in a completed smoothed image.

Since we are mainly interested in the pore region and its morphology, in this work we applied a *Non-Local Means* filter. This filtering process has the advantage of removing the high frequency noise without losing information of the object's borders. By border we mean any region with steep transition between two grayscale values. This way we can remove the noise and preserve as much as possible the morphology of the pore space.

Filtering is an important step because of the segmentation step. Using the same commercial software, we manually set a threshold value in which any voxel with intensity under the set value, will be assigned to pore space. This is the binarization step, in which we transform the grayscale image into binary information where 0 is the grain region, and 1 is the pore space. If the filtering step is skipped, the binarization step will be prone to errors because neighboring voxels might have very different intensity values due to high frequency noise. The filtering step smooths the images so continuous regions will have voxels with similar grayscale intensities.

3.2 SIMULATIONS ON THE VOLUMETRIC DATA

After the volumetric data is segmented, this information can be used to simulate fluid flow and current flow inside the pore space in order to estimate petrophysical characteristics of the samples. In this work, we use the simulations in the volumetric data to observe the correlation of the topological and morphological features of the networks with the petrophysics measurements of the samples.

Two simulations were used: the absolute permeability simulation and the formation factor simulation. All simulations were run on the commercial software PerGeos.

3.2.1 Absolute Permeability

The absolute permeability is a measure of the ability of a porous material to transmit a single-phase fluid. The relationship between the absolute permeability and the flow rate is given by Darcy's law⁵¹:

$$Q = -\frac{\kappa \Delta P}{\mu L} S \quad (3.5)$$

where Q is the flow rate, κ is the absolute permeability constant, μ is the fluid's viscosity, ΔP is the pressure difference applied, L is the sample's length and S the sample's cross section in which the fluid goes through. The pressure difference is an approximation for the actual pressure field that is applied to the sample. The permeability is described as tensor, but for the global petrophysical characterization of a porous sample, it can be estimated as a constant, given a direction in which the pressure difference is applied to the sample.

The simulation takes as input parameters the fluid viscosity μ , the pressure difference ΔP (or the input/output pressure and the fluid flow rate) and the direction $\mathbf{x}, \mathbf{y}, \mathbf{z}$ the pressure/flow is applied. For the purposes of this work, the default values were used for all experiments: $\mu=0.01$, input pressure $P_{in} = 1,3 \times 10^5 Pa$, output pressure $P_{out} = 1 \times 10^5 Pa$.

The simulation then solves the stokes equations for the missing parameter:

$$\begin{aligned} \vec{\nabla} \cdot \vec{V} &= 0 \\ \mu \nabla^2 \vec{V} - \vec{\nabla} P &= \mathbf{0} \end{aligned} \quad (3.6)$$

where $\vec{V}$ is the fluid velocity field. These equations take into consideration that the fluid is incompressible, Newtonian and that the flow is in a steady state and it is laminar. The dynamics is simulated through a finite volume model until a convergence criterion is reached.

Figure 5 - Permeability simulation experiment. The grey regions represent the solid phase of the sample. One voxel wide surface is added to each side of the sample on the direction of the applied pressure so the sample is isolated. The flux is set in a way that the region near the entry face and outlet face is homogeneous in terms of pressure and fluid velocity.

Source: By the author

3.2.2 Formation factor

There are many different measurements that are routinely done in the petroleum industry to estimate the quantity/type of hydrocarbonate fluids and the production of a reservoir.⁵² Amongst these is the measurement of permeability of the rock, that was discussed before, and the electrical resistivity log, which is used to calculate the porosity and the saturation of the reservoir rock. The laboratory characterization of the electrical resistivity is usually done by the measurement of the bulk resistivity of a rock core saturated with brine solution. The *formation factor* of the sample is defined as:

$$F = \frac{R_0}{R_l} \quad (3.7)$$

where R_0 is the bulk measurement of resistivity and R_l is the known liquid resistivity.

There are many physical properties that will be correlated to the resistivity measurements, such as the conductance of the solid surface and the fluid characteristics that permeates the porous space. However, there is also a dependence on the rock's lithology such as the porosity. This dependence was first defined by Archie, 1942⁵³:

$$F = C\phi^{-m} \quad (3.8)$$

where ϕ is the porosity of the sample and m is called the cementation factor.

Equation (3.8) is often referred to as Archie's Law. The determination of the cementation factor has been theme of discussion in the scientific community^{52,54–58}. It depends on the rock's lithology (sandstones will have different cementation factors than bioclastic carbonates, for instance). Also, more recent studies agree that the C factor on (3.8) is correlated with the sample's *tortuosity*^{56,59–62}:

$$F = \tau^\alpha \phi^{-m} \quad (3.9)$$

where τ is the tortuosity, F is the formation factor and ϕ is the porosity of the sample. The factor α may change according to the rock's heterogeneity.^{54,63}

However, the definition of tortuosity is also an open question. Usually, there are four possible definitions of tortuosity that depends on the application^{59-60,62}: *geometric*, *electrical*, *hydraulic* and *diffusive*.

Geometric tortuosity is usually defined as the ratio of the mean length of all flow paths through the medium and the straight-line length across the medium:

$$\tau_g = \frac{\langle L_{flow} \rangle}{L_{line}} \quad (3.10)$$

This definition does not take into account that the particles may follow *preferential paths* of flow, given the different cross-section diameters of the paths. To account for that, the *hydraulic tortuosity* was defined. The hydraulic tortuosity is given by the ratio of a *flux-weighted* average path length $\langle L_h \rangle = N L_h$ to the straight-line length, where N is the number of streamlines going through that path:

$$\tau_h = \frac{\langle L_h \rangle}{L_{line}} \quad (3.11)$$

Closely related to the hydraulic tortuosity, we have the *electrical* tortuosity:

$$\tau_e = \frac{\langle L_e \rangle}{L_{line}} \quad (3.12)$$

where $\langle L_e \rangle$ is the average electrical flux path length. The tortuosity correlated to the previous discussed formation factor would be the electrical tortuosity. The electrical tortuosity and hydraulic tortuosity are usually larger than the geometric tortuosity. The reason is that the conductance of the paths will take an important role in their determination. So, even if a path is *longer* than another in geometrical terms but its conductance is higher than the rest, the tendency is that the flow will choose to pass through it.

The diffusive tortuosity is usually defined as the ratio of the diffusing species in free fluid d_f to the restricted diffusion on the tortuous paths inside the porous medium d_p :

$$\tau_d = \frac{d_f}{d_p} \quad (3.13)$$

The restrictive diffusion coefficient can be determined by NMR relaxometry⁶⁴.

In this work, we focused on the electrical tortuosity, so we could correlate to the formation factor simulations. The simulation is done by applying a constant electric potential difference on two opposing faces of the sample. The other faces are considered closed by an electric insulator. So, the simulation solves for the current flux:

$$\frac{j_{tot}}{S} = \sigma \frac{V_{in} - V_{out}}{L} \quad (3.14)$$

where j_{tot} is the current flux going into the sample, S is the sample's cross section area, σ is the electrical conductivity of the material, V_{in} is the input imposed electrical potential, and V_{out} the output electrical potential. Two border conditions are imposed: that the sample is homogenous (σ doesn't vary in space) and the sample is completely saturated.

To find the conductivity of the saturating fluid, Ohm's law is applied:

$$j_{tot} = \int_S -\sigma_{solution} \vec{\nabla} v \, dS \quad (3.15)$$

Where v is the electric potential.

3.3 SAMPLES

3.3.1 Rock samples

We applied the extraction method to samples with very different lithology with two objectives in mind. The primary objective was to validate the developed software of network extraction. Secondly, by choosing samples with very different petrophysical characteristics, we wanted to evaluate the correlation of the networks structural and functional properties to the measured petrophysical characteristics of the samples.

The porous media used in this part of the work were composed by two rock samples: a sandstone (Berea) and a carbonate sample (Estailades). Another porous sample used was an artificially constructed porous medium composed by the packing of glass spheres. This was a sample prepared for the study of molecular diffusion through NMR measurements and simulations, work done by our colleague PhD candidate Everton Lucas de Oliveira, and was also used in this work. The diameter variation of the glass spheres used was 150 μ m to 300 μ m.

The Berea sandstone is well established in literature as having a homogenous structure, and is often used as a reference material ^{65,66}. It is a sedimentary rock whose grains are predominantly sand-sized and composed of quartz held together by silica.

The Estailades limestone, (Estailades, France), in the other hand, has a more complex porous matrix. It is a bioclastic limestone, meaning that its structure is formed from fossil fragments or other organisms as well. It is composed of more than 99% calcite ^{67–69}

The μ CT images of the Berea sample and the sphere packing sample were obtained by our group, with voxel resolution of 3.3 μ m and volume dimensions of 505x362x532 for the Berea sample, and 504x504x750 for the sphere packing sample, with voxel resolution of 3.0 μ m. The Estailades sample was downloaded from the Digital Rock Portal. ⁷⁰ The sample also has voxel resolution of 3.3 μ m and its volume dimensions are 650x650x650.

3.3.2 Acidification samples - wormholes

The productivity of a reservoir is of major importance in the oil industry. There are various factors which can lower a reservoir's productivity. The rock formation with low porosity region, due to lamination on its formation, might induce low permeability in the direction of the fluid extraction and even the drilling itself may cause damages to the reservoir that reduces its productivity.

One of the stimulation procedures that is often applied to carbonate reservoirs is the acid treatment, because of the high reaction of the acid to the carbonate formations. It consists of a reactive fluid flow that is injected to the inner rock of the reservoir. This procedure creates a conductive preferential path, known as wormhole, that optimizes the extraction of the hydrocarbon fluids.⁷¹

However, determining the efficiency of the technique is a difficult task. There is the question of the optimum pathway formation for maximum fluid extraction, with minimum use of acid. For this determination, there are many variables involved: the total volume of acid used, the original petrophysical characteristics of the rock and the injection rate. All these will influence on the formation of the wormhole pathway's morphology. Therefore, the characterization of the wormhole's topology is of vital importance to assess the efficiency of the method

All the acidification samples were acquired through a joint project with Petrobras/Cenpes. The acidification and imaging was done by the Cenpes team. The samples are composed by 5 Indiana Limestones rock plugs (E2, E4, E5, E8, E9) (region of Indiana, US). Each sample is cylindrical, with 3.8 cm of diameter and 7cm in length. All samples were treated with HCl, with injection rate 10cc/min. The μ CT images were acquired at 40 μ m resolution (with some variations), so the wormholes could be visualized.

