Random Walk simulation of Nuclear Magnetic Resonance for characterization of reservoir rocks using micro-CT data

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Abstract. Random walk algorithms have been used to simulate nuclear magnetic resonance (NMR) transverse relaxation (T2) decay in porous media since the early 1990's. Since the time of their first implementation, they have been primarily based on geometric models of pores and grains such as the grain consolidation model. These models have been useful for examining mismatches between the actual T2 distributions and the pore size distributions from mercury injection capillary pressure (MICP) and those from X-ray microtomography (micro-CT) images. Noticeable success has been achieved, particularly in complex carbonate rock samples where the T2 distributions may represent an average pore size between the macro-pores and the micro-pores due to diffusive coupling. In typical random walk simulations, the position of the walker is calculated geometrically in terms of the radius of the macro-pore to determine if it has arrived at the grain surface. This approach is useful for geometric models with Euclidean geometry pores. Currently, micro-CT images would require an intermediate step, where the image is converted and approximated to Euclidean geometries such as spheres and prisms to represent the macro-porosity. An alternative approach would be to construct a binary cube for 3D simulations (or square for 2D). In this approach, the position of the walkers is linked to the binary cube index where 0 would represent macro- pores and 1 would represent the micro-porous grains. Comparison between the results of these two approaches shows similar computational times and the indexed method is more suitable for binary images from micro-CT.

Keywords: porous media, Nuclear Magnetic Resonance, Random Walk, diffusive coupling, Python simulation.

1 Introduction

NMR logs are routinely used in the Pre-salt carbonate formations offshore Brazil to help identify the most productive intervals as shown by Machado et al [1]. These intervals typically have a larger proportion of macro-pores while the least productive intervals are dominated by micro-pores. T2 distributions from downhole NMR logs and from laboratory NMR of core samples are often compared to pore size distributions from micro-CT images to validate the relation between T2 and pore size based on the harmonic average between bulk (B), surface (S) and diffusion (D) relaxation as shown by Toumelin et al [2],

$$\frac{1}{T_2} = \frac{1}{T_{2B}} + \frac{1}{T_{2S}} + \frac{1}{T_{2D}}. \quad (1)$$

For most porous media applications, the effects of bulk and diffusion are minimal, and eq. 1 can be reduced to the relationship between T2 and surface relaxation parameter ρ and surface to volume ratio (S/V) of the porous media,

$$\frac{1}{T_2} = \rho \frac{S}{V}. \tag{2}$$

As in eq. 3 below, T2 can also be expressed as a time constant for the exponential decay of the magnetization M(t) as it decays from initial amplitude A, which is proportional to the number of hydrogen nuclei. The decay occurs as a function of time(t) due to the relaxation processes occurring at the surface of the pores from the interaction between the polarized hydrogen nuclei and the paramagnetic sites that influence surface relaxation.

$$M(t) = \sum_i A e^{\frac{-t}{T_{2,i}}}. \tag{3}$$

When there are mismatches between the T2 distributions and the pore size distributions it is useful to examine whether they are caused by diffusive coupling between the micro and macro pores as per Ramakrishnan et al [3] and Carneiro et al [4] or if there is another cause such as strong internal magnetic fields due to heavy minerals as described by Saidan and Prasad [5], increased surface area proposed by El-Husseiny and Knight [6] or very large pores as in Kleinberg [7]. Random walk simulations can be designed to evaluate all these effects as shown by Toumelin et al [2], but Random walk simulations are especially useful for evaluating diffusive coupling between macro-pores and micro-porous grains as first presented by Ramakrishnan et al [3].

2 Methodology

2.1 Random Walk Simulations for Micro-Porous Grains: Geometrical Models vs CT Images

Geometrical models were first utilized by Schwartz [8], to evaluate electrical properties and the flow of viscous fluids in porous media by modeling diffusion using random walkers. The random walkers were placed randomly within a spherical or elliptical pore and their position was noted by the distance from the center of the pore. The walker then advanced +/- one grid unit in the z, x, y directions and the clock would advance with each step until the walker strikes the pore-grain interface. For modeling diffusive coupling between macro-pores and micro-porous grains the walk can be then terminated at the time of the strike as described by Ramakrishnan et al [3] and Carneiro et al [4]. A strike was determined when the distance of the walker from the center exceeds the known radius of the pore space. This method is satisfactory for spherical pores but is not easily adapted to realistic pore shapes from micro-CT images. To overcome this limitation, a voxel based random walk can be done on a binary cube constructed from micro-CT images with indices as shown by Jin et al [9]. Comparing the two methods yields similar computational times, with the voxel-based method being faster by about 10-20%. Tab. 1 below is a comparison of computation times for 10-, 30- and 50-micron radius spheres using both the geometrical model and the binary cube voxel model for 1000 and 10000 random walkers where the walk ends at the first collision with the grain boundary as there is an assumption the walker will remain in the micro-porous grain.

