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A NEW APPROACH TO RANDOMLY GENERATE POROUS MEDIA TO PERFORM CFD SIMULATIONS

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Abstract. *Flow and transport in porous media have been subject in researches due to its wide range of applications like chemical, pharmaceutical and food as well as petroleum and groundwater engineering and in many other industrial applications. In this way, to improve the physical understand for such flows and the accuracy of existent models, the study of more realistic geometries would be necessary. In the current work, we present a strategy to generate a highly complex three-dimensional porous media. The porous media is generated by a controlled random function. Frequency points are controlled by a Fast Fourier Transform algorithm, allowing control the region with more pores or fractures. Afterward, a constructive solid geometry software is applied to create the domain. Pore-scale simulations have been conducted on porous media using OpenFOAM, for single and two-phase flow for Newtonian fluids. The accuracy and stability of the numerical method have been verified through the development of several test cases. The results showed the potential of the method to predict multiphase flow and the viability of the porous media generator to perform computational fluid dynamics simulations of different materials.*

Keywords: *porous media, artificial structure, pore-scale simulation, Newtonian multiphase flow*

1. INTRODUCTION

Understanding multiphase flow at pore-scale is of great importance for a wide range of applications: from environmental understanding, like aquifer and site-pollution, to industrial process improvements (oil recovery and waste management), (Aboukhedr *et al.*, 2015; Icardi *et al.*, 2016). The intrinsic complexity of multiphase systems and multi scale heterogeneity of geological formations represent major challenges to understand and model immiscible displacement in porous media. Porous materials can be described by the unique shape and connectivity of the internal void structures which give rise to a large range of macroscopic transport properties.

Upscaled descriptions based on Darcy's law are extensively used to study Newtonian fluid flow in porous media. However, these techniques fail to predict accurately the pressure drop because many flow parameters are not considered while simplifications are made for the multi-scale structure of the rocks. To increase the accuracy of upscaling techniques, a fundamental understanding of the physical characteristics of the porous medium and fluids within the pore space is necessary. These include hydraulic conductivity, capillary pressure and relative permeability. Numerical representation is also important with respect to a proper selection of boundary conditions, because a small part of the actual porous medium is investigated, algorithms to capture the interfaces between the fluids and the quality of the mesh. In this way, to improve the physical understand for fluid flows on porous medium and the accuracy of existing models, there is a need for realistic geometries to be investigated (Soulaine *et al.*, 2016; Sahimi, 2011).

To perform an accurate numerical simulation of fluid flow in porous media is crucial importance use geological realistic characteristics, which should include geometric properties like pore or particle shape and volume, and topological properties such as pore interconnectivity. A larger number of models to represent the microstructure of porous media have been proposed over the years (Biswal *et al.*, 1999). The process to obtain a representative porous medium can be based on image reconstruction (Okabe and Blunt, 2004; Mosser *et al.*, 2017) or purely based on numerical models. The image reconstruction process depends from dataset of high-resolution micro computed-tomography (micro-CT) images and image reconstruction techniques. In the image reconstruction process and in many cases of numerical methods high computational resources are involved, limiting their applications. Therefore, it is important to construct models capable

of closely mimicking the heterogeneity of the real porous media and, at the same time, are efficient enough to allow the simulation of flow and transport phenomena with reasonable computational effort (Yeong and Torquato, 1998; Ioannidis and Chatzis, 2000; Lehmann *et al.*, 2008). In Fig. 1 it is possible to see the morphology difference of eight rock samples.

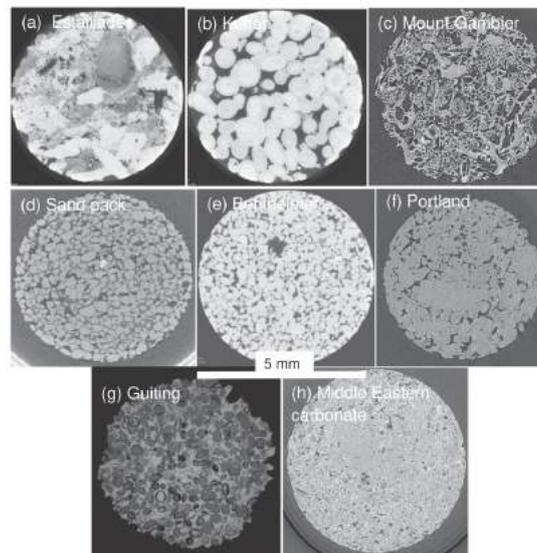


Figure 1. Two-dimensional cross-section of 3D micro-CT images of different samples (Pore space is shown dark). Source: Blunt *et al.* (2013)