4 METHOD DEVELOPED

Even though the volume extracted from the μ CT images can be directly used in fluid flow simulations, there are advantages on the simplification of the volumetric data by describing it as a network. One is simply the amount of computer resources needed to simulate directly into the total captured volume of the pore space. The complex system of the porous structure for a small sample of millimetric size can be composed of millions of voxels or even larger.

Moreover, the simplification of the volume into a network opens the possibility of capturing information of the morphological and topological features of the porous structure. If we can simplify the complex porous space problem into basic elements and the interaction between these elements, we could find common features between porous samples. This can help us understand the process that lead to their shape and formation and how their structure influences on the dynamics of the permeating fluid.

When we are dealing with flow in porous media, two main features are of interest: pore sizes, which are the regions that the fluid is stored and the connection between pores, which limits the extraction of the fluid inside the rock. These two characteristics differ from the sample's morphology (size and shape of the pores) and the samples topology (position of the pores and how they are connected).

This is the main motivation for our study of the different algorithms of network extraction and the development of a new method. In general, the algorithms either focus on the total topology of the sample through medial axis methods, or focuses only on the separation of pores and throats, oversimplifying the samples' topology.

To reduce the information loss, we have proposed a new way of viewing the interconnection of pores. We use the well stablished maximum spheres algorithm to divide the pore space into sphere cells. This allows a simplification of the pore space with minimum original data loss. The sphere cells are connected as a graph, leading to a complex network of regions. The final algorithm doesn't ignore that knowing the position of the regions considered as pores, and their morphology is an important information. We see as well, the importance of knowing the regions of constriction, which can limit the extraction of fluid

from the pores. So, a pore-throat separation method is also proposed, which aims to be applicable to any porous medium. Here, we will first discuss the main methods used for pore-network extraction from μ CT data: medial axis, watershed algorithm and the maximum spheres algorithm. Then the proposed method will be presented.

This chapter is organized as follows: First the pre-processing steps required for the network extraction are presented, then the different approaches for pore space separation will be presented and finally the proposed alterations to the Max Ball algorithm will be discussed and the final algorithm of the developed software is shown.

4.1 PRE-PROCESSING

The data from the μ CT scanners is usually stored as a set of 2D images. To use this information to extract the morphological characteristics of the porous matrix, is necessary first to reconstruct these images into volumetric data. There are several software that perform this task, such as *ImageJ*, which is a open source software, free to download.

Each volumetric point is called *voxel* ($v^i = v(x^i, y^i, z^i)$), where $x, y, z \in \mathbf{N}^3$ are coordinates on the tridimensional space. The *voxel* is the equivalent to the pixel, in volumetric objects. It will represent the intensity on each point of the space.

When we are dealing with porous media, each voxel will either represent void space or a specific kind material. Since we are interested on the void portion, we segment the volumetric data into void voxels v_{void} and material representative voxels $v_{material}$. Void voxels are defined as follows:

$$\begin{aligned} v_{void}^i &= v^i \in N | v^i(x, y, z) < t, i = 0, 1, 2, \dots, N \\ N &= \text{total number of voxels} \end{aligned} \tag{4.1}$$

Where t is a threshold parameter, a greyscale level set by the user that sets all the voxels under a defined limited of brightness into pore space. There are several proposed methods to choose this threshold value.

Now the volumetric data is segmented into voxels that belong to the pore space and to the sample material. This is the input data for all digital rock experiments, so minimum loss of the original data on the segmentation procedure described above is paramount. As we discussed before, usually this is achieved by using minimum loss filters on the original μ CT images before the segmentation procedure, such as Non-Local Means.

4.2 DEFINITION OF PORES AND THROATS

After the pore space is defined by the volume segmentation described before, the space can be further simplified by capturing the two main entities that will be the descriptors of the fluid flow: pores and throats.

The identification and separation of pores and throats in the final volume is a difficult problem, but before discussing the different approaches for the pore-network extraction, we need first a definition of what will be considered a pore and a throat in the volumetric pore space. The most accepted definition of a pore is a wide region of the pore space that is limited by narrowing regions, namely throats. So, the pores' total volume is representative of the bulk volume of the permeating fluid and the throat radii are representative of the capillary pressures.

A more precise description of this definition has been done by M. J. Blunt, 2017⁵¹, through a mathematical model that defines the position of a pore's center.

Figure 6 - Pore space, pore and throat definitions. (a) The porous space is defined as the empty space in the matrix, the grains compose the solid space and surface. (b) Example of discretization of the pore space, and definition of the pore center (red) and throats (green dashed lines) through the distance transform on the pixels.

Source: By the author

The pore space, as shown on a 2D representation on Figure 6 (a), is a continuum space with complex morphology. The pore center is represented by the red pixel on Figure 6 (b) and the throats are the dashed green lines. To find the position of the pore's center, we apply to the image an operator called *distance transform*. The distance transform assigns to each *object pixel* the distance between its position and the nearest border pixel, such as:

$$DT(v_{void}^i) = \min_{0 < k < N^{border}} (\|v_{void}^i - v_{border}^k\|) \quad (4.2)$$

If we considered the pore space as a continuum, the local maxima, minima, or saddle point of the continuous distance transform would be the points (x,y) in which the gradient of the transform is zero, such as:

$$\nabla d(x,y) = \mathbf{g} = 0 \quad (4.3)$$

The local maxima will be defined amongst these extreme points as the positions (x,y) in which the second derivative is negative. In more general terms, the local maxima would be the positions in which the eigenvalues of the Hessian matrix are all negative:

$$H_{i,j} = \frac{\partial^2 d(x_i, x_j)}{\partial x_i \partial x_j} \quad (4.4)$$

$$H_{i,j} e_j = \lambda e_j$$

The position of the local maxima can be considered the pore centers, in other words, the regions where the bulk fluid will be concentrated.

The definition of the throat's centers, on the other hand, can be a more difficult task. M. J. Blunt, 2017⁵¹, imagines a streamline starting from pore i and ending on pore j in which the direction of this line is always parallel to the gradient field $\mathbf{g}$. The throat would be the surface perpendicular to the regions of saddle point that belongs to this streamline.

Even though these definitions are straightforward for a continuous medium, the application to digital rock samples encounters several difficulties. The local maxima in a

discreet region may not be well defined (two or more neighboring voxels can have similar distance to the walls). There is also the question of recovering the pore's morphology (the shape and geometry), which holds important information of the sample's formation. Moreover, for sheet like pores, the local maxima won't be representative of the real cross section of the pore space (Figure 7).

Figure 7 - Representation of “sheet-like” pore. The local maxima will be the distance represented by the circle's radius. This simple representation won't be able to capture the real cross section of the pore space which can lead to erroneous interpretation of the data.

Source: By the author

The task of capturing the correct shape of the pores and throats, as well as the complete topology of the sample has been tackled by three main approaches: volumetric medial axis, distance transform combined to watershed methods and finally the maximum spheres algorithm. These three approaches usually are interconnected and each has its limitations which we will discuss here briefly.

The medial axis approach tries to reduce the volume of pores into a topological equivalent of interconnected lines. This is done by the morphological operation of Erosion on the tridimensional pore space.⁷²⁻⁷³ Erosion, as the name states, is an operator that erodes away the boundaries of the regions considered as objects in a volume.

Let A be a binary matrix representing an image in which the object of interest (the pore space) is represented by voxels set as one and the solid matrix represented by voxels set as zero. In this case, the *object* of interest is the pore space. The erosion takes two pieces of information as input: the binary matrix A and a structuring element B . This structuring element is also a binary matrix that defines the neighboring region of the voxel a in the border of A that should be eroded. If X is the subset of coordinates of the object voxel positions on A , the mathematical definition of erosion would be:

$$A \ominus B = \{x \in X | Bx \subseteq A\} \quad (4.5)$$

Where Bx defines the translation of B to the center point in x . Basically, the erosion operation on A defines the removal of pixels that are in the border of the object, limited by the structuring element B . The medial axis is acquired by the repeated erosion, done pixel by pixel, in the object, until the current pixel has at least two neighboring background pixels.

Figure 8 - Example of the process of repeated Erosion on a 2D image. Pixels that are on the border of the object are chosen for removal. This is done interactively until only one pixel is left.

Source: By the author

After the procedure is done, the result is called the morphological skeleton of the image. This process is interesting because it preserves the original *topology* of the pore, capturing the tortuosity of the space. However, the definition of *pores* can be ambiguous. The frequently used method to define pores on the skeleton are the regions where the skeleton branches into two or more pathways. The problem with this approach is that these regions of branching aren't necessarily regions of larger volume. In fact, the branching regions could be more representative of throats than pores.

This ambiguity on the pore definition can be visualized on Figure 9. The shape of the border of the region creates subdivision of the skeleton into multiple branches. Even though there are many proposed methods to remedy the over branching of the medial axis with good results on porous media,^{25,74–77} there is still the problem of losing the information on the pore's original shape. Usually the recovering of the pore's shape is done by applying the watershed algorithm to the treated data of the skeleton.

Figure 9 - Example of medial-axis application to a complex porous structure (a) pore space, (b) morphological skeleton. The branching happens because of the shape variations of the border pixels.

Source: By the author

The watershed based methods uses the image processing object separation algorithm watershed transform, and it is used frequently on pore space separation.^{32,78-79} The watershed transform is a region-based segmentation approach, and its intuitive idea is based on topographical separation of a landscape. Imagine a landscape with mountains with different heights being flooded with water. The flooding process continues until the deepest valley is completely flooded and reaches the highest peak. The outcome of this process is the landscape partitioned into regions separated by “dams”, the watershed lines (Figure 10).

Figure 10 - Example of the steps of the watershed algorithm. (1) The valleys represents the local maximum of the distance transform. The flooding procedure would be a pixel neighbor clustering step. (2) a tag is assigned to each local maximum, signaling different objects (or in the pore space, pore locations). (3) the clustering process on a region continues until it meets a different region .The limit between two regions are called watersheds.

Source: By the author

The image equivalent of a landscape is acquired through the inverse distance transform (Figure 11). Instead of the local maxima representing a peak, it represents a valley. These are the starting points of the algorithm (seeds of the algorithm). Then, the algorithm checks the neighboring pixels of the starting points. If the neighbor pixels are closer to the walls than the current pixel, they are tagged as the same object.

Figure 11 - Example of the distance transform applied to the pore space model. (a) pore space (b) distance map: blue are the pixels closest to the border (c) the inverted distance map used as entry data for the watershed algorithm.