Table 1. Execution time comparison of geometric- vs voxel-based models

Number of random walkers	One thousand			Ten thousand		
Macropore radius (microns)	10	30	50	10	30	50
Geometric-based execution time (s)	1.0	7.4	19.8	9.9	77.0	196.0
Voxel-based execution time (s)	0.8	5.9	17.1	9.2	57.6	159.6

In addition to faster execution time, the voxel-based method is better suited for micro-CT images where the pore shapes are often non-spherical. The micro-CT images must be binarized though, based on a grey-scale threshold selected so that the calculated porosity from the image matches the expected value for the visible porosity based on the image resolution.

2.2 Random Walk Simulation for Micro-porous grains vs solid grains

When doing random walk analysis in carbonates a key consideration is whether the grains are treated as micro-porous or solid. For solid grains, when a walker strikes a grain boundary the walker will bounce back to the previous position and continue the random walk with the clock advancing. The decay rate for the walker is a combination of bulk effects and surface relaxivity ρ, given by eq. 3 below, where ε=1 when the walker is within a step of the grain boundary and 0 while in the macro-pore, and δr is the step length as described by Toumelin et al [2].

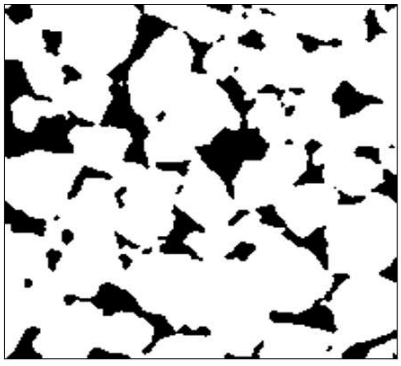
$$\frac{1}{T_2} = \frac{1}{T_{2B}} + \varepsilon \frac{3.84\rho}{\delta r}. \tag{3}$$

For micro-porous grains, the walker will not rebound after striking a grain boundary but would enter the micro-porosity and will remain within the micro-pores decaying at a known rate (ε =1), thus the walk ends, and the time is recorded as per Ramakrishnan et al [3] and Carneiro et al [4], and then a new walker starts the process again.

As a typical random walk consists of at least 2000 steps as recommended by Jin et al [9], the difference in computation time between the micro-porous vs solid grain simulations can be significant. Response time for the solid grain simulation could be improved considerably by parallelization as each walker is independent of the others but for a typical laptop computer with an Intel Core i5-2467M and CPU @1.6GHz running the simulation written in Python code, Tab. 2 below shows the results for 100 random walkers for 3 different size simulation cubes with 1 micron resolution from a micro-CT image for Berea sandstone.

Table 2. Comparison of computation times for micro-porous versus solid grains

Grain type	Microporous grains			Solid Grains		
Cube width (microns)	50	100	200	50	100	200
Macro porosity (%)	18.5	18.5	19.6	18.5	18.5	19.6
Average Number of Steps	20.4	17.8	28.5	667	1595	2175
Execution Time (s)	29.1	28.2	31.1	667	928	1473