In the current work we present a strategy to generate a highly complex three-dimensional (3D) porous media. The flow and mass transport through a porous media are described, characterized and simulated, with objective of better understand the underlying mechanisms and the influence of the medium structure. This study is limited to Newtonian fluids. The porous media reconstruction technique can be made from pictures from literature (e.g. Fig. 1), maintaining the porosity and the permeability of the original material. With the aid of a software for creating 3D Computer-Aided Design (CAD) models the porous media material can be approximated by spheres, cylinders, polygons, etc., maintaining the grain characteristics (size geometrical features, etc) of the real sample. The software provides two main modeling techniques: First there is constructive solid geometry (aka CSG) and second there is extrusion of two-dimensional (2D) outlines (OpenSCAD, 2016). For instance, ketton limestone (see Fig. 1-b), an oolitic quarry limestone of Jurassic age. The grains are smooth spheres with large pore spaces (Blunt *et al.*, 2013), that can be approximated by an artificial generation of spherical void phases porous media micro-structure.

2. METHODOLOGY

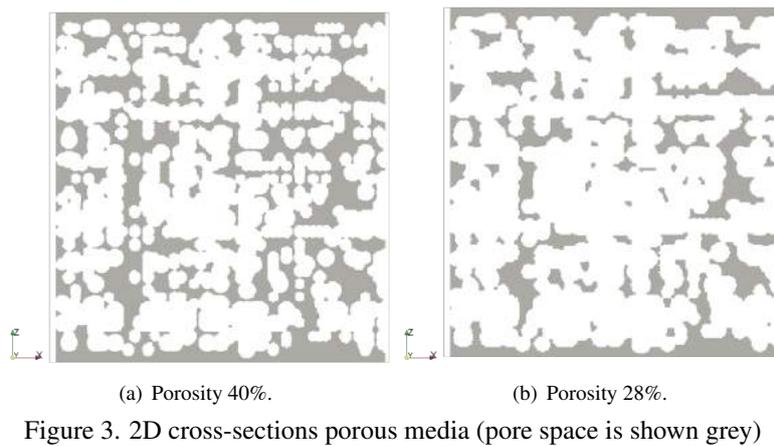
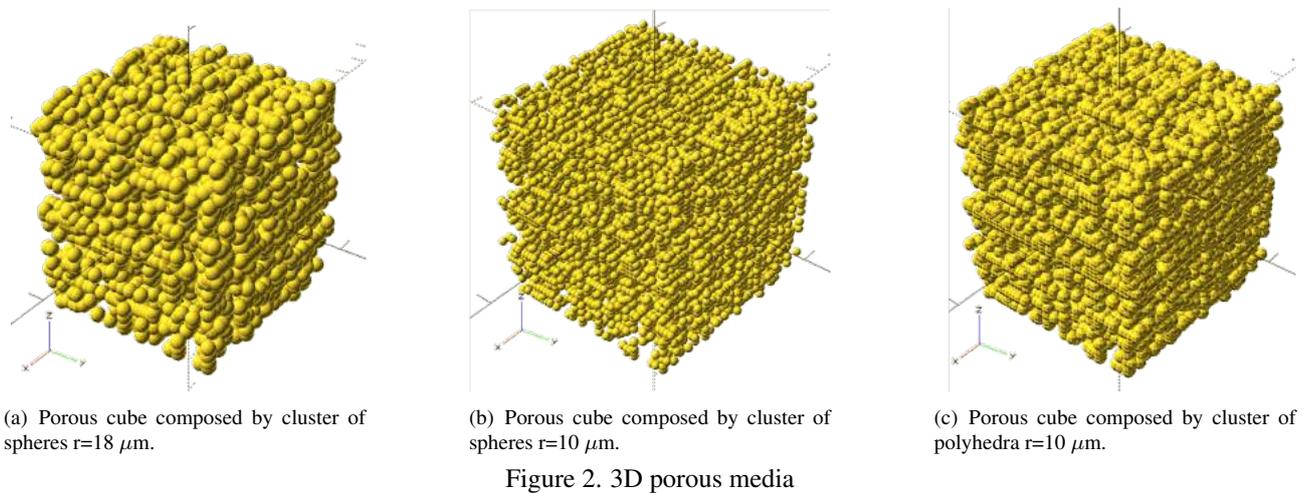
2.1 Porous media generator

The development of strategies for the 3D generation of porous media as close to real cases to analyze the internal flow with the aid of computational fluid dynamics (CFD) tools is a major obstacle to the study of porous media. Thus, a software tool to generate a highly complex 3D porous media was developed. The 3D porous media is generated by a controlled random function. In this version of the code, the points frequency is controlled by a Fast Fourier Transform (FFT) algorithm, allowing control the region with more pores or fractures. All geometric and topological parameters, characterizing pores or fractures are related to porosity and preferential paths. The porous media reconstruction technique can be made from pictures from literature, maintaining the porosity and the permeability of the original material.