Source: By the author

The algorithm proceeds until all pixels are tagged. This procedure recovers the complete shape of each pore. However, the final separation is completely dependent on the starting points of the algorithm. These starting points can either be defined through the medial axis junction points (after a correction is applied to avoid over branching), or through a threshold parameter set by the user.

The problems of over branching of the skeleton and the minimization of over segmentation due to the problems of the discrete distance transform was tackled by the development of the maximum spheres algorithm (MS)^{28-31,80}. The algorithm is based on mathematical morphology, and its basic steps are as follows (see Figure 12):

- (1) Pore space binarization and definition;
- (2) The volumetric pore space is subdivided into maximum inscribed spheres. A sphere is said to be maximum if it is not contained by any other sphere and touches the volume surface at least on one point;
- (3) The spheres' centers with the largest radius in each region is the center of a pore, and a tag is assigned to it;

- (4) Other spheres that touches a pore sphere, are assigned the same tag and are said to belong to the same pore. This tag is passed through to neighboring spheres interactively. This is similar to a breath-first search on a graph. Each sphere with smaller radius that is connected (by touching another in some point) to another with larger radius is given the same tag. This procedure is often compared to the pore's "family name" being passed through to the smaller spheres that compose its volume.
- (5) If a sphere already tagged is found by a sphere with a different 'family name', this sphere is tagged as a throat, or connection between pores.

Figure 12 - Maximum spheres (MS) algorithm for pore space separation. (1) pore space definition (2) maximum spheres are localized (3) maximum spheres are tagged as different pores (4) smaller spheres that are connected to a pore sphere is given the same tag and composes the pore's volume. Spheres that share two or more pore tags are defined as throats.

Source: By the author

This method is an elegant solution to the main problem with the previous approaches: the over-segmentation of the pore space due to the shape of its borders. As we have shown before, the direct application of the erosion procedure and watershed transform on the voxels can lead to over-branching and to over-separation respectively. The MS algorithm gives an intermediate step between processing the voxels directly and separating the pore space, reducing problems with noise in the pore-grain interface.

Another important advantage of this process is that there is no loss on the pore's morphology. Since we can divide the pore-space into spheres as small as the image resolution, with proper guidelines, the complete surface of the pore is recovered and assigned to each individual pore. However, even though there is considerable reduction on errors due to the pore's surface shape, there can be still issues with over segmentation due to the definition of the throat spheres. Since the only condition on a sphere being assigned as a throat is that it will belong to two (or more) pore families, a small variation on the pore's surface can lead to a region being separated into two different ones. Usually this is corrected by setting a threshold parameter, limiting the size of a sphere that can be considered as throat³⁰:

$$\frac{r_{throat}^j}{r_{pore}^i} < \lambda, \quad 0 < \lambda < 1 \quad (4.6)$$

Equation (4.6) states that the ratio between the radius r_{throat}^j of a throat sphere j to the radius r_{pore}^i of all i pores it connects must be lower than a threshold value λ . If it isn't, the smallest of the pore sphere's is merged with the largest neighboring pore. This can be problematic since different choices of λ between implementations of the algorithm can provide different results on the pore-throat separation for the same sample, which in turn, can lead to different interpretations of the pore structure.

We have summarized the three approaches positive outcomes and issues on Table 1.

Table 1 - Summary of the different pore space separation approaches.

Algorithm	Positive outcomes	Problems
Medial axis	Topological description of the medium.	Over-branching; Loss of morphology (can be remedied by the use of watershed); Dependent on user tuned parameters
Watershed+distance transform	Morphological description of the pores.	Over-segmentation; Loss of topology; Dependent on user tuned parameters
Maximum Spheres	Morphological description of the pores; Avoids over segmentations	Loss of topology; Dependent on user tuned parameters

Source: By the author

Based on the positive outcomes of the MS algorithm, we propose studying the morphology of our samples based on its concepts. The idea is to use the segmentation of the pore space into spheres instead of working directly with the voxel data. In the next section of this chapter the MS algorithm will be presented in more detail and the proposed method for capturing both the pore-space morphology and topology through network analysis.

4.3 CONSTRUCTION OF THE REGIONS NETWORK

After the pre-processing, the volumetric data becomes binary information, so we can see the pore space in a True/False perspective. Since our region of interest is the void space, we set the final tridimensional matrix as:

$$v_{void}^i = v^i \in N \mid v^i(x, y, z) = 1 \quad (4.7)$$

$$v_{material}^i = v^i \in N \mid v^i(x, y, z) = 0$$

The original MS algorithm does a search on each of the pore space voxels to find the maximum inscribed sphere with each voxel as center. In the developed software, this step is done by performing a *Euclidean Distance Transform (EDT)* on the volumetric data.

As we discussed before, DT is a known transform for binary image processing. It sets to each pixel on the image, that is considered as an object of interest, the minimum distance of that pixel to the object's borders. The EDT uses the Euclidian distance for this calculation. So, since we are interested on the $v_{void}^i(x, y, z)$ voxels, EDT applied to this volumetric data will measure the minimum distance of each v_{void}^i to all v_{border}^k voxels. If we have N^{border} border voxels, EDT applied to v_{void}^i will result as:

$$EDT(v_{void}^i) = \min_{0 < k < N^{border}} (\|v_{void}^i - v_{border}^k\|) \quad (4.8)$$

$$\|v_{void}^i - v_{border}^k\| = \sqrt{(x_{void}^i - x_{border}^k)^2 + (y_{void}^i - y_{border}^k)^2 + (z_{void}^i - z_{border}^k)^2}$$

An example of the application of the EDT on a binary 2D image is shown on Figure 13. This the case of the EDT applied to a slice of a BEREa sandstone μ CT image.

Figure 13 - Example of EDT applied to a 2D slice of the μ CT data of a Berea sandstone sample. (a) the binary original image (b) the resulting EDT. The color scale represents the calculated distance of each pixel to the wall.

Source: By the author

As shown, each pixel is colored per its minimum distance to the borders. This distance will be the radius of the maximum inscribed sphere MS^i centered at voxel $v_{void}^i(x, y, z)$. At this point of the original algorithm, all possible inscribed spheres are stored.

The next step is to exclude the information of the spheres which are included on others with larger radius, which bring redundant information of the morphology. A sphere a is included in a sphere b with larger radius R^b , if:

$$\|v^a - v^b\| < (R^b) \quad (4.9)$$

The resulting information after this process is the complete recovery of the porous matrix. We have applied the process to the same Berea sandstone slice of Figure 13 on a 2D version of the software, the result is in Figure 14. We see that the porous matrix is filled by the resulting spheres, and no information of morphology is lost.

Figure 14 - Final network of spheres. (a) the original distance transform of the image. (b) the maximum spheres found on the image.

Source: By the author

The final step of the original MS algorithm is the definition of pores and throats. This is done by ordering the remaining spheres per their radius in descending order and checking the *connection* between spheres. Even though the algorithm eliminates spheres which are included in others with larger radius, it still allows spheres to touch under the limit imposed by equation (4.9).

Figure 15 - The construction of the network of regions. Two separate networks are constructed: a network composed of the complete set of spheres (middle image) and a second one composed only of the medial axis spheres (right image).

Source: By the author

The developed software finds the spheres' connections and builds a weighted network, in which the node locations are the spheres' centers and to each edge is assigned a maximum

flow capacity (Figure 15). For each sphere pair, we consider that the maximum possible flow from sphere i to a neighboring sphere $i+1$ can be approximated by the area of the cross section of the adjoining regions (Figure 16).

The capacity of each edge is defined as:

$$Capacity(e_{i,i+1}) = \pi R_{cs}^2 \quad (4.10)$$

with R_{cs} being given by:

$$R_{cs} = \left(\frac{R_i - R_{i+1}}{d} \right) (d - R_{i+1}) + R_i \quad (4.11)$$

where $R_i > R_{i+1}$ are the spheres' radius and d is the distance between the spheres' centers.

The final network stores in each node the sphere's center position, the original sphere's radius and the capacities assigned to each edge. This way, the original spheres can be reconstructed and visualized.

Figure 16 - The model used for the capacity assigned to each edge of the graph. The edge's capacity of node i to $i+1$ will be the area of the full blue circle on the image, given by equation (4.10).

Source: By the author

After the complete regions network is constructed, a medial axis network can be extracted using the topology of the complete network. This is done by applying the throat

concept in the original MS algorithm. When a throat sphere is found, this signals that a path between two pores exists. To find the medial axis, we search for the shortest path between the two pore nodes by defining the shortest path as the path that will offer the least resistance for fluid flow. So, we set the weight of each edge as:

$$weight(e_{i,i+1}) = \frac{1}{Capacity(e_{i,i+1})} = \frac{1}{\pi R_{CS}^2} \quad (4.12)$$

Then, the shortest path is found through Dijkstra's algorithm⁸¹ that searches for the path of minimum length based on the edges' weight. An 2D example of both networks are shown on Figure 17.

Figure 17 - Example of the two networks constructed on the 2D slice of the μ CT data of a Berea sandstone sample. On the left is the complete network, and on the right the medial axis network. The spheres of the medial axis network are the spheres considered as pores in the algorithm, and the cylinder edges are the path found between the pores.

Source: By the author

We see that by defining the shortest path as the path of least fluid flow resistance, the path will be composed by the largest possible spheres. By setting a path connecting these spheres' centers, it will follow the medial axis of the object. This way, we recover the sample's topology without having to treat the problem of over-branching of the skeletonization of the sample.

A comparison between applying directly the skeletonization procedure through erosion and the network method is shown on Figure 18. We have enumerated 1-5 examples of over-branching of the medium that is remedied by our method. We see that the spheres represent a single pore as being a region of largest volume, as it was proposed before, and the edges capture the tortuosity of the path between pores as it was expected.

However, one of the limitations of this simple method is pointed out by branching 6. If multiple paths between two pores exists, only the least resistance path will be considered. To get all possible paths, a “path removal” approach can be applied. If a path is found, it is removed from the original network and the algorithm tries to find another path. This is costly computationally. Another solution would be to enforce the throat node to be a part of the path. The problem with this approach is that the throat node may not be representative of the medial axis.

Figure 18 - Comparison of the network shortest path and the skeletonization procedure for finding the medial axis. 1-5 are examples of the over-branching problem mentioned before of the erosion procedure (grey lines). 6- limitation of finding one single pathway between pore nodes.