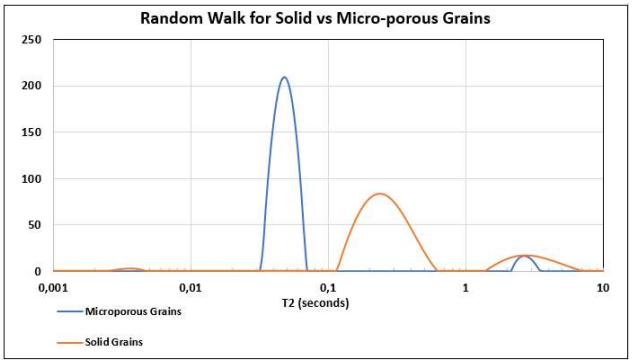
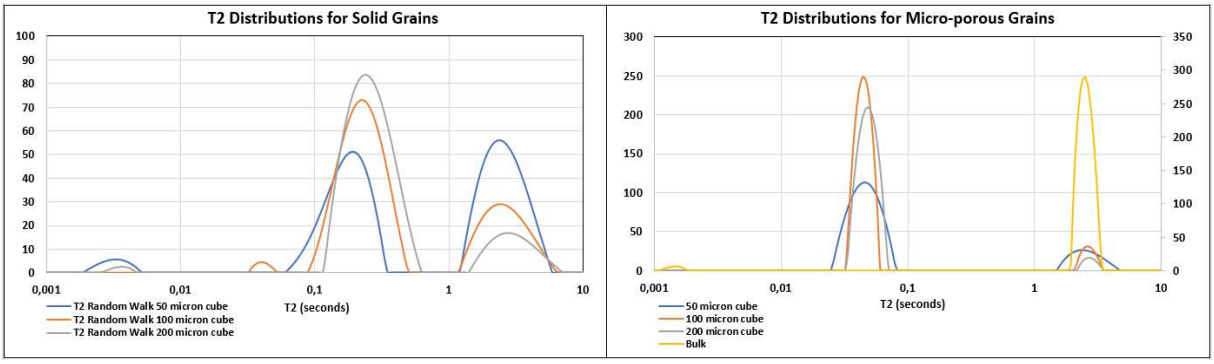


Figure 1. (left) Berea sandstone micro-CT 200x200 pixel slice from 3D image with 1 micron/pixel. Pore space is black, and grains are white. Figure 2. (right) Random walk simulation results for solid and micro-porous grains for Berea Sandstone. Cube size is 200x200x200 microns at 1 micron resolution.

For the 200x200x200 cube, there is a distinct difference in the T2 distributions for the micro-porous grains versus the solid grain simulations. Berea is not expected to have micro-porous grains and in section 2.4 we will examine this in more detail. Both the micro-porous and solid grain simulations show the edge effects with the longer time T2 humps at 2.5 s due to the walkers in the pores on the edges of the cube relaxing at a T2 bulk rate of 2.5 s seconds. The bulk effect is stronger for the solid grain simulation as the walkers are free to continue their walk for longer times and hence eventually arrive in a pore at the cube boundary. Both the solid grain and micro-porous grain simulations assumed a surface relaxivity parameter ρ = 11 microns/second, which is typical for Berea as per Washburn et al [10].

2.3 Random Walk Simulation for sub-cube

As can be seen in Tab. 2, computation time can be reduced considerably by selecting a sub-cube to perform the computation. By reducing the size of the sub-cube however the edge effects associated with pores contacting the border of the sub-cube must be considered. As the results may be compared with Lab NMR measurements it is common practice when doing lab NMR on vuggy carbonates with visible pores on the surface of the core to wrap the core with Teflon tape to keep the saturating fluid within the exposed pores. If the saturating fluid is



water, the Teflon tape would present a non-relaxing boundary and the water in such pores will often appear as water relaxing at bulk rate. For this reason, we have chosen to let walkers that strike the boundaries of the micro-CT image to decay at bulk rate (ε=0 in eq. 3). These edge effects become more significant with smaller sub-cube sizes as the proportion of surface area to volume increases as the width of the cube becomes smaller.

Figure 3. (left) T2 distributions for Solid grain Random Walk simulation for cube sizes of 50, 100 and 200 microns. Figure 4. (right) T2 distributions for Micro-porous grain Random Walk simulation for cube sizes of 50, 100 and 200 microns. Bulk relaxation at 2.5 seconds is shown for reference.

Figures 3 and 4 both indicate greater edge effects as the sub-cube size decreases, and the edge effects are significantly greater for the solid grain simulations. For the solid grain simulation 50x50x50 cube, the edge effects represent about 60% of the NMR signal, for the 100x100x100 cube the edge affects are about 30% of the NMR signal and for the 200x200x200 cube the edge effects are about 15%. As the surface to volume ratio of a cube is 6/W where W is the width of the cube, these ratios are consistent with the cube size differences. For the micro- porous grain simulations, the edge effects are minimal, and the execution times are similar regardless of the cube size as the simulations used only 100 walkers to be consistent with the solid grain simulations. Increasing the number of walkers to 1000 would still have reasonable execution times for the micro-porous grain simulations but would take over four hours processing for the 200-micron cube. In addition to the varying edge effect for the different cube sizes, there is a noticeable increase in the T2 value of the main peak of the T2 distributions as the cube size increases, which implies that the large cube sizes encounter larger pores. This will be examined in more detail in section 2.4.