With the aid of an open source software (OpenSCAD) (OpenSCAD, 2016) for creating 3D CAD models, the porous media material can be approximated by spheres, cylinders, polygons, etc., maintaining the grain characteristics (size geometrical features, etc) of the real sample. The software provides two main modeling techniques: First there is constructive solid geometry and second there is extrusion of 2D outlines (OpenSCAD, 2016). Figure 2 shows three examples of a 3D porous media with $500\mu\text{m}$ generated by the methodology described above. Different grains diameters and geometrical formats are used resulting in different porosities, as can be seen on the Fig. 3.

2.2 Mesh generation

After the 3D generation and renderization of the porous media, a STereoLithography (STL) file is exported with the domain data information. With the STL containing the information of the porous medium, the mesh is generated representing the pore-space of the sample allowing perform the fluid flow simulation. The domain is then discretized by one of



the native meshers of the open-source CFD toolbox OpenFOAM®, *SnappyHexMesh*, which creates hexahedral meshes. The mesh approximately conforms the surface obstacle via successive refinement and snapping a starting background hexahedral mesh until a predefined precision level is reached. Figure 4 shows an example of the geometry and mesh around the obstacles.

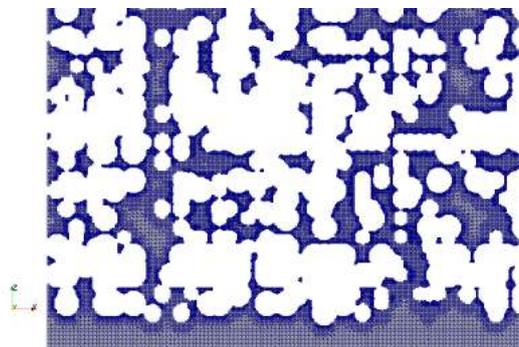


Figure 4. 2D cross-section porous media- Computational mesh - porosity 40%

To perform a precise and stable simulation, the quality of the mesh is checked before the CFD simulation. The test had been controlled using *checkMesh* a built in tool for mesh quality check.

The work of Guibert *et al.* (2015) highlights how important a correct meshing for the numerical study of permeability of different materials. It is also highlighted in the work the importance of a correct balancing for parallel processing of porous media for cases with mesh refinement.

Table 1. Fluid properties and initial conditions

Parameter	Symbol [units]	Value
Volumetric flow rate (single phase)	Q [m ³ /s]	8.33E-11
Volumetric flow rate (two-phase)	Q [m ³ /s]	1.00E-10
Fluid density (water)	ρ [kg/m ³]	998
Fluid dynamic viscosity (water)	μ [$\frac{Ns}{m^2}$]	8.88E-04
Fluid density (oil)	ρ [kg/m ³]	835
Fluid dynamic viscosity (oil)	μ [$\frac{Ns}{m^2}$]	1.00E-01
Surface tension (water/oil)	N/m	4.80E-02

2.3 CFD setup

The computational fluid dynamics package OpenFOAM was applied to solve the governing fluid flow equations. Single-phase (water injection through a 3D porous medium) and two-phase flow (oil drainage by water injection) simulations were performed. The goal was to analyze how the behavior of porous media artificially generated and the mesh quality affects predictions of flows through the specific domain.

The standard laminar Navier-Stokes equations of mass and momentum conservation were applied for the single-phase simulations. The Volume of Fluid (VOF) method (Hirt and Nichols, 1981) was used for the analysis of oil-water of the porous medium. This method tracks the interface between the two fluids while an additional term accounting for surface tension forces between the two liquids was added to the momentum equation.

Both single- and two-phase simulations were assumed incompressible, isothermal and immiscible. The fluids properties of water and oil adopted as well as the inlet conditions are presented in Tab. 1. The reference values used were taken according to the work of Aboukhedr *et al.* (2015). Due to the presence of interphase and the use of VOF method in order to track it would require a low Currant number to ensure the stability which demands high processing time.

The schematic representation of the boundary conditions can be seen in Fig. 5-a.