Source: By the author

Another clear advantage of using the network approach is demonstrated on Figure 19. (a) shows our result by using the shortest path method. Both pore locations and path tortuosity are captured. (b) shows a pore-throat network acquired by a commercial software. The edges

connect two identified pores, losing information of the medial axis, which is preserved on the network approach.

Figure 19 - Comparison of the network extraction method (a) and a pore-throat network.

Source: By the author

4.4 ACQUISITION OF THE PORE MORPHOLOGY

As discussed before, the recovering of pore's morphology on the original MS algorithm is done by a breath-first search of the spheres, starting from the pore's central sphere, and adding the subsequent spheres of smaller radius until a sphere tagged as throat is found. The problem with this approach is that little noise originating from the pore's surface can lead to an erroneous qualification of a sphere as a throat. This, in turn, can lead to an over-separation of the pore space in which the pores won't be representative of the regions of larger volume limited by constrictions.

The original correction is done through a user tuned parameter. In this work, we propose a different approach based on the network's node current flow betweenness centrality. We propose merging nodes considered as pores which present low centrality scores, to neighboring pore nodes with high centrality scores. The idea behind this correction procedure is that pore nodes that present low centrality scores are not relevant for information transmission, so they act as part of the volume of a neighboring pore node. To validate the correction procedure, we created a sphere packing model to simulate an ideal pore space (Figure 20).

Figure 20 - Simulated pore space considered for first pore morphology tests. The medium is an ideal sphere packing of spheres of equal radius. To simulate a fully connected pore space the spheres are separated by two voxels from each other. (a) sphere packing with sphere radius of 30 voxels (b) cross section of the packing. (c) pore space formed. (d) complete sphere's network acquired from the space.

Source: By the author

The simulated pore space and the measured centralities based on current flow are shown on Figure 21. The current flow centrality measure was chosen for its precision, compared to other centralities measures, as we discussed in the previous chapter. Since the pore nodes are highly connected, as it was expected, they presented higher centrality than the rest of the nodes.

Figure 21 - Comparison of the centralities scores for each node type: pore nodes, throat nodes and other nodes in the network. (a) a visualization of the complete network each node color represents its centrality value. (b) normalized distributions of centralities of each node group (black other nodes, blue throat nodes and red pore nodes)

Source: By the author

The comparison of centralities of each group shown on Figure 21 (b) gives a good overview of the behavior of the nodes on the complete network. We see that pore nodes are most central, even though there are pore nodes with relative low score comparing to the mean centrality of the group. This reflects the pore nodes that are on the border of the volume. Similar phenomenon happens to the throat nodes group, which shows wide distribution of centralities. Based on these preliminary results, we proposed a correction procedure as follows:

- (1) Pore nodes are sorted according to their centrality in descending order.
- (2) A breath-first search starts on the pore node with highest centrality cf^i . Then, the centralities cf^j of the neighboring nodes are checked. While $cf^j < cf^i$, the search continues. If j is a pore node, it is no longer considered a pore. The same procedure is applied to the throat nodes.
- (3) The search stops when the neighboring node j has centrality such as $cf^j > cf^i$.

We have applied the procedure to the simulated pore space of Figure 20, the results are shown on Figure 22. Each node group distribution is normalized by the number of the nodes in that group.

Figure 22 - Comparison of the centralities scores for each node type (a) before the correction procedure (b) after the correction procedure.

Source: By the author

However, there was a correction on the number of throat nodes. This is due to redundant throats spheres: two or more spheres tagged as throats that connect the same pores. This can happen when the throat has a large diameter and is described by more than one maximum

sphere. The algorithm removes this redundant information by removing the throat spheres with low centrality.

After the correction procedure is done, the pore's morphology is recovered by a region-growing technique starting on the remaining pore nodes. We use these as “seeds” for the region growing algorithm. Each pore node adds to its body its neighbors interactively. The procedure stops when no more spheres can be added, or a high centrality throat is found.

We have applied to the simple pore space of Figure 20. Since it is an ideal sphere packing space, we can have an analytical solution for each pore's volume.

Figure 23 - The expected equivalent volume V of the pores is the volume of the darker region of the figure.

Source: By the author

Since the grains are composed of spheres of same radius, the volume of the largest space between the spheres will be the form based on Figure 23:

$$V_{pore} = V_{cube} - V_{sphere} \quad (4.13)$$

If we consider a sphere of radius R_{eq} , such as the sphere's volume equals V_{pore} , we have:

$$\frac{4}{3}\pi R_{eq}^3 = (2R)^3 - \frac{4}{3}\pi R^3 \quad (4.14)$$

So,

$$R_{eq} \cong 0.96R \quad (4.15)$$

This will be the expected *equivalent radius* of the pores. Using the case of Figure 20, in which the sphere's radius $R=30$ voxels, the expected equivalent radius of the separated pores will be $R_{eq} \cong 28.8$ voxels .

Figure 24 - Results for the sphere packing of Figure 20. (a) the pore space separation acquired through the developed method. (b) The equivalent radius distribution of the pores.

Source: By the author

The results are presented on Figure 24. The image on (a) is a representation of the separated pores, each pore is the cluster of spheres with the same random color. We see on (b) that the distribution of pore radius is close to the expected value, with some variations due to the discrete characteristic of the volume. These are mainly due to the volume's borders. We have applied the same method to other sphere packing examples of Figure 25, with expected equivalent radius of 48 voxels (sphere radius of 50 voxels), 24 voxels sphere radius of 25 voxels) and a mixture of 9.6 and 24 voxels (sphere radius of 10 and 25 voxels respectively).

Figure 25 - Simulated ideal sphere packing examples. Left, spheres with R=50, middle R=25 and right a mixture of small and large spheres: R=10 and R=25.

Source: By the author

We see that the expected pore sizes were recovered correctly from all examples we applied the algorithm to. The mixture example was assembled such as we had 200 small spheres and 20 larger spheres, which reflected on the number of smaller pores in comparison to larger ones (see Figure 25 histograms). The radius variations due to the volume's borders are pointed as transition regions, same as the transition from the larger spheres to smaller spheres in the mixture example. These preliminary results show the method can acquire the pore's morphology with good reliability.

Finally, after the correction procedure is done, a pore-throat network is constructed based on the remaining pore's center position. To better account for the samples morphology, we use the medial axis network to find the tortuosity and mean diameter of the paths between pores to set the capacity parameter of our final network such as:

$$capacity(e_{i,i+1}) = \frac{\langle A_{throat} \rangle}{\tau} \quad (4.16)$$

Where $\langle A_{throat} \rangle$ is the average cross section area of the throat connecting pore's i and $i+1$ and τ is the tortuosity of the path. The idea is to account for the morphological variables that will give the connection between the morphology of the medium and the observed permeability and formation factor experiments. The final pore-throat network for the first example is shown on Figure 26

Figure 26 - Pore-throat network extracted from the sphere packing example with $R=25$. Spheres represent the pore locations, and the channels represent the throats. The throat's diameter for all connections is 25 voxels.

Source: By the author

5 RESULTS

5.1 APPLICATION ON ROCK SAMPLES

The network extraction method was applied to the three-different porosity and origin samples: Berea sandstone, Estailades carbonate and the syntherized sphere packing (Figure 27).

Figure 27 - Samples used for the pore network extraction method and analysis. (a)-(c) Reconstructed volume and dimensions of the Berea Sandstone, Estailades carbonate and syntherized sphere packing samples. (e)-(f) visualization of the pore space for the Berea, Estailades and sphere packing samples. All images were obtained by the developed software, using python mayavi.mlab library.

Source: By the author

The volumetric images were first pre-processed and binarized (with the exception of the Estailades sample which was obtained already binarized.). Then, the data was input to the developed software, and the space was subdivided into sphere's cells. The output of the software at this stage is the complete network of spheres cells and the medial axis network of each sample.

Table 2 - Pore-space morphological data from the samples. Samples' porosity ϕ , the pore space surface area S and volume V , and the specific surface area SSA (surface area per solid volume).

	ϕ	S	V	SSA
Berea	0.18	72 mm ²	0.6 mm ³	25 mm ⁻¹
Estailades	0.13	83 mm ²	1.3 mm ³	10 mm ⁻¹
Spheres	0.35	79 mm ²	2.3 mm ³	18 mm ⁻¹

Source: By the author.

The process was partially parallelized by using the SCOOP parallel library for python and run on a DELL PWS TOWER 7910. The computational time needed to get the complete network of spheres and the medial axis network varied between 1h30m for the Berea sample and 3h for the sphere packing sample. The porosity percentage of the samples escalates the processing time, according to the resolution of the captured μ CT. The complete network of sphere's cells of each sample is shown on Figure 28.

Figure 28 - Complete sphere cells networks for the three porous samples: Berea Sandstone, Estailades carbonate and the synthesized glass sphere packing. The results show that the division of the pore space into sphere cells is coherent with the pore-space of each sample.

Source: By the author

The pore-space division into sphere cells eliminated a great portion of the required information for the characterization of the pore-space, as we can see on Table 3. Since the sphere cells are allowed to overlap, the distance between nodes are usually smaller than the sphere's radius, as we see on the graph of Figure 28. It is interesting to note that the mean sphere-cell distance is small, 20 μ m, and it is independent on the sample. However, for the larger pore-space volume samples Estailades and Sphere packing, the distance between nodes can get to 100 μ m.

The radius of the sphere cells varies according to the sample's pore-space volume, the percentage of spheres obeying an exponential decay with the sphere's radius. The sphere-packing presented the cells with larger radius, characteristic of its formation, which relates to larger pore sizes. The Estailades carbonate presented larger cells than the Berea sample, even though its total porosity is smaller, signaling that the pore size distribution may be more correlated to the total pore-space volume than to the sample's porosity.

Table 3 - Comparison between the total number of pore-space voxels and the total number of nodes of each sample's network.

	voxels	Nodes
Berea	18.002.989	205.164
Estailades	35.517.594	290.727
Spheres	67.785.996	533.766

Source: By the author.

Next, the medial axis network for each of the samples was evaluated, the results presented on Figure 29. As we can see, the distance between sphere cells differ greatly from the complete network. The reason for this is that intermediate cells between the medial axis spheres were removed, leaving just the longest connection between the remaining sphere cells. The range of the radius distributions of the cells remained the same, just varying in proportion to the complete network. This means that the medial axis cross section variation is within the entire range of the complete network sphere cell's radius.

Figure 29 - Medial axis networks for the three porous samples: Berea Sandstone, Estailades carbonate and the synthesized glass sphere packing.