2.4 Comparison of converted micro-CT images with voxel based Random walk

To validate the random walk simulations, the Berea micro-CT images were processed with PORE* simulation software developed by ESSS based in Florianopolis, Santa Catarina, Brazil. With PORE software the pores are approximated as spheres using the maximum sphere algorithm developed by Silin & Patzek [11]. This was done for the 3 sub-cube sizes of 50, 100 and 200 microns as discussed in sections 2.2 and 2.3 and the pore size distributions were converted to T2 distributions using eq. 2, assuming spherical pores with a surface to volume ratio of 3/R where R is the radius, and a surface relaxivity parameter ρ= 11 microns/second, to be consistent with the value used for the random walk simulations.

Figures 6, 7 and 8 below show the comparison between the T2 distributions derived from the Maximum spheres and the T2 distributions from the solid grain Random walks. There is a good correlation between the two methods indicating that as the cube size increases some larger pores are accessed during the random walk.

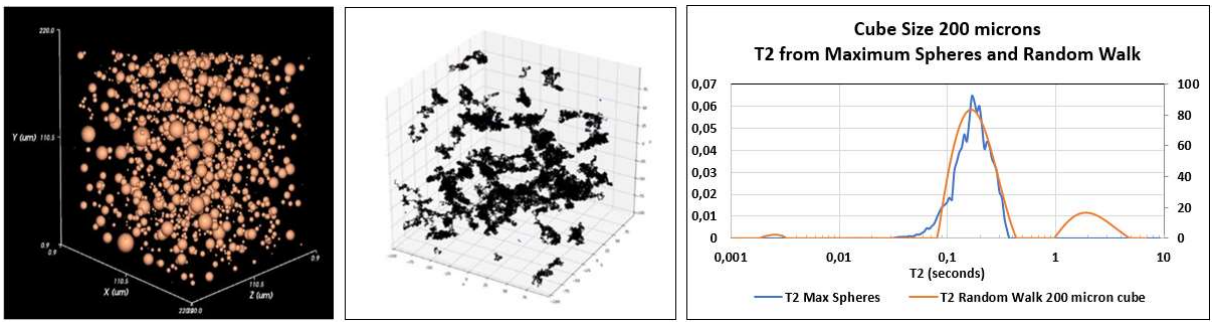


Figure 5. From left, Maximum Sphere processing for 200-micron cube, Random Walkers positions and overlay of T2 distribution calculated from Maximum Spheres with T2 from Solid Grain Random walk.

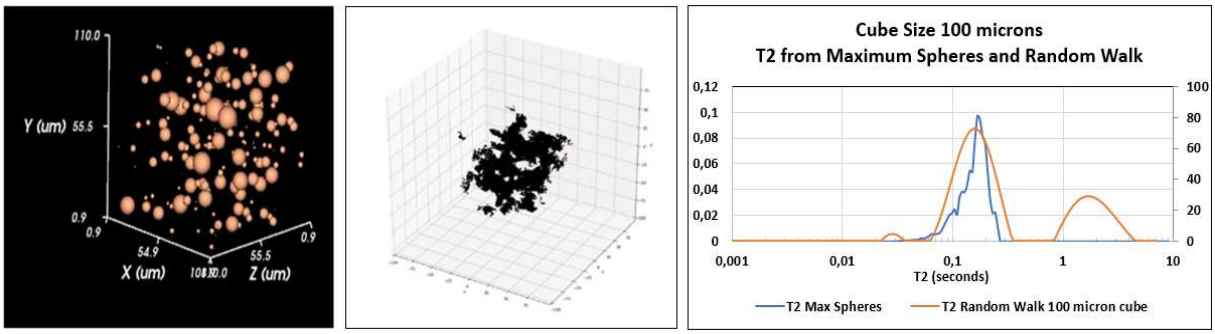


Figure 6. From left, Maximum Sphere processing for 100 micron cube, Random walkers positions and overlay of T2 distribution calculated from Maximum Spheres with T2 from Solid Grain Random walk.