A pressure outlet condition was set for the outlet surface. All walls (porous media and channel) were so-called no-slip boundaries that are characterized by a velocity of zero at the wall. These boundary conditions were based on Jungreuthmayer *et al.* (2015) work's, where CFD simulations and experimental analysis were performed. The domain was filled by water for the single-phase calculations and for the case of oil drainage by water injection the domain was initialized with oil and water as shown in 5-b.

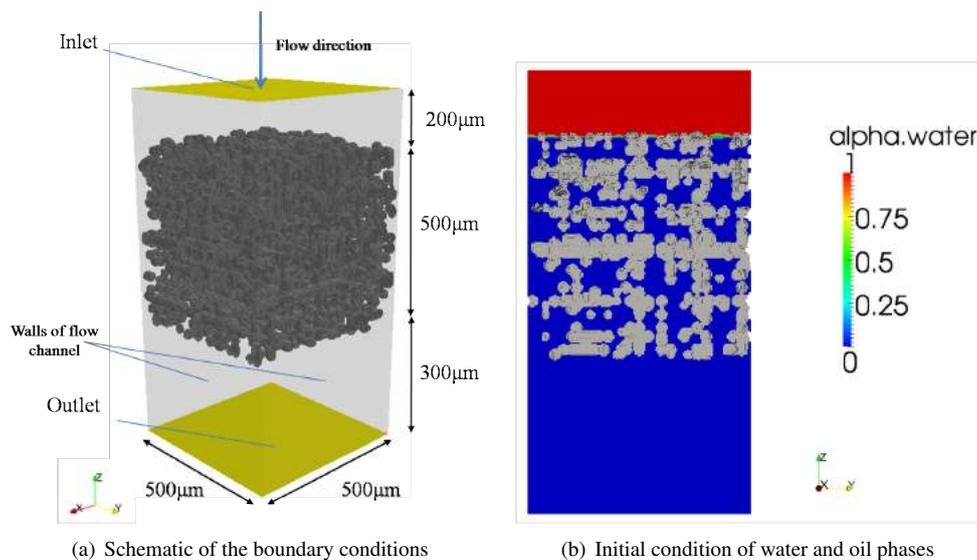


Figure 5. Schematic representation of the computational domain

Computer simulations were performed at supercomputer Euler from Center of Mathematical Sciences Applied to Industry CeMEAI - ICMC/USP. Hardware and software details about the supercomputer Euler can be found at <http://www.cemeai.icmc.usp.br/Euler/index.html>. To perform the simulations in this work a processing node with 20

cores (40 threads) was used.

3. RESULTS

3.1 Single flow simulation

According to Guibert *et al.* (2015) the mesh quality is very important for the numerical study of permeability of different materials. In order to verify if the mesh resolution was sufficiently high, the CFD simulation were performed with meshes that contained approximated 20.5, 5.2 and 2.7 million elements which meant an increase of the elements by a factor of 7.6 and 3.9, as can be seen in Tab. 2. These tests were performed on a porous medium with porosity of 40%.

Darcy's law was used to estimate the permeability k , as shown by

$$k = -Q \cdot \mu \cdot L / (A \cdot \Delta p), \quad (1)$$

where, Q is the volume flow rate, A is the inlet surface area, μ is the dynamic viscosity, L porous media length and Δp is the pressure difference between inlet and outlet.

Table 2. Mesh quality analysis

Case	# hexaedric volume	Δp [Pa]	Permeability [m ²]	Maximum velocity [m/s]	Relative error velocity	Relative error Δp	Comp. time [s]
1 (Fine grid)	20510570	6945.082	2.183E-12	1.300	-	-	75900
2	5262582	7089.992	2.138E-12	1.279	1.62%	2.04%	16144
3 (Coarse grid)	2708945	7196.378	2.107E-12	1.263	2.88%	3.49%	7500

The results showed in Tab. 2 that the mesh with 5 million of element shows a change of the obtained pressure and velocity near 2% indicating that the applied mesh was sufficiently accurate.

In order to show the potential of the approach developed to generate artificially porous media, a comparison with the Aboukhedr *et al.* (2015) was done. Aboukhedr *et al.* (2015) performs numerical simulations on porous media obtained from reconstruction of 2D images of Berea sandstone samples. The porosity experimentally determined and applied on numerical simulation was 40%. The properties of the fluid are the same as those used in our tests, as shown on section 2.3. The average permeability obtained by Aboukhedr *et al.* (2015) was compared to the calculated permeability in the direction of flow, as can be seen in Tab. 3. The permeabilities calculated show a good agreement with the numerical results obtained in Aboukhedr *et al.* (2015).