Source: By the author

Next, the complete network data from each sample was used to acquire the sample's pore sizes through the procedure described in the previous chapter. The results from the correction stage, in which we remove low centrality nodes, is shown in Figure 30.

Figure 30 - Centralities of each node group: throat, pore and other before and after the correction was applied to the network data of each sample. (a) Berea sample, (b) Estailades sample (c) sintherized sphere packing. Each node group is normalized by their total number of nodes.

Source: By the author

All samples presented a decrease on the number of nodes classified as throats which have high centrality, at the same time there was an increase in proportion of the number of high centrality pore nodes. This implies that there was a removal of nodes classified as pores in each sample. However, as we can see, not all nodes with low centrality were removed. Indeed, if the centrality scores of two neighboring pore nodes are similar, both nodes keep their classification as pores since they represent the same relevance in the total flow of the sample.

The Berea sample presented the largest correction in number of nodes, having 38% of the original nodes classified as pores removed from the pore nodes group. Similar percentage of pore nodes was removed from the Estailades sample, 36% of nodes. The syntherized sphere packing sample had only 17% of the pore nodes removed from the group.

If we compare the results from the idealized sample from the chapter before to the results for the sphere packing sample, we see that there is similar behavior. The majority of nodes that were classified as representative pore regions were correctly captured by the direct application of the MS algorithm, with no issues of over-separation of the region. However, as expected for rock samples, the larger variation of pore shapes leads to an over separation on the number of pores.

Table 4 - Comparison between the total number of pore-space voxels and the total number of nodes of each sample's network.

	Pore nodes before	Pore nodes after
Berea	8921	5495
Estailades	6501	4160
Spheres	1104	912

Source: By the author.

A representation of the final pore-throat networks can be visualized in Figure 31. In this image, (a) presents the final clusters of sphere cells that represent the pores found by the process. The color coding is the calculated equivalent diameter of each cluster. The throats are represented as cylinders, and the calculated mean diameter of the channels is coded in grayscale range.

The pore size distribution shown in (b) makes clear that the pore sizes of the rock samples are very similar. The sphere pack sample, on the other hand, presented much larger pore sizes. It is interesting to see that the shapes of the curves are very similar to the shape of the radius distribution curves presented on Figure 29 of the medial axis network. This could indicate that the medial axis network could be used as a preliminary tool for the comparison of the expected pore sizes of different samples.

The mean throat diameter distributions presented on Figure 31 (c) shown that, even though the carbonate sample and sandstone samples are similar in pore sizes, the structure of their connections differ. The throat diameters of the sphere packing sample are slight smaller than the pore sizes, as expected from the morphology of this sample.

Figure 31 - Comparison of the pore diameter measured by the developed software (new method) to the analysis of a commercial software (Pergeos). (a) Application of the method to a Berea Sandstone sample. (b) Application of the method to a Estailades carbonate sample.

Source: By the author

5.1.1 Comparison to commercial methods of pore space analysis

The validation of the extraction method was done by comparing the network's pore size distributions of the developed software to that of the commercial software PerGeos. The measure used to define each pore's size was the pore's equivalent diameter, using two separate methods: Chamfer is a conservative approach to the pore separation which uses a different distance transform in acquiring the seeds for the watershed based pore -separation. The skeleton approach uses the erosion technique discussed before. The comparison of the results for each sample is shown on Figure 32.

Figure 32 - Comparison of the pore diameter measured by the developed software to the analysis of a commercial software (Pergeos). (a) Application of the methods to the Berea Sandstone sample. (b) Application of the methods to the Estailades carbonate sample (c) Application of the methods to the Sphere packing sample.

Source: By the author

We see on Figure 32 that the range of pore sizes were correctly captured by our method of analysis for all samples. Discrepancies between the pore sizes were expected, but it occurred only for a small percentage of pores found. The low variation between the commercial software results and the developed method shows that we can predict the pore size distributions with the same reliability as well-established commercial methods.

Even though the range of pore sizes is coherent between the methods, we see that the behavior of the separation of the developed method correlates better to the CHAMFER conservative approach. One explanation for this is that the direct application of the reduction of the volume to its topological equivalent skeleton could have led to an over branching of the pore's volume, which is avoided in the correction stage of the developed software.

5.1.2 Global morphology evaluation of the networks

The final networks of the samples were used to find the correlations from the morphology and topology of the networks with petrophysical simulation measurements done directly on the binarized tridimensional volume. We concentrated our study into two characterizations of

the samples: the resistivity formation factor, and the absolute permeability. The resistivity Formation Factor was used to characterize the structural measurement of tortuosity through the medial axis networks, to show an application of the medial axis network directly. We measured both the geometrical tortuosity and we estimated the electrical tortuosity to see if the formation factor results were correlated to the tortuosity found through the network method.

The measurement of the absolute pore space permeability was used in the application of the separated space. Instead of using the medial axis network, we tested the pore-throat network in terms of the capacity for flux assigned to each throat. The topology of the final networks was characterized in terms of connectivity and capacity of flux and these results compared to the absolute permeability found for each sample.

First the structural analysis will be discussed and then the topological characteristics and permeability of the samples will be presented.

5.1.3 Structural Analysis

To estimate the samples' electrical tortuosity, we proposed the following method: pore nodes presented in each opposing face of the samples were selected as starting and end points of the possible paths that the flux could follow. To measure the tortuosity of these paths, we used the definition of tortuosity:

$$\tau = \frac{L_a(\text{real path})}{L_b(\text{straight line})} \quad (5.1)$$

The real path (L_a) was acquired through the application of *Dijkstra's algorithm* to the weighted network, which finds the shortest paths between two nodes in a graph. The total distance of the path is calculated by adding the distance between each node's (sphere) center, such as:

$$L_a = \sum_i^{N_a-1} \sqrt{(x_i - x_{i+1})^2 + (y_i - y_{i+1})^2 + (z_i - z_{i+1})^2} \quad (5.2)$$

Where (x_i, y_i, z_i) is the center position of the i th node, in a path with N_a nodes. The distance L_b is simply the distance between the first and last nodes in the calculated path. Channels with larger diameter will have higher capacity for flux, this is accounted for in the

capacity attribute of the edges of the medial axis networks. So, the closest path will be the path with least resistance to fluid flow. This is very similar to the definition of the electrical tortuosity discussed before.

To compare between methods, we also acquired the geometrical tortuosity, simply defined by the shortest path between the start and ending points. The geometrical tortuosity was measured on the network not weighted, so all edges were considered to have equal weight. The distribution of paths' tortuosity for the weighted network in comparison to the unweighted is shown on Figure 33.

Figure 33 - Comparison between geometrical and electrical tortuosity distributions acquired through network walk. (a)-(c) show the geometrical tortuosity found for the Berea sample, Estailades sample and Sphere packing sample respectively. The graphs (d)-(f) show the tortuosity distribution of the paths considering the diameter of the channels and the mean centrality of the nodes. (d) Berea sample, (e) Estailades sample and (f) sphere packing sample.

Source: By the author

The graphs on Figure 33 show that the geometrical tortuosity is always smaller than the tortuosity found by measurement of paths of least resistance for flux. These results are in accordance with the experimental results from literature that show that the geometrical tortuosity tends to be smaller than the electrical tortuosity.

Table 5 - Mean path tortuosity results for each direction. Geo stands for the geometrical tortuosity, EL. Stands for the estimated electrical tortuosity.

Direction	Berea Geo $\langle \tau \rangle$	Berea EL $\langle \tau \rangle$	Estailades Geo $\langle \tau \rangle$	Estailades EL $\langle \tau \rangle$	Spheres Geo $\langle \tau \rangle$	Spheres EL $\langle \tau \rangle$
X	2.3	2.9	2.3	2.8	1.4	1.6
Y	2.4	2.6	2.4	3.6	1.4	1.6
Z	2.0	2.4	2.0	3.2	1.5	1.5

Source: By the author.

Table 5 summarizes the mean tortuosity found for each direction. The mean values found for the sphere packing and Berea samples of the geometrical tortuosity is very similar to the mean value found for the estimated electrical tortuosity. This result indicates the homogeneity of these samples. The carbonate sample, on the other hand, presented a large difference between methods, the tortuosity of the paths for the estimated electrical tortuosity is much wider than for the geometrical case. This is coherent with the expected heterogeneity of the paths of a carbonate in comparison to a sandstone sample.

Figure 34 - Estimated electrical tortuosity distributions in comparison to the porosity profiles of each sample. (a)-(c) electrical tortuosity distributions for Berea, Estailades and sphere packing respectively. The graphs (d)-(f) show the porosity profiles for the Berea, Estailades and Sphere packing volumes, respectively.

Source: By the author

The heterogeneity of the samples can also be observed on their porosity profiles (on Figure 34 d, e and f). We see that the dispersion found for x direction on the tortuosity of the

paths was also observed on the porosity profile for the Berea sample. We also observed that, on the z direction, Berea sample's porosity profile had little variation, which is also coherent with the narrow distribution of the paths' tortuosity.

The wide distributions seen on the Estailades sample indicates high heterogeneity, which is also present on the porosity profiles of the images. The sphere packing sample presented a small range of porosity variation on its profiles in all chosen directions, indicating the high homogeneity of the sample.

Figure 35 - Distribution of the Euclidian distance between pores and the arc distance of the connecting channels. (a) Euclidian distance (b) arc distance. We see that the distance between pores is similar for the Berea and Estailades. On the other hand, the number of paths with a higher arc distance between pores is much higher for the Estailades than the Berea sample.

Source: By the author

The homogeneity level of each samples could also be assessed by the mean distance between pores (figure 35) and the normalized variance of the data, presented on Table 6.

Table 6 - Mean pore separation for each sample: $\langle L \rangle$ is the mean of the straight path distance between each pair of pores in the sample (identified by the new method). The quantity $\sigma_L^2 / \langle L \rangle^2 = \langle L^2 \rangle / \langle L \rangle^2 - 1$ is a measure of the statistical fluctuations of the data. $\langle S \rangle$ is the arc length of the distance between pores, measured using the same method described for the tortuosity evaluation (through the Dijkstra algorithm), and $\sigma_s^2 / \langle S \rangle^2 = \langle S^2 \rangle / \langle S \rangle^2 - 1$ is the statistical fluctuations of S .

	$\langle L \rangle$	$\sigma_L^2 / \langle L \rangle^2$	$\langle S \rangle$	$\sigma_s^2 / \langle S \rangle^2$
Berea	15.27 μm	0.25	20.10 μm	0.45
Estailades	22.75 μm	0.23	36.38 μm	1.04
Spheres	63.02 μm	0.15	73.76 μm	0.23

Source: By the author.

