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Representative elementary volume for *NMR* simulations based on X-ray microtomography of sedimentary rock

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ABSTRACT

In porous systems like natural rocks, many phenomenological models have been developed in order to study the correlations between physical properties and the pore structure of these systems. The high resolution obtained with X-ray microtomography (μCT) images (micro or nanometer scales) has allowed exploring in details the complex morphology of the pore space in natural rocks. This has promoted the development of numerical simulations at the pore-scale level aiming to improve our comprehension about the correlations between pore structure and macroscopic physical properties. In this respect, simulations of nuclear magnetic resonance properties performed directly on μCT images are very important, since petrophysical properties can be predicted using a realistic model for the heterogeneous porous structure. Also these simulations can include a specific morphology of the pore geometry, which can be controlled in order to verify the different hypotheses introduced during *NMR* interpretation of physical properties, like for example, permeability predictions and/or fluid typing. In addition, *NMR* simulations allow to study the existence of a representative volume of the whole system, whose experimental determination is a major challenge. In this work, nuclear magnetic relaxations are simulated on a pore geometry obtained from microtomography of a natural rock formation, localized in the southeast of Brazil. The simulations were performed through a discrete random-walk algorithm computed at the pore scale. In the simulations bulk relaxation was not considered, while the relaxation rate at the surface of the pores was assumed constant. Our results indicate that the relaxation curves can be considered representatives of the whole system for volumes above a representative volume with dimensions of some cubic millimeters. In addition, this representative elementary volume seems to be of the same order that the one found from the analyses of the porosity on the same digital rock. In summary, this study points out to the importance of verifying the existence of this characteristic volume during *NMR* simulations directly on images obtained from tomography, in order to ensure the reliability of the information obtained from the numerical simulations.

1. Introduction

In nature, many systems show a complex behavior with many macroscopic physical properties being determined by several processes or mechanisms at microscopic scale (Anderson, 1972). A porous rock, formed by an entanglement network of grains and pores, represents a typical example of such a complex system (Sahimi, 1993). These porous rocks are ubiquitous components of oil reservoirs, mineral deposits, soils, and so on. The interplay between the physical properties of porous rocks and their porous structures is a point very studied in the literature. In this sense, nuclear magnetic resonance has been widely used to explore the porous space and its morphology in natural rocks (Song, 2012). Basically, the use of this technique explores the fact that the surfaces of the pores substantially modify the relaxation and diffusion properties of molecules of the fluid (or fluids) that occupies the interstitial space inside the pores (Song, 2012). In general, these studies provide information on the pore-size distributions, surface to volume ratio of the pores, pore-through distributions, fluid typing, etc. (Song, 2012).

In a classical experiment of nuclear magnetic relaxation (*NMR*) the system of spins is initially oriented by an applied magnetic field, then the field is removed and the system relaxes to a new not organized

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equilibrium state. This relaxation process can be experimentally quantified by the relaxation of the two components of $\overrightarrow{M}$; the longitudinal projection (characterized by the constant time T_1) and the transverse component (quantified by T_2). In any case, the basic equations governing the *NMR* relaxation effects in porous rocks are (Cohen and Mendelson, 1982; Brownstein and Tarr, 1979; Mendelson, 1990):

$$\frac{\partial M}{\partial t} = D\,\nabla^2 M - \frac{M}{T_{1,2}} \tag{1}$$

$$(D\,\vec{n}\,\vec{\nabla} M + \rho\, M)|_S = 0 \tag{2}$$

$$M(\vec{r}, t = 0) = M_0 \tag{3}$$

Here D represents the bulk diffusion coefficient (usually considered isotropic) of the fluid; the time constants T_i can be T_1 (spin-lattice relaxation) or T_2 for spin-spin relaxation; M is the respective component of $\overrightarrow{M}$ (vector magnetization); $\vec{n}$ is a unit vector normal to the surface of the pores; and finally ρ represents an empirical parameter (supposed a constant) that quantify the average spin relaxation at the surface of the pores. The solution of the equations system $(1-3)$ can be represented as a combination of different normal modes, each one characterized by a specific relaxation time τ_n, i.e., $M(\vec{r}, t) = \sum_{n=0}^{\infty} A_n\, T_n(\vec{r})\, e^{\frac{-t}{\tau_n}}$ (Brownstein and Tarr, 1979). Finally, the physical quantity (component of $\overrightarrow{M}$) that is experimentally measured can be described as $\sum_{n=0}^{\infty} I_n\, e^{\frac{-t}{\tau_n}}$ (Brownstein and Tarr, 1979). The equations $(1-3)$ basically content the fundamental elements in order to analyze nuclear magnetic relaxation experiments in porous media (Mendelson, 1990).

On the other hand, in recent years the micro-scale X-ray tomography μCT has been consolidated as a useful technique in the study of porous systems, like for example, natural rocks extracted from petroleum reservoirs. This technique provides a $3D$ image of porous systems at a reasonable resolution, from which the pore structure and its particular morphology can be characterized. This pore-scale representation, not only can be statistically characterized through different descriptors, as reviewed in (Torquato, 2002), as also it can be used as a mathematical domain in order to solve differential equations that describe different physical phenomena.