Table 3. Comparison between different permeabilities

Model	Permeability [m ²]
Numerical 10M (Fine grid) (Aboukhedr <i>et al.</i> , 2015)	1.024E-12
Numerical 1M (Coarse grid) (Aboukhedr <i>et al.</i> , 2015)	6.700E-13
1 (Fine grid)	2.183E-12
2	2.138E-12
3 (Coarse grid)	2.107E-12

Hydraulic conductivity (K) is a property that describes how easily a fluid can move through pore spaces or fractures. It depends on the permeability, the degree of saturation, and on the density and viscosity of the fluid. Given the value of hydraulic conductivity the permeability can be calculated as follows

$$k = K \frac{\mu}{\rho g}, \quad (2)$$

where g is the acceleration due to gravity. Based on the Eq. (2) the hydraulic conductivity, K , for the analyzed case is equal to 2.406E-05 m/s.

Different porous media cases were generated with the aid of the software, in order to verify its use viability. A computational fluid dynamics simulation was performed. The cases analyzed and the results obtained are shown in the Tab. 4. The pressure inside the flow channel and porous media is shown in Figure 6. It can be seen the pressure drop Δp occurred along the porous media length.

Figures 7 and 8 show the water velocity distribution through the simulated channel (horizontal and vertical slices). It is possible to observe that the flow accelerates not only on small pores, as is expected due the pressure difference, but also through wider throats. This is a phenomenon associated with surrounding material structure. The presence of areas with higher velocities can be considered an indicator of the existence of preferential flow path, see Figure 9. A maximum

Table 4. Analyzed cases: single-phase flow

Case	Porosity	# hexaedric volume	Δp [Pa]	Permeability [m ²]	Maximum velocity [m/s]
p28	28%	4738533	21269.596	7.129E-13	2.604
p40	40%	5262582	7089.992	2.139E-12	1.279
p46	46%	5829301	2960.657	5.122E-12	0.895
p57	57%	4480140	1069.038	1.418E-11	0.619
p65	65%	5326174	964.637	1.572E-11	0.436

velocity of 2.604 m/s was found inside the porous media case p28, which is more than 76 times higher than applied fluid velocity. In case p65 (porosity 65%) the maximum velocity found was 0.436 m/s, which is more than 12 times higher than applied fluid velocity. The velocity profiles and streamlines allowed a more detailed insight into the flow pressure behavior of porous media artificially generated. For qualitative verification with the literature (Kaviany, 1995), the typical permeability sandstone permeability can vary between $5,0 \times 10^{-16}$ a $5,0 \times 10^{-12}$ m² where the values calculated in this work fits.