We see that even though the dispersion of the mean pore distance $\langle L \rangle$ is similar for both rock samples, the dispersion on the arc distance (related to the tortuosity) for the Estailades is

twice the dispersion for the Berea data. So, even though the pores are distributed in similar form in the pore space, the path between each pore is, on average, more tortuous on the Estailades sample. The opposite could be seen for the sphere packing sample. The dispersion of both the arc lengths S and real distance L were small, which implies high homogeneity of the sample.

Figure 36 - Behavior of the tortuosity distributions for each sample in each chosen direction.

Source: By the author

We see from Figure 36 that, in most cases, the path chosen most frequently was the same, as we can see by the behavior of the distributions. The exceptions were the paths on the x direction for the Berea sample and the path on the y direction on the Estailades sample. We can understand from these results that, in these cases, the probability that the flux will follow either a tortuous path or a straight path is very similar. This is correlated to an intrinsic heterogeneity of these samples on these directions.

Since the electrical tortuosity is correlated to the paths in which we have the largest density of flux, we compared the tortuosity correlated with the highest frequency on the graphs of Figure 36 to the results for resistive formation factor simulated on Pergeos (Table 7).

We see that the direction in which we had largest tortuosity correlates to the formation factor result on that direction. The Estailades sample y direction distribution didn't have a clear largest frequency, so both the tortuosity related to the largest peak ($\tau=3.0$) and the mean tortuosity ($\tau=3.6$) is shown.

Table 7 - Tortuosity of paths found more frequently for each direction compared to the Formation Factor results.

Direction	Berea max(τ)	Berea Formation Factor (Pergeos)	Estailades max(τ)	Estailades Formation Factor (Pergeos)	Spheres max(τ)	Spheres Formation Factor (Pergeos)
x	2.7	41	2.1	88	1.6	4.3
y	2.6	38	3.0-3.6	383	1.5	4.4
z	2.0	18	3.2	263	1.5	4.8

Source: By the author.

We applied the formula (3.9) to estimate the formation factor using the results of tortuosity from Table 7. The parameter $\alpha=2$ was used for the rock samples, and $\alpha=1$ for the sphere packing sample. For the Estailades sample, we estimated the cementation factor $m=1.5$, using the tortuosity results on the x direction as an adjustment. For the Berea sample and sphere packing we let $m=1.0$.

Table 8 - Results for the calculated Formation Factor (NN) of the samples compared to the apparent Formation Factor acquired with the software PerGeos.

Berea			Estailades			Spheres		
Direction	F (NN)	Apparent F (Pergeos)	Direction	F (NN)	Apparent F (Pergeos)	Direction	F (NN)	Apparent F (Pergeos)
X	40,5	41	X	94	88	X	4.6	4.3
Y	37,5	38	Y	192-276	383	Y	4.3	4.4
Z	22	18	Z	218	263	Z	4.3	4.8

Source: By the author.

There is good agreement between the simulated formation factor and the estimated values from the application of (3.9). The homogeneity of the sphere packing sample led to a linear correlation of tortuosity and the formation factor, as we can see on Table 8. The results for the Berea sample were also very close to the expected formation factor value, showing that the method of using the medial axis networks to estimate the sample's tortuosity, not simply the geometric tortuosity, but the electrical tortuosity, leads to coherent results.

The high levels of the apparent formation factor on the y and z directions provided by for the Estailades sample are not unusual for carbonate samples.^{51,63,82-83} This indicates high

heterogeneity on the pore size distributions on y and z directions. However, we could get coherent results on the directions in which the tendency of tortuosity was well defined.

5.1.4 Topology study of the extracted networks

Another important measure of the porous structure is the pore network's coordination number, (the number of connection of each pore node), which is a measure of the sample's connectivity and it is correlated with the sample's permeability^{1,61,84–86}. The coordination number distributions for the pores identified by the developed software are presented on Figure 37.

Figure 37 - Pore coordination numbers (k) for the Berea sample (black) and the Estailades sample (red) Sphere packing sample (blue). (a) Degree probability distributions (k), (b) power law fitting (c) cumulative degree distributions $P(K > k)$ compared to an exponential decay of the form $P_{exp}(k) = e^{-(k/\langle k \rangle)}$, with $\langle k \rangle = 5 - 10$.

Source: By the author

The Kolmogorov–Smirnov goodness of the fit test⁸⁷ was applied to the cumulative pore coordination number distributions for power law fits. The results presented high p values for all data ($p > 0.01$). This suggests that the distributions aren't described by power laws, as we can see on the attempt fit to the data on Figure 37 (b). Applying an exponential decay fit to the data, we got $R^2 > 0.98$ for all distributions, the exponential decay following the form:

$$P_{exp}(k) = e^{-(k/t)}, t = 5 \text{ rock samples and } t = 10 \text{ sphere packing} \quad (5.3)$$

There have been reports of real networks that present exponential behavior on the node degree distributions with characteristic exponential decay parameter close to the network's mean degree^{88,89}. The Berea sample presented an average pore coordination number $\langle k \rangle = 2.64$, the Estailades sample, $\langle k \rangle = 2.83$, and sphere packing sample $\langle k \rangle = 4.7$. We

see that the exponential decay parameter is not close to the mean degree of the networks, but it is correlated $= 2 * \langle k \rangle$.

This shows that the mean degree alone may not give enough information on the networks' topology, since the variation of connectivity indicates that we find highly connected nodes with relevant frequency. The exponential behavior instead of a power-law heavy tail curve for the degree distribution might be associated to the pore distribution in the tridimensional space. This gives a low probability of long range connections.

The mean connectivity reported in the literature for Berea samples is $\langle k \rangle \sim 3$ and for Estailades samples $\langle k \rangle \sim 2.8$ ^{51,80}. One explanation for the lower values found in the extracted networks are the pore nodes on the border of the volumes. These pores present $k=1$, leading to an unrealistic low connectivity. After eliminating these pores from the distributions of the rock samples, the average connectivity found was $\langle k \rangle \sim 3.14$ for the Berea sample and $\langle k \rangle \sim 2.9$ for the Estailades sample, which is in agreement with values from the literature.

We compared the mean values of connectivity with the mean permeability found by direct simulation on the pore space volume using the commercial software Pergeos. The results are summarized on Table 9. We see that mean absolute permeability found in the simulations is highest for the sphere packing, which presented the highest mean coordination number as well. We had a slight difference in permeability between the carbonate and sandstone samples, which agrees to the mean connectivity found in the proposed network model.

Table 9 - Mean absolute permeability $\langle p \rangle$, simulated on the binary data using the commercial software Pergeos, in comparison with the mean connectivity $\langle k \rangle$ calculated in the network model.

Samples	$\langle p \rangle \mu\text{m}^2$	$\langle k \rangle$
Berea	2.14	3.14
Estailades	1.69	2.9
Spheres	120.2	4.7

Source: By the author.

The absolute permeabilities of the samples were also compared to the flow capacity of the pore-throat networks models. We choose to evaluate the absolute permeability on Z direction, in which the distinction of the absolute values found on the simulations for each sample were more evident. The total flow capacity of each sample was acquired by finding the paths of maximum flow, setting a *super source* of flow connected to the pores nodes in the

border of the network at $Z=0$ and a *super sink* connected to the pore nodes in the border of the network at $Z=$ sample size.

The simulations on the volumetric data are shown in Figure 38. The color encoding represents the magnitude of the z component of the fluid velocity on the region, normalized to 0-255.

Figure 38 - Flow paths observed resulting from the permeability experiment on Z direction, simulated on the original volume data of the samples on the software PerGeos. Left: Berea sample, middle: Estailades sample, right: sphere packing sample. The color coding represents the magnitude of the Z direction velocity component of the fluid, normalized 0-255.

Source: By the author

The comparison between the maximum flow paths in Z direction found on the networks and the flow paths of the simulated experiments are shown in Figure 39. As we can see, the paths in which we had more density of flux are equivalent to the calculated paths found through the network model.

If we consider the maximum flow value, calculated by the sum of the edge's capacity of the minimum cut of the networks, we see that there is correlation between the predicted absolute permeability values and the maximum flow values (Table 10).

Table 10 - Maximum flow found on the networks compared with the simulated permeability p_z in Z direction.

Samples	$p_z \mu\text{m}^2$	<i>max flow</i>
Berea	3.20	2929
Estailades	1.19	1708
Spheres	123.7	52489

Source: By the author.

This is good evidence that the network model is able to capture the morphology of the channels without critical loss of information from the volume data.

Figure 39 - Flow paths from the simulated permeability experiment on the complete volume, and the network maximum flow paths found for each sample. 1: the network color coded according the the edge's total flow capacity. 2- the network color coded according to the used capacity of each edge. 3: simulated permeability experiment (PERGEOS). The spheres represent the inlet and outlet points used for the max flow calculations on the networks. (a) Berea sample, (b) Estailades sample and (c) Sphere packing sample.

Source: By the author

We also see that the throats' morphology changes significantly the topology of the networks. We measured both the current flow centrality distributions and closeness centrality distributions. The current flow betweenness centrality distributions remained with the same shape if we considered the weighted networks or unweighted networks, with a slight increase of the percentage of nodes with higher score (Figure 40).

Figure 40 - Comparison of the current flow betweenness centrality distributiona of the networks without considering the edge weights (A) and considering the edge weights (B). We have a slight increase of higher centrality nodes.

Source: By the author

However, the change in topology between the weighted and unweighted networks were evident on the closeness centrality scores of the nodes. The results from Figure 41 show that, if we consider the pore positioning on the network without taking into account the diameter and tortuosity of the connecting channels, the mean distance between nodes increases, given by the relative percentage of nodes that presented low closeness centrality.

This is especially true for the Estailades sample. We see that the mean distance between nodes decreases considerably when we take into account the morphology of the throat channels. This could indicate that there can be pore nodes acting as bridges between two different pore clusters.

Figure 41 - Comparison of the closeness centrality distribution of the networks without considering the edge weights (the distance between nodes is the number of steps in the network) and considering the edge weights. We see that when we consider the edge weights, the number of nodes with high closeness centrality tends to increase.

Source: By the author

Even though the results of the closeness centrality distributions could indicate high heterogeneity on the mean node strength, the measurement of the local entropy shows that the majority of nodes presented a homogeneous distribution on the distance and arc distances between pores Figure 42 (c).