One area, which has been intensely developed in the last years is the numerical simulation (or numerical calculation) of physical properties, performed directly in pore-scale representation of a porous rock obtained from microtomography images (Spanne et al., 1994; Auzerais et al., 1996; Arns, 2004; Jin et al., 2009; Arns et al., 2011). These simulations are usually done by using discrete element theories (finite element and finite difference methods) aiming calculate or predict transport properties, like for example, permeability and/or conductivity (Spanne et al., 1994; Auzerais et al., 1996). Meanwhile, other simulations performed at the same conditions (i.e. at pore-scale) have been addressed on *NMR* properties, like for example, diffusion and relaxation processes (Arns, 2004; Jin et al., 2009; Arns et al., 2011). In general, *NMR* simulations of petrophysical properties performed directly on a pore distribution obtained from high-resolution μCT images are very important, since these studies improve the understanding of *NMR* experiments performed on natural rocks, as the heterogeneous character of the pore structure is included during the calculations. This redresses simple hypotheses introduced in different models commonly used to analyse the results from *NMR* experiments, which do not consider the heterogeneity present in natural rocks (Song, 2012; Arns, 2004; Jin et al., 2009; Arns et al., 2011).

In this respect, a critical property which is related to the complexity of a particular system is its heterogeneity in space and/or time. This aspect implies that the scale of observation used during a simulation or experiment on a porous system is an important point to be observed (Al-Raoush and Papadopoulos, 2010; Vik et al., 2013). The influence of the scale in the quantification of the non-homogeneity is represented through the representative elementary volume (*REV*) concept (Al-Raoush and Papadopoulos, 2010; Vik et al., 2013; Nordahl and Ringrose, 2008; Bear, 1988; Fitch et al., 2015; Liu et al., 2016). This parameter represents a scale or data population size above which the observed physical property does not depend on the size of the data, in other words, the *REV* parameter is a volume that allows to verify the representative heterogeneity of the whole system (Bear, 1988; Vik et al., 2013). It should be noted that, in principle, physical properties obtained from simulations performed on volumes above the *REV* should be almost independent of the volume.

Also, it is very important to note that the *REV* can be different for the same system, depending on which physical property is being studied (Vik et al., 2013). Usually, the representative elementary volume is determined based on the porosity of the studied sample (Baveye et al., 2002; Razavi et al., 2007). Nevertheless, the *REV* concept can be also determined through the study of other macroscopic parameters (Al-Raoush and Papadopoulos, 2010). The use of the porosity as a standard parameter to determine the *REV* can be a consequence of the facility for the determination of the porosity for a particular system. Note that simulations, like for example, those related with *NMR* relaxation demand time consuming depending of the volume of data used in the simulations, thus from computational viewpoint, the connection between data volume (i.e. computational cost) and accuracy of the simulations is a very important point (Liu et al., 2016).

Regarding the *REV* concept, it is also important to stress that the experimental determination of a representative volume through a *NMR* experiment is really challenging. Taking into account these ideas, one point which deserves special attention is to verify the *REV* concept in *NMR* simulations performed directly on μCT images. This manuscript explores this last point, and also it tries to answer the following question: representative elementary volumes obtained via porosity and *NMR* simulations performed on μCT images are equivalent? This question is not so simples, since in theory, the relaxation rate in *NMR* depends on the surface area/volume ratio of the pores, it means, the relaxation is not directly correlated with the porosity level of the samples (Brownstein and Tarr, 1979).

In order to address this problem, μCT images were obtained on a plug from a rock formation, which resembles the presalt carbonate rocks found in oil reservoirs along the cost of Brazil (South Atlantic). The images were segmented by a k-means algorithm that allowed identify the geometry of the pore space. In essence, this procedure allowed to identify a pore space representation of the plug, on which, porosities and *NMR* simulations were conducted at different volumes. Our results confirm that, first there exist a *REV* which should be taking into account in *NMR* simulations on μCT images, and second, there seems to be a coincidence in the representative elementary volume as determined by both, *NMR* simulations and porosity.

2. Image processing

The μCT images were obtained on a rock formation located in the northeast part of the state of Rio de Janeiro and called *Lagoa Salgada*. The place is a salty lake containing stromatolites, thrombolites and oncolites formations which are sedimentary deposits that represent records of ancient rocks. This rock formation can show some similarities with the carbonate rocks found in the presalt reservoirs along the Brazilian cost. A plug from this deposit was explored by using X-ray microtomography. The μCT technique provided a $3D$ image of the plug in the form of a set of $2D$ slices separated by the resolution used in the measure. The images were obtained with a microtomography scanner GE phoenix v|tome|x L 300. The in-plane resolution of the μCT images was 17.2 μm/pixels. Initially the images were pre-processed by using a Matlab filter named imadjust to adjust the contrast of the images.

The images used in the calculations of this work were chosen inside cubes, which were centered on the center of the digital rock (image of the plug). This avoids possible surface effects that can modify the experimental data. The images were segmented through a k-means