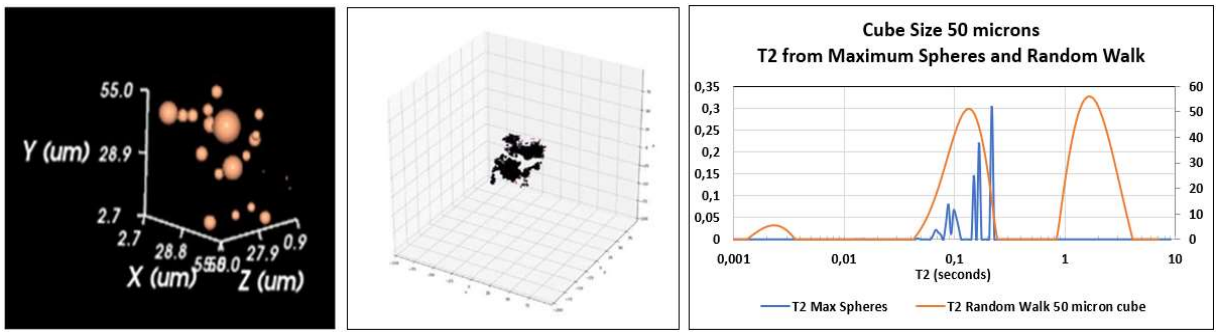


Figure 7. From left, Maximum Sphere processing for 50-micron cube, Random Walkers positions and overlay of T2 calculated from Maximum Spheres with T2 from Solid Grain Random walk. The small number of pores in the 50-micron cube results in spiky T2 distribution from Maximum spheres.

3 Results and Discussion

The original goal of this project was to develop a voxel based Random walk for NMR T2 simulation for micro-porous grains with Python that could be run on a normal laptop to process 3D images from micro-CT scans. This goal has been achieved for micro-porous grains but to extend the application to solid grains will require parallelization of the code to achieve reasonable execution times. Selecting a smaller sub-cube to reduce the execution time for doing solid grain simulations will increase the edge effects and should only be done if a more powerful computer is not available. To eliminate the edge effects, a geometrical model could be used instead of a micro-CT image by placing the pore in a solid or micro-porous cube such that the pore boundary does not contact the sides of the cube. If the pore sizes are known from either a micro-CT image or thin section slide, this can be done with a simple geometrical model using either a spherical or elliptical pore.

In addition to micro-porous coupling, other researchers such as El-Husseiny and Knight [6] have suggested that higher surface roughness and irregular pore shapes which increase the surface to volume ratio could lead to faster T2 relaxation. With sufficient resolution, voxel-based Random walk analysis of micro-CT scans,

combining back-scattered electron microscopy (BSEM) and Focused ion beam SEM (FIBSEM) images as described by Sok et al [14] would be required, but this will require merging images with different resolutions and more powerful computational resources.

It should also be emphasized that the Random walk simulations presented here were for water saturated samples as most Lab NMR measurements are performed on water saturated cores. Partially saturated cores with water and oil can be simulated with Geometrical based Random walk simulations as shown by Carneiro et al [4]. This could be adapted to a voxel-based model with micro-porous grains where the micro-pores are assumed to be water saturated and the macro-pores oil saturated. Then the key consideration would be whether the macro-pores are oil-wet in which case the grain contact represents a relaxing surface or whether the macro-pores are water wet with a thin layer of water on the grain surface which represents a non-relaxing surface to the hydrogen protons in the oil molecules. Such a simulation will also require allowing the walkers to start their walk within the micro- pores. This was not done for any of the examples here but was examined using geometrical models where the main consideration is whether the walkers starting in the micro-pores can enter the macro-pores and whether walkers starting in the macro-pores can enter the micro-pores and re-enter the macro-pores as discussed in Toumelin et al [2]. These scenarios will require more advanced computational resources also and will be addressed in a future paper.

As mentioned previously, the micro-CT image analyzed was Berea sandstone which was selected as it was available in 1 micron per voxel resolution. There was no Lab NMR available from this Berea sample but the T2 distribution from the solid grain simulation is within the range of expected values for Berea and matched well with the analytical solution based on Maximum sphere processing. Berea is not considered micro-porous but was chosen to minimize any complications from larger voxel sizes as described by Jin et al [9]. We expect to next apply this methodology to carbonate micro-CT images with resolutions of 3.5 microns per voxel, 7 microns per voxel and 14 microns per voxel to fully investigate which resolution is preferred for Random walk NMR simulations of Pre- salt carbonates. The final goal is to improve the accuracy of transforming T2 distributions into pore-size distributions such that oil recovery factors can be better understood in these complex carbonates.