The networks also presented a non-trivial correlation between the number of connections a node has and the mean strength of the nodes. The correlation of the node's connectivity and the mean distance between nodes and the total channel length s are shown in Figure 42 (b) and

(a) respectively. This means that highly connected pores usually are also connected to the more tortuous paths.

Figure 42 - (a) Correlation between the mean edge distance and the number of connections of the pores. (b) Correlation between the arc distance of the edges and the number of connections of the pore. (c) local entropy of edge weights for all samples.

Source: By the author

There is also evidence of homogeneity on the clustering scores distribution of the nodes (Figure 47)

Figure 43 - Clustering score distribution of the nodes for each sample.

Source: By the author

It is interesting to note that, both the estallades and Berea samples presented similar shape of the distributions. We see that the majority of nodes for these samples have low clustering score, which is expected, given the sparse nature of geographical networks.

The sphere packing sample, on the other hand, presented a more homogeneous distribution. This a very interesting characteristic present only in this sample. This result is correlated to a high connectivity of the sample, which could in turn be correlated to the high permeability results in the simulations.

A verification of the correlation between the topological evaluation and permeability of the samples was done through a robustness test. This test was performed through the measurement of the maximum flow in the network as chosen nodes were removed. The

choice methods were: nodes with high closeness centrality scores, nodes with high current flow betweenness centrality scores, largest pore nodes and finally through a targeted edge removal, removing edges with high capacity.

Table 11 - Number of nodes removed to interrupt flow through closeness centrality targeted attack

sample	% nodes removed
Berea	0.02
Estailades	0.09
Spheres	1.50

Source: By the author.

What we observed is that the closeness centrality of the nodes (Table 11) is that, indeed, nodes with higher closeness centrality play a major part on the flow. The results from Table 11 show that very small percentage of node needed to be removed such that the flow was interrupted.

A different result was observed when we targeted the edges with high capacity. As we can see on Figure 44, the distribution of the edges capacity is very heterogeneous for the rock cores.

Figure 44 - Edge capacity distribution of each sample. We see that for the estailades and Berea samples, a majority of nodes presented edges with low capacity. The Sphere packing sample presented, on the other hand, a more homogeneous distribution.

Source: By the author

The homogeneity of the sphere packing sample is evident, on the other hand. However, even if the edges capacity distribution is heterogeneous for the Berea sample, the directed attack was not as efficient on interrupting flow as it was when choosing nodes with high closeness centralities.

Figure 45 - Comparison between the maximum flow variation with the target attack for the Berea and Spheres samples.

Source: By the author

However, the Estailades sample had its flow interrupted faster than the target node attack through closeness centrality. Only 0.03% of the edges were removed for the complete interruption of flow.

The comparison on figure 45 shows that, the attack based on edge capacity had a similar effect on flow as the current flow attack (CF) and the removal of the largest pore nodes.

Figure 46 - Variation of the maximum flow (Z direction) as pores were removed from the network. Red spheres represent the variation as the largest pores were removed, black squares represent the variation as the most central pores were removed. (a) Berea sample, (b) Estailades Sample, (c) Sphere packing sample.

Source: By the author

On Figure 46 we see the comparison for all three samples for the contrast between largest pores removed and current flow betweenness centrality target attack. It is very interesting to note that the sandstone sample variation of flow first was more influenced by the removal of

the largest pores, and then by the highly connected pores. The Estailades sample, in the other hand, is more dependent on larger pores for the fluid flow, as we can see on Figure 46 (b).

The sphere packing sample showed that the high homogeneity on pore sizes makes the network more dependent on the highly connected nodes. Even though the size of pores is large, the centrality of the pores is more relevant for the connectivity of the sample.

5.2 APPLICATION ON ACIDIFICATION SAMPLES - WORMHOLES

On the acidification samples, the study aimed at the characterization of the final morphology of the channels (wormholes) formed after the acidification process. The μ CT data from the samples contained the original pore space and the wormhole, so, to focus only on the wormholes, first we processed the volume to find the largest connected region which percolated in the direction of the acidification. The characteristics of the samples after this process are on Table 12.

Table 12 - Characteristics of μ CT data of the wormhole samples. Resolution, number of images slices, volume of the selected wormhole, surface area of the selected wormhole and the porosity ϕ of the sample considering only the wormhole.

Sample name	Resolution (μ m)	N slices	Sample Volume (cm^3)	Wormhole Volume (cm^3)	Wormhole Surface Area (cm^2)	ϕ (%)
E2	42.7	(775x775)x1500	85	1.8	5.8	2.1
E4	45.2	(775x775)x1500	85	1.3	6.7	1.5
E5	45.2	(775x775)x1500	85	2.3	17.7	2.7
E8	45.2	(775x775)x1500	85	1.3	3.5	1.5
E9	45.2	(775x775)x1500	85	3.1	22.6	3.6

Source: By the author.

The surface of the structures formed from the acidification procedure can be visualized in Figure 47. As we can see from the data in Table 12, sample E9 presented the largest surface area, follow by sample E5. These two samples differ greatly from the E2, E4 and E8 samples, which presented more structured channels.

Table 13 - Porosity ϕ and absolute permeability of the samples previous to the acidification procedure

Sample name	ϕ (%)	Absolute permeability (mD)
E2	16.2	>40
E4	15.3	>40
E5	15.4	>40

E8	14.7	>40
E9	17.8	>40

Source: By the author.

All samples, previous to the acidification, were samples with high permeability (larger than 40mD) and porosities around 20% (Table 13). We see that, from the porosity and permeability data alone it is not possible to infer the final structure of the wormholes. In fact, E2 had the second highest porosity percentage, but it's structure is more alike to the formation in sample E4. E5 and E4 both had 15% porosity before acidification and the wormholes' structures are completely different between samples.

Figure 47 - Structure of the wormhole formations for each sample. The grey surface represents the wormholes.

Source: By the author

5.2.1 Structural analysis

We were able to quantify the differences between structures by the extraction of the medial axis networks of the samples. We see from Figure 48 that the algorithm could capture the structures without loss of the morphology from the wormholes.

Through the networks, we separated the percolating paths in the direction of the acidification from the ramifications paths.

Figure 48 - Medial axis networks from the wormhole samples. The diameter variation of the paths is shown in color code.

Source: By the author

The definition of what were considered main paths and ramifications is explained on Figure 49. The extremity nodes at $Z=0$ of our network are the acid inlet points, and the other nodes at the extremity on $Z=$ sample length, are the outlet points. The *main paths* are *all* the *minimum distance* paths that connect *all* the inlet points to *all* the outlets, considering the networks' edges' capacity. The minimum distance between each inlet-outlet pair is the path which presented the least resistance for fluid flow.

The radius variation of the main paths for all samples followed the same exponential behavior, in terms of frequency in which the channels presented that radius in its cross section (Figure 50 (a)). This implies that, even though the structures of the porous space of the samples prior to the acidification could be different, this didn't influence significantly on the acid corrosion on the final diameter of the preferential paths.

Figure 49 - Definition of the separation between main paths and ramifications, using sample E2 as an example. We defined the main paths as the minimum distance paths between the inlet points of the acid influx to the outlet points at the limit of the sample. All other paths are considered ramifications from the main paths.

Source: By the author

However, we see that samples E8 and E2 presented larger percentage of nodes with $\text{radius} > 0.8 \text{ mm}$ (more than 10% of the total diameter variation of the channels), than the other samples. If we look on Figure 48, we could already visualize that these samples presented fewer ramifications from the main paths than the rest. This, in turn, could be evidence that the acid reaction focused on one preferential region. So, instead of opening other paths, the acid opened the main paths further.

On the graph (b) from Figure 50, we analyzed the radius distributions for the ramification paths. We observed two behaviors: samples E9 and E5 presented much less percentage of ramifications with $\text{radius} > 0.4 \text{ mm}$ than samples E8 and E2. This larger number of small radii

ramifications explains the high surface to volume ratio measured for these samples ($E5 = 7.7 \text{ mm}^{-1}$, $E9 = 7.3 \text{ mm}^{-1}$).

Figure 50 - Radius distribution from the samples. (a) main path radius distributions. (b) ramification channels radius distributions (c) comparison between ramification and main path radius distributions (d) radius variation of the main paths with the distance of the acid entry point.

Source: By the author

Sample E4 presented an intermediate behavior between the two groups. Even though its structure presented many possible paths between the inlet and outlet points, we observed through a simulation of maximum flow that there was one main path in the middle of the sample which presented much less resistance to fluid flow than the rest (Figure 51 (c)). For that reason, all other paths were considered as ramifications.

This lead to the transition behavior observed on Figure 50 (b). The sample presented the same frequency on ramifications with radius $< 400 \mu\text{m}$ that of samples E8 and E2. For larger radius, on the other hand, the frequency of channels found for this sample correlates with the frequency of samples E5 and E9.

Figure 51 - Definition of the separation between main paths and ramifications for the E4 sample. (a) complete sample color coded according to the path's diameter. (b) main paths selected from the sample, color coded according to the path's diameter. (c) maximum flow passage in each edge.

Source: By the author

We can see that, even though the main paths have a much larger diameter in comparison to the ramifications, we still need many small diameter spheres to represent the paths completely, as we see on Figure 50 (c): 90% of the spheres representing the main paths are in the same range as the ramifications. We have two reasons for this: paths smaller in diameter need a great number of maximum spheres to capture its structure than paths with larger diameters. The second reason is that the extremities of the samples are composed mainly of paths with small diameter, which are connected to the main paths.

The method also allowed the measurement of the variation of the diameter of the main paths on the direction on the acid influx (Figure 50 (d)). Up until the 50mm limit, we have no discernible correlation of the samples' z direction length and the diameter of the paths. The mean radius of the entire sample group measured in this case was $0.7 \pm 0.3mm$.

We observed that, after the 50mm limit, the main channels' radii start to decrease. This could indicate that there is a loss on the effectiveness of the chemical reaction at this point.

The electrical tortuosity of the main paths was also evaluated, with the same process as we have applied to the rock samples. The inlet and outlet points were chosen on either extremity on the Z axis of the samples, as it is shown on Figure 49. Then, the lengths of all the

possible paths of connection between the outlets and inlets were measured. This resulted on the tortuosity distributions shown on Figure 52.

