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Computational approach to integrate 3D X-ray microtomography and NMR data

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Abstract: Nowadays, most of the efforts in NMR applied to porous media are dedicated to studying the molecular fluid dynamics within and among the pores. These analyses have a higher complexity due to morphology and chemical composition of rocks, besides dynamic effects as restricted diffusion, diffusional coupling, and exchange processes. Since the translational nuclear spin diffusion in a confined geometry (e.g. pores and fractures) requires specific boundary conditions, the theoretical solutions are restricted to some special problems and, in many cases, computational methods are required. The Random Walk Method is a classic way to simulate self-diffusion along a Digital Porous Medium. Bergman model considers the magnetic relaxation process of the fluid molecules by including a probability rate of magnetization survival under surface interactions. Here we propose a statistical approach to correlate surface magnetic relaxivity with the computational method applied to the NMR relaxation in order to elucidate the relationship between simulated relaxation time and pore size of the Digital Porous Medium. The proposed computational method simulates one- and two-dimensional NMR techniques reproducing, for example, longitudinal and transverse relaxation times (T_1 and T_2 , respectively), diffusion coefficients (D), as well as their correlations. For a good approximation between the numerical and experimental results, it is necessary to preserve the complexity of translational diffusion through the microstructures in the digital rocks. Therefore, we use Digital Porous Media obtained by 3D X-ray microtomography. To validate the method, relaxation times of ideal spherical pores were obtained and compared with the previous determinations by the Brownstein-Tarr model, as well as the computational approach proposed by Bergman. Furthermore, simulated and experimental results of synthetic porous media are compared. These results make evident the potential of computational physics in the analysis of the NMR data for complex porous materials.

Keywords: NMR, Digital Porous Media, Computational Methods, Relaxation, Diffusion

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