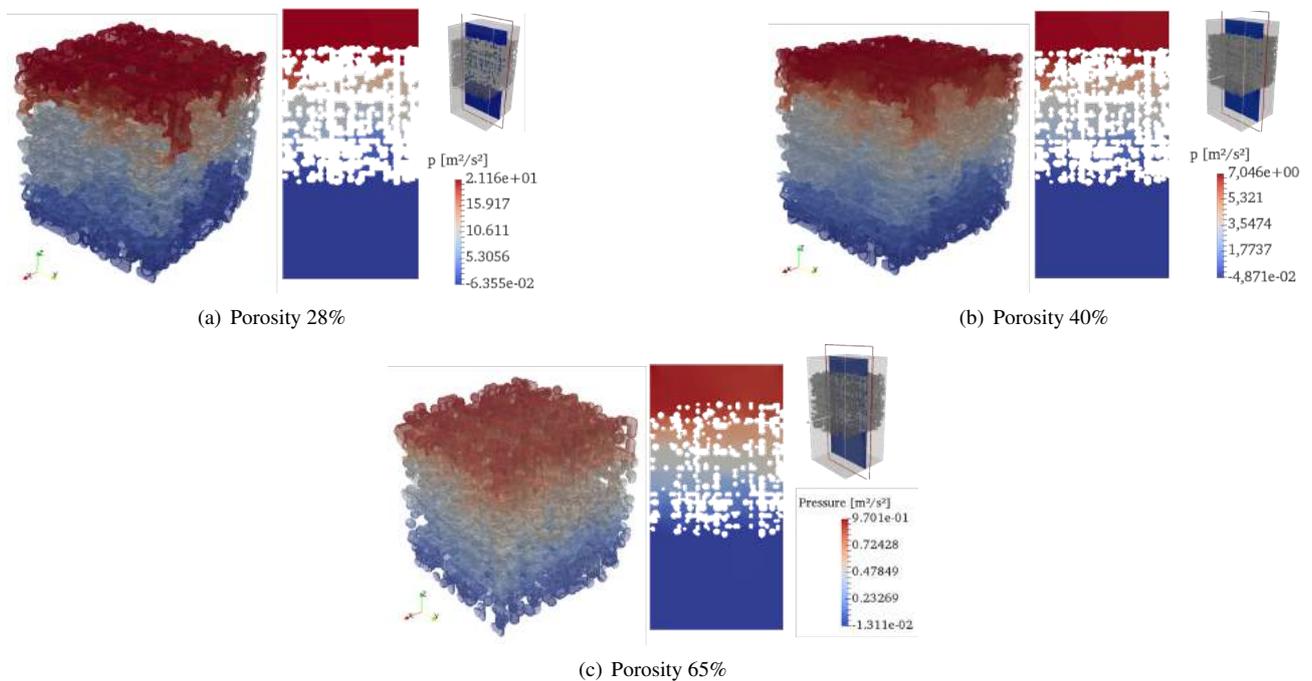


Figure 6. Porous media pressure values

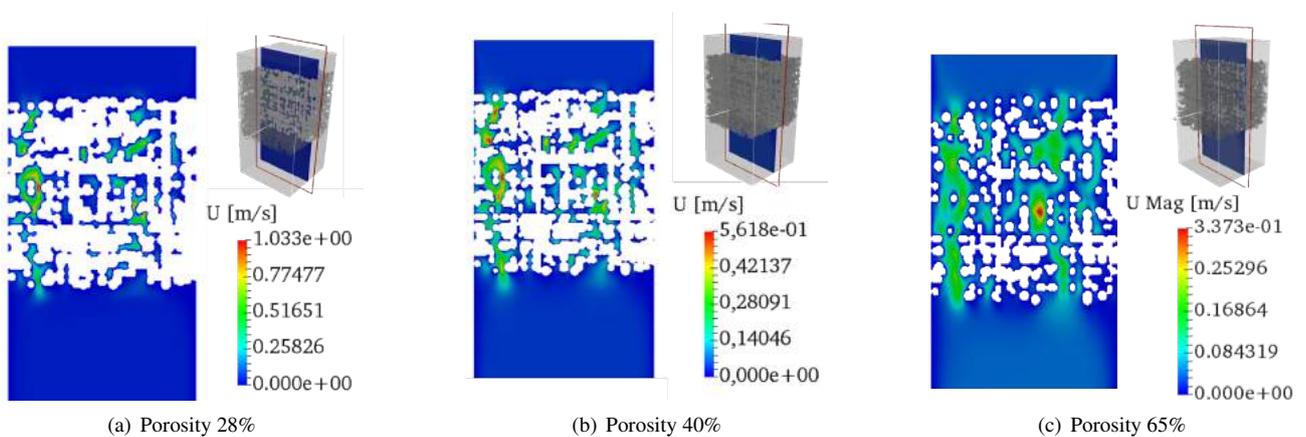


Figure 7. Fluid velocity inside flow channel - cross section side view

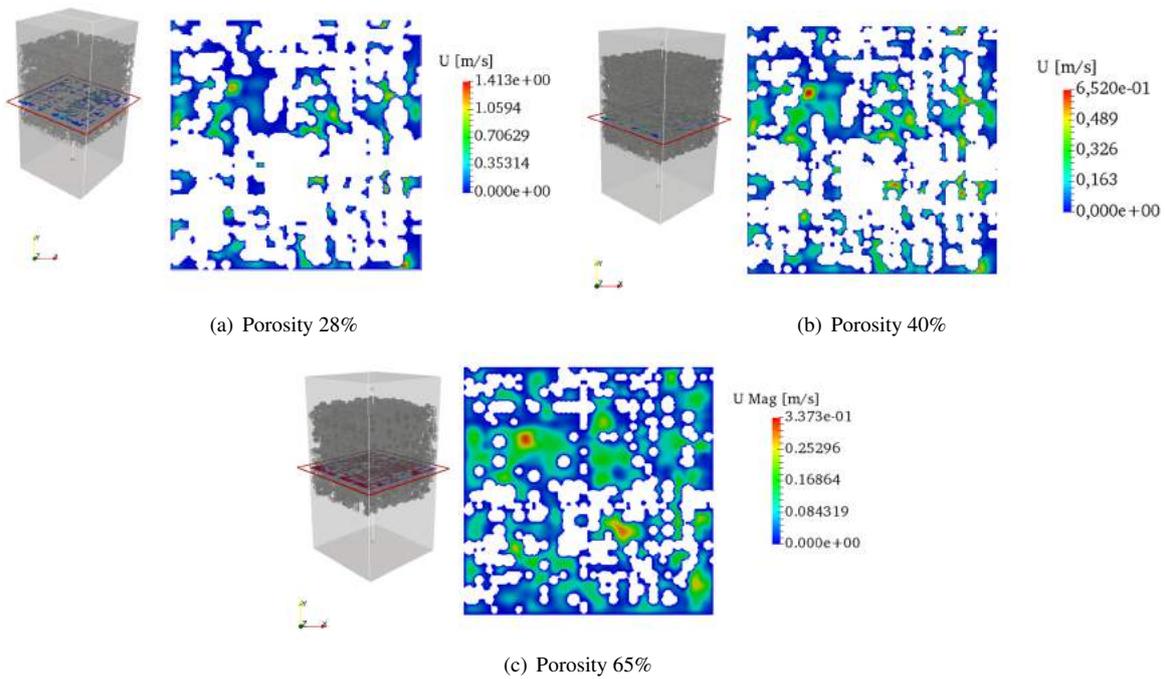


Figure 8. Fluid velocity inside flow channel - cross sectional top view

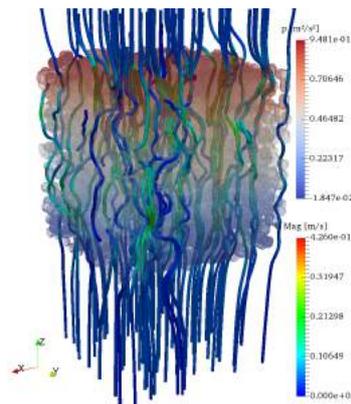


Figure 9. Velocity streamlines occurring inside flow - porosity 40%

3.2 Multiphase flow simulation

In order to study the oil drainage by water injection on artificially generated porous media multiphase CFD simulation was performed. The CFD simulation setup was presented on Section 2.3. The porous media case p40 with 40% porosity was used to perform the multiphase simulation. Figures 10 and 11 shows the oil recovery process simulation computationally on the artificially generated porous media. It is possible to see in the figures the formation of preferential paths due the lower viscosity of the injected water decreasing the oil displacement efficiency.

Figure 10 shows the temporal evolution of water in the pore space at six different snapshots. These results were obtained in order to verify the correct implementation model for flow simulation with two immiscible fluids in porous media generated artificially. For the presented results, the use of adaptive mesh was not used for capturing accurately the interface curvature. The application of the adaptive mesh allows to capture the thin film of oil between the water and the pores' wall that is numerically very challenging to capture. The use of adaptive mesh and a more detailed analysis of two-phase flow in porous media will be a subject for the future work.

4. CONCLUSIONS

With improvements of imaging techniques, high performance computers architectures and simulation capabilities, pore simulations are used to characterize the flow properties of real porous formations. Single- and two-phase flow calculations have been performed inside a randomly generate 3D porous media and have allowed estimation of preferential