We see that most samples presented wide distribution of tortuosity of the paths. Samples E4 and E9 presented the widest distributions, in which we have paths connecting inlets to the outlets that are twice as long as the straight line connecting them. This is due to the number of ramifications that appeared on the acidification process. Sample E5 and E2 presented a tendency of most paths presenting the same tortuosity (30% of the paths), which means that a particle will follow the same path 30 percent of the times, independent on the inlet-outlet pair chosen.

Sample E8 was the only one that presented a small variation on the tortuosity measured. This shows that the morphology of the wormhole followed basically one main channel, as we could see already qualitatively by the visualization of the network extracted. This information could implicate that the flow is entirely dependent on a single channel.

Figure 52 - Tortuosity distributions in the direction of the acidification for each sample.

Source: By the author

5.2.2 Morphology evaluation through random walk simulation

Through the tortuosity direct measure, we could assess the morphology of the main paths. In order to verify the influence of the samples' ramifications, we proposed a particle diffusion experiment through random walk. The particles start at a randomly chosen node in the medial axis network, then at each step the particle can move to a different node or remain on the current node, with the probability:

$$p_{i,j} = \frac{c(i,j)}{s(k)} \quad (5.4)$$

Where $c(i,j)$ is the edge's capacity and $s(k)$ is the total strength of the node. So, there is a larger probability that a particle will move to nodes with larger diameter. Then, the particles are allowed to diffuse in the network until one of two things happens: either the particle finds an outlet node, meaning that the particle was allowed to leave the wormhole, or the simulation reaches a time limit.

Figure 53 - Mean frequency that a site was visited in the simulations for each sample.

Source: By the author

The simulation was run for 10000 events for each sample, and the number of times a node was visited and the number of different sites that were visited were measured.

The result for each simulation of the visited frequency of the nodes are shown in color coding in Figure 55. We see that, for this model, there are region of the samples in which the particles choose more frequently to pass through then others. This is expected since we gave preference for regions with larger diameter in the simulations. What is interesting to note is that there are some specific sites that seemed to act as bridges, being visited far more times than others.

Figure 54 - Percentage of the total unique visited sites versus the simulation time for each sample. Here only the results of the particles that reached the outlet points in shown.

Source: By the author

The coverage results for the samples shown on Figure 54 gives another view on the tortuosity results from before. We see, as expected, that the high number of ramifications present on samples E9 and E5 leads to a need for the particle to, in average, walk a larger number of steps in order to reach the outlet points. However, we see that the number of distinct sites visited is not as high as the other samples. So, even though the ramification paths add a new level of complexity for these samples, the particles tend to follow common paths to find the outlet points.

Table 14 - Compared results of the mean number of steps need to reach the outlet points and the number of nodes in each network.

Sample name	$\langle Nsteps \rangle$	Nnodes	$\langle Nsteps \rangle / Nnodes$
E2	30498	12420	2.4
E4	31063	10391	2.9
E5	81434	39759	2.0
E8	49924	4490	11.1
E9	98112	65017	1.5

Source: By the author.

Another important result from these simulations concerns sample E4. Sample E4 presented a wide distribution on the tortuosity of its main paths. However, the diffusion simulations show that, even though the paths are tortuous, they act as shortcuts for the particles to reach the outlet points. We see this from the results of Table 14. The mean number of steps needed for a particle to walk from its starting point to the outlets is in average the same of sample E2, which presented a lower mean tortuosity of the main paths.

This means that, even though the branching on the main paths might lead to wide distributions on tortuosity, this branching can also be positive if we are interested in the diffusion of a solute through the region, given that the diameter of the branching channel is large.

The results from Table 14 for sample E8 also show that the number of steps needed for the particles to reach the outlet points surpassed the number of nodes in the network. This is a consequence of the model not being self-exclusive. Since the acidification on this sample acted on one main channel, the particles didn't have a preferential pathway to follow. So, the probability of the particle moving inside the channel or staying put was very similar. We can make the analogy that the particle acts as it is in free diffusion, instead of restricted by the morphology of the sample.

5.2.3 Network robustness evaluation

To assess the dependence on the main paths and the dependence on certain regions of our samples saw on the diffusion simulations, the robustness of the networks was evaluated similarly as it was done for the rock samples. The variation of the maximum flow in the Z direction was measured as the nodes of the networks were removed. The inlets and outlets chosen as it was done in the main paths evaluations. The difference here is that there wasn't a

separation on pore nodes and throats. The nodes to be removed were selected directly from the medial axis network.

We measured the effectiveness of the centrality measures to find the major throughputs nodes for fluid flow with the robustness test as well. We have applied the target attack using page rank, betweenness centrality, current flow betweenness centrality and eigenvector centrality. We had two interesting results with the current flow betweenness centrality measures and the eigenvector centrality measures. We saw that the current flow betweenness centrality was the most efficient centrality measure to find the critical nodes for the continuity of the flow on the networks.

Figure 55 - Visualization of the current flow centrality scores for each sample.

Source: By the author

The current flow betweenness centrality scores can be visualized on Figure 52. We see that the regions in which we had high centrality scores correspond to regions of bifurcation of the paths. Figure 56 (a) shows the variation of the maximum flow measured with the removal of nodes with high current flow scores. We see that the flow decays fast for all samples, especially for the E2, E8 and E5. The least effective case was for the E4 sample, but even for

this sample, we needed under 1% of the nodes removed for the flow to stop completely. Comparing to the random case, Figure 56 (c), in which the nodes were chosen randomly for removal, there was a minimum of 2% of node removal for the maximum flow to fall to half the initial value, and a minimum of 4% for the flow to stop completely. The random case was run for 1000 of events.

Figure 56 -Variation of the maximum flow measured with the removal of nodes. (a) nodes were removed according to the current flow centrality scores. (b) nodes were removed according with its eigenvector centrality score. (c) nodes were removed randomly (d) comparison of the robustness test for samples E5,E8 and E9 of the results by current flow scores (black) and eigenvector centrality scores (red).

Source: By the author

The results of the attack using the eigenvector centrality scores are shown on Figure 56 (b). We see that, for some samples, more specifically E5, E8 and E9, the eigenvector centrality score was a very efficient measure to find the critical regions for the fluid flow, on the other hand, for the samples E4 and E2 that wasn't the case. This points out to two morphologies found: the wormholes that are dependent on one path for the flow to pass in the Z direction and the ones that branched into many large diameter paths.

The dependence on one path seemed to be the case for the E8 sample, however E5 and E9 also presented that behavior, even though we had a large variation of the paths tortuosity for these samples. We see from Figure 56 (d) that still the current flow centrality scores were

more effective on finding the critical nodes, except for sample E9, in which the eigenvector centrality was even more efficient.

The explanation for this behavior lies in the mass conservation of the maximum flow calculation and in the characteristic of the eigenvector centrality scores. A node will have a high eigenvector centrality score if it is connected to other nodes with high relevance on the network. For sparse networks, such as these, most nodes will have 0 eigenvector scores, since they are poorly connected, leaving just few highly connected nodes with relevant eigenvector centrality scores.

This means that this is a very directed and targeted attack in a concentrated region of the network. If the attack succeeds in stopping the flow, this means that, due to mass conservation, there were only one possible path that the particles could follow (Figure 57).

Figure 57 - The main path for fluid flow, highlighted in black, for sample E5. We see that, to maintain the conservation of mass, if the black path is broken, the flow isn't able to divert to other paths.

Source: By the author

However, this is only valid for the maximum flow calculations in the networks. In a flow simulation on real samples, the total flow might not stop, but we could argue that the flow rate would decay if one of the critical regions found by the eigenvector centrality measurements were clogged. This experiment has not yet been done in this work, but it is one of the proposed future works.

6 CONCLUSIONS AND FUTURE WORK

We have proposed the use of network theory as a complementary tool to understand the topology of porous materials. In our work, we developed a powerful method of network extraction that could recover the morphological and topological features of our samples.

The *medial axis* networks proved to be efficient for the tortuosity measurement of the samples. The modelling of the networks' *capacity* was able to capture the paths with least resistance for fluid flow, so the electrical tortuosity of the samples was recovered. This shows that the topology of the final networks could describe correctly the features from the volumetric data from the samples.

The test of the recovering of morphology of the samples was also successful. The pore size distributions of the developed method corresponded to the pore size distribution captured by commercial methods. However, the developed method has some advantages over the commercial application:

- (1) The pore space is divided according to the relevance of the pore centers inside the complete network, this removes the necessity of adjustments made by the user of the software;
- (2) The regions identified as throats will always be regions with high connectivity in the network, meaning that the throats will be the regions of preferential paths of fluid flow.

The correspondence between the paths of flux observed in the direct simulations and the paths found through maximum flow measurement in the networks showed that the final pore-throat networks are also robust models for fluid flow, which, in turn, permitted that the structure of the networks could be evaluated through network theory.

The evaluation through network theory showed that the pore-throat networks are not free-scale, but follow an exponential decay on the connectivity of nodes. We were also able to show that the closeness centrality distribution of the nodes provides important information on the dynamics of fluid flow. Even though the local entropy of the nodes is low, meaning that the variation between capacities of each throat connected to the pore is not very large, we still find nodes with high closeness centrality on the sample with lowest absolute permeability

measured. This is an indication of the existence of nodes acting as bridges for the passage of flux.

The nodes that were more important for flux was also determined through the robustness test. Indeed, closeness centrality of a pore is correlated to the total flux of the sample. We observed as well, that, for more homogeneous samples, there is little difference between removing a pore with large volume from a more central one. However, for the heterogeneous sample, removing a large pore is very crucial for fluid flow.

On the wormholes study, we could show that the method developed is an important technique to evaluate the final structures after acidification. We could separate the influences of the main channels of that of the ramifications. We were also able to show that, even though the tortuosity of the sample is large, the ramification structure can play an important part on the fluid extraction. Also, the robustness test was able to verify which sample channeling structure could be more fragile to flaws.

We believe that this work is an important contribution to continue development of methods and characterization of porous materials.

6.1 FUTURE WORK

For future work, we intend to use the development extraction method for the simulation of dynamics of diffusion and NMR experiments inside the porous media.

We also intend to apply the method for more rock samples, carbonates and sandstones. We see that complex network theory applied to porous medium is a powerful tool, so we intend to apply for a large range of samples to make a statistical analysis of the porous space.

A first visualization of this application is shown on Figure 58, in which the *sphere cell* network is used for the separation of the pore space into regions with long relaxation times (larger radius) in contrast with regions with short relaxation times (smaller radius).

Figure 58- Separation of the pore space into regions of large relaxation times and small relaxation times. Example applied to the Berea sample.

Source: By the author

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