4 Conclusions

As computational speeds continue to increase and as parallel processing becomes more routine, using Random walk techniques to analyze NMR response based on micro-CT images of rock samples will become more common place. This paper demonstrates that a simple Random walk to evaluate diffusive coupling between macro pores and micro-porous grains can be achieved using Python code with a laptop computer. More complex simulations to evaluate varying surface relaxivity as described by Benevides et al [12] and strong magnetic field gradients as described by Toumelin et al [2] will require parallel processing to achieve reasonable processing times. The effects of increased surface roughness on NMR as described by Ma [13] will require higher resolution images and the smaller voxel sizes will in turn require more powerful processing to perform the random walk simulations.

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References

[1] V. Machado, P. Machado, P. Netto, R. Bagueira, A. Boyd, A. Souza, L. Zielinski and E. Junk, "Carbonate Petrophysics in Wells Drilled with Oil Base Mud," SPWLA 52nd Annual Logging Symposium, May 14-18, 2011.
[2] E. Toumelin, C. Torres-Verdin, B. Sun and K.J. Dunn, "Random-walk technique for simulating NMR measurements and 2D NMR maps of porous media with relaxing and permeable boundaries" J. of Magnetic Resonance., vol. 200, pp. 313–320, 2009.
[3] T. S. Ramakrishnan, L. M. Schwartz, E. J. Fordham, W. E. Kenyon and D. J. Wilkinson, "Forward Models for Nuclear Magnetic Resonance in Carbonate Rocks," The Log Analyst, vol 40, no. 4 (July-August 1999).
[4] G. Carneiro, A. Souza, A. Boyd, L. Schwartz, Y.Q. Song, R. Azeredo, W. Trevizan, B. Santos, E. Rios and V. Machado, "Evaluating Pore Space Connectivity by NMR Diffusive Coupling," SPWLA 55th Annual Logging Symposium, May 18-22, 2014.
[5] M. Saidan and M. Prasad, "Effect of mineralogy on nuclear magnetic resonance surface relaxivity: A case study of Middle Bakken and Three Forks formations," Fuel., no. 161, pp. 197-206, 2015.
[6] A. El-Husseiny and R Knight, "A Laboratory Study of the Link Between NMR Relaxation Data and Pore Size In Carbonate Skeletal Grains and Micrite," Petrophysics, Vol. 58, No. 2; pp 116–125, April 2017.
[7] R.L. Kleinberg, "Utility of NMR-T2 distributions, connection with capillary pressure, clay effect, and determination of surface relaxivity parameter ρ" from Magnetic Resonance Imaging (Elsevier), Vol. 14 – No. 7/8, 1996.
[8] L. M. Schwartz., "Modeling transport in granular porous media," SPWLA 31st Annual Logging Symposium, June 24- 27, 1990.
[9] G.Jin, C.Torres-Verdín and E.Toumelin, "Comparison of NMR simulations of porous media derived from analytical and voxelized representations" Journal of Magnetic Resonance., vol. 200, no. 02, pp. 313–320, October 2009.
[10] K. Washburn, M. Sandor and Y. Cheng, "Evaluation of Sandstone Surface Relaxivity Using Laser-induced Breakdown Spectroscopy," Journal of Magnetic Resonance, 2018.
[11] Silin, D. Patzek, T., 2006. "Pore space morphology analysis using maximal inscribed spheres". Physica A: Statistical Mechanics and its Applications, 371(2), pp.336–360.R, 2006.
[12] F. Benavides, R. Leidermana , A. Souza, G. Carneiro and R. Bagueira, "Estimating the surface relaxivity as a function of pore size from NMR T2 distributions and micro-tomographic images." Computers & Geosciences 106, (200-208) 2017.
[13] S. Ma, G. Leu, S. Chen and M. Eid,, "Objective Driven Solid Surface Roughness Characterization for Enhanced Formation Evaluation," SPE-201689-MS SPE Annual Technical Conference, Denver, Colorado, USA, 5 – 7 October 2020.
[14] R.Sok, T.Varslot, A. Ghous, S. Latham, A. Sheppard and M. Knackstedt, "Pore Scale Characterization of Carbonates at Multiple Scales: Integration of Micro-CT, BSEM, and FIBSEM," Petrophysics, Vol. 51, No. 6, Dec. 2010