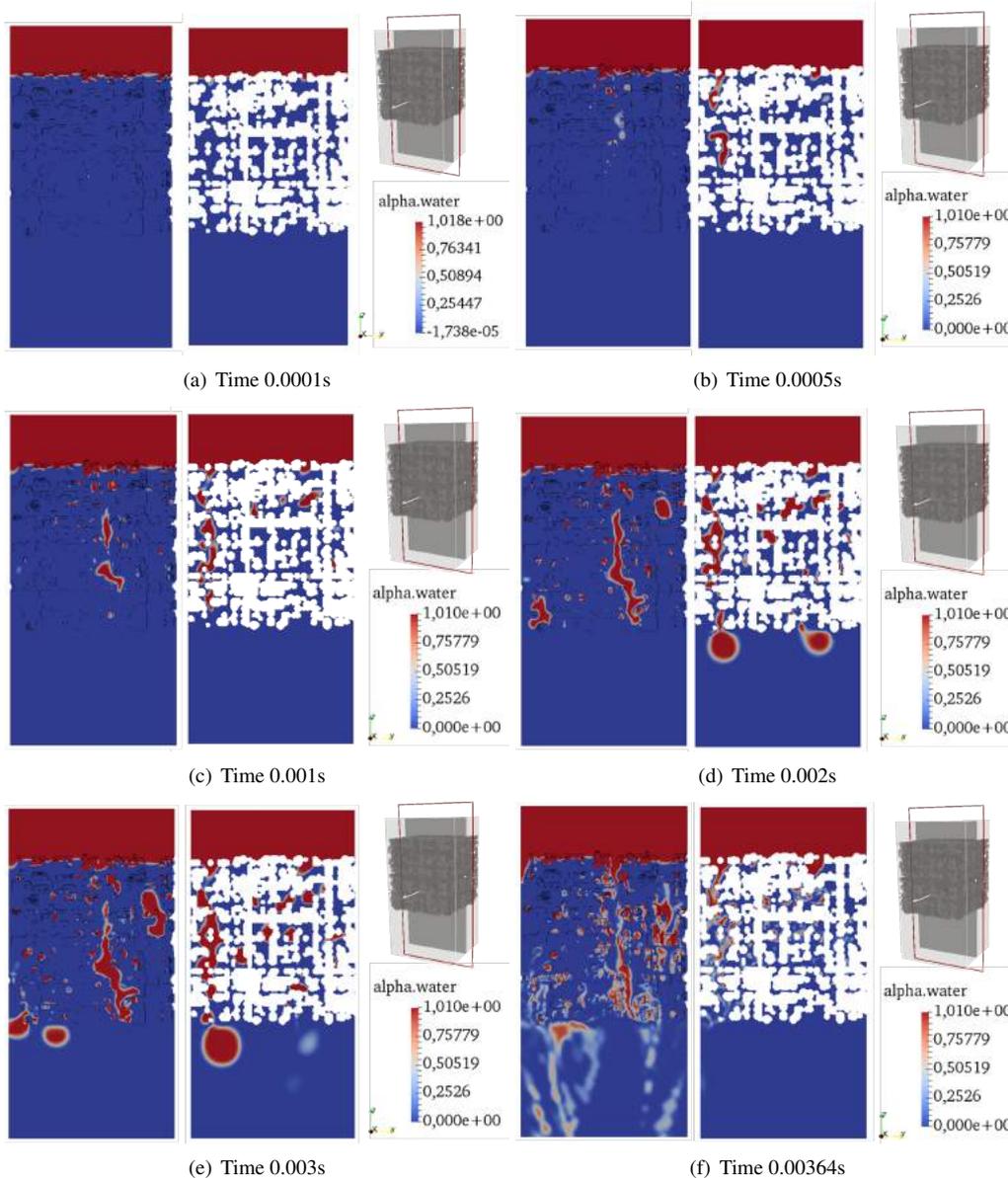


Figure 10. Water injection process in porous media containing oil simulated computationally

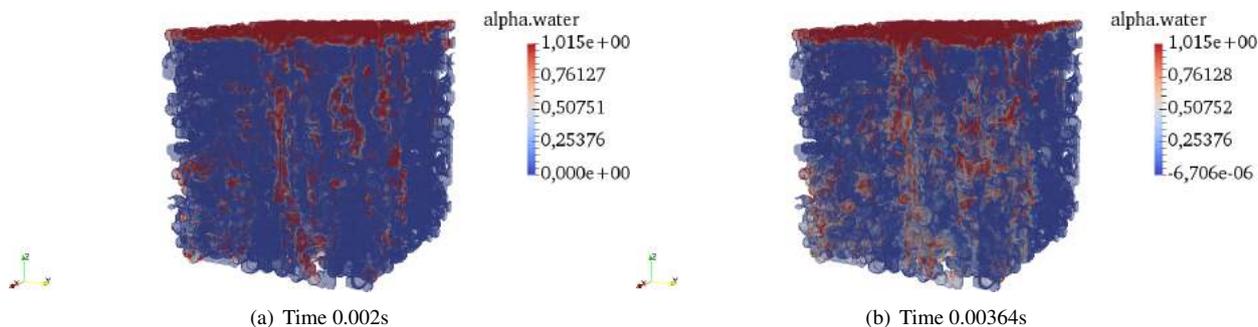


Figure 11. Oil drainage computationally simulate

flow path and permeability. The strategy of random generation of 3D porous media shows to be feasible, thus allowing its application to the study of different numeric models.

The random generator of porous media allows control of the particle frequency and the use of different combinations of geometric shapes. Thus, is possible to obtain extremely complex porous media. The method can be applied to randomly generate porous media to study applications for problems such as stochastic upscaling and propagation of uncertainty from microscopic fluid and rock properties for multi-phase flows. Another possibility of using this technique is the 3D

printing of the porous medium or filters, allowing performing experiments to validate the numerical simulations.

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