NUMERICAL MODELING OF NMR SURFACE RELAXATION IN POROUS MEDIA WITH IMPROVED PORE SURFACE AREA EVALUATION AND DERIVATION OF INTERFACIAL ABSORPTION PROBABILITY

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ABSTRACT

In digital rock physics, surface relaxation of NMR decay on a 3D porous media is often simulated with Random-Walker methods, where Brownian walkers representing the magnetized nuclei are absorbed by the solid surface under an interfacial absorption probability. Previous simulations usually neglected the blocky pixel appearance of 3D pore space images, which results in over estimation of the surface area, particularly for unconventional reservoir rocks with large fractions of micropores, such as tight sandstones or shale. This leads to arbitrary adjustments of the interfacial absorption probability by tuning the value of the surface relaxivity strength (SRS) in order to match simulation results with experimental measurements. However, this arbitrary adjustment violates the fact that SRS is a rock dependent physical property. In this study a new interfacial absorption probability for NMR simulations is presented that honours the physical principles. This new absorption probability computation depends on accurate evaluation of the surface area, which is assured by a new approach of 3D pore space surface area evaluation. The new algorithm is verified by performing NMR Random-Walker simulation tests on both standard geometries and realistic 3D heterogeneous porous media.

INTRODUCTION

In Random-Walk NMR simulation the decrease of random walkers, which simulates the

transverse decay of magnetization, is controlled by an absorption probability of the solid grain surface, usually called the killing probability, which is proportional to the surface relaxivity, the random walker step size, and is reversely proportional to the bulk diffusivity [1]. Traditionally, the expression of killing probability derived by Bergman and Dunn [1] was used as an input to the simulation program [2-4]. However, this expression of killing probability, based on the assumption of random walkers hitting a planar surface was neglecting the discretized voxel effect and thus, required unphysical adjustment of input parameters. This effect is increasingly evident in unconventional rock types, with high surface-to-volume ratio (S/V).

In this study two aspects are discussed to reduce the uncertainties from the previously used killing probability approaches. Firstly, an updated killing probability is derived based on the physical process of transverse magnetization decay. The new killing probability effectively includes the surface-to-volume ratio and the global hitting probability of the entire pore space geometry and is adaptable to any rock type. Secondly, an algorithm is proposed, which more accurately evaluates the surface area and reduces the voxel discretization effect. The new NMR simulation is verified by testing on both standard geometrical pore spaces and digital images of realistic rock samples of various rock types and shows that the previously shifted T2 distribution is successfully corrected.

THEORY AND METHODS

Nuclear magnetic resonance occurs when an ensemble of spinning hydrogen protons performing Larmor precession in a uniform magnetic field $\boldsymbol{B_0}$ are tilted by an oscillating magnetic field pulse $\boldsymbol{B_1}(t)$ with oscillation frequency the same as the Larmor precession frequency and perpendicular to $\boldsymbol{B_0}$. The net macroscopic magnetization $\boldsymbol{M_0}$ previously along the direction of $\boldsymbol{B_0}$ is tilted away from its longitudinal direction to the transverse plane. As the magnetic pulse is turned off, the tilted magnetization relaxes back to its longitudinal direction and the transverse component of macroscopic magnetization $\boldsymbol{M}_\perp$ follows an exponential decay [5],

$$\boldsymbol{M}_\perp(t) = \boldsymbol{M}_\perp(0)e^{-t/T_2} \tag{1}$$

where T_2 is determined by three effects, bulk relaxation, surface relaxation and bulk relaxation, which is defined as the combination of [6]

$$\frac{1}{T_2} = \frac{1}{T_{2bulk}} + \frac{1}{T_{2surface}} + \frac{1}{T_{2diffusion}} \tag{2}$$

It is well understood that in pore space, where the scale satisfies the fast diffusion limit,

the surface relaxation time $T_{2surface}$ is related to the mineralogy on the pore solid surface and the surface-to-volume ratio of the pore space [7],

$$\frac{1}{T_{2surface}} = \rho \frac{S}{V} \tag{3}$$

where ρ is the surface relaxivity, S the pore surface area and V the pore space volume.

In this study, the surface relaxation described by Eq. (1) is simulated by Random-Walk methods, in which an ensemble of random walkers representing the spinning hydrogen protons is seeded into porous space to imitate diffusive Brownian motion [1]. The random walkers travelling to the image pixels near to the solid-void boundary are absorbed by the solid interface, leading to the decrease of random walkers, analogous to the surface relaxation process in which the spinning nuclei is relaxed by interaction with the solid grain surface.

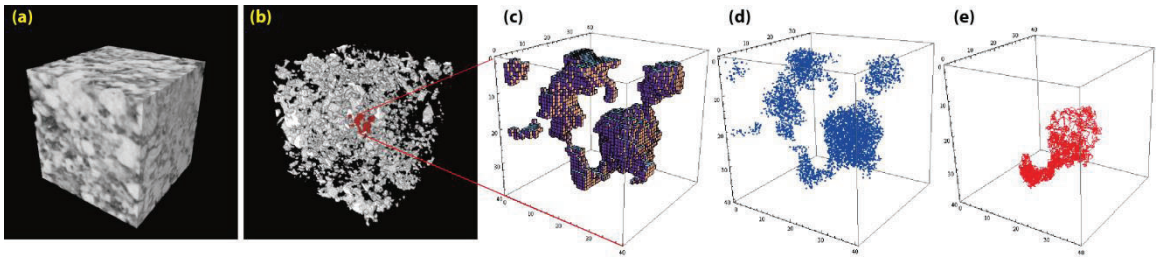

Figure 1. Scheme of Random-Walk NMR simulation on MCT image: (a) a typical MCT greyscale image with lighter area indicating the high density grains and darker area the pores. (b) segmented pore space extracted from the greyscale image. (c) zoom-in of a part of the pore space shows the pore space is compiled by cubic voxels. (d) random walkers (blue) seeded into the pore space. (e) the track of one random walker in one pore space.

Initially, a number of N random walkers are uniformly seeded into a 100% wetting phase saturated pore space. After an infinitesimal time Δt, the number of random walkers decreases by $Nh\gamma$, where h is the global probability of random walkers hitting the pore surface and γ the probability of random walkers being absorbed by the surface. Relating the decrease of random walkers with the decay of magnetization in Eq. (1), we obtain

$$h\gamma = \frac{\Delta t}{T_2} \tag{4}$$

In our simulation the time step Δt is determined by the law of Brownian motion of

spatial diffusive particles in a 3D space, $\epsilon^2 = 6D_0\Delta t$, where D_0 is the bulk fluid diffusivity and ϵ the diffusion distance of random walkers within a time step. Therefore Eq. (4) can be rewritten as the expression for killing probability,

$$\gamma = \frac{\rho\epsilon^2 S}{6D_0 hV} \tag{5}$$

Effective implementation of Eq. (5) into the whole process of NMR simulation requires both accurate evaluation on the surface area S and the global hitting probability h of the pore space. In this study, an optimized marching cubes algorithm [8] is employed to evaluate the pore space surface area by interpolating a virtual smoothed surface along the discretized solid-pore interfaces and random walkers hitting the surface are determined by judging whether the random walkers cross this virtual surface. The hitting probability h depends on the structural geometry of the pore space and is calculated as

$$h = \sum_{i=1}^{N}(1 - Z_i)(h_s \sum_{s=1}^{6} Z_i^s + h_c \sum_{c=1}^{8} Z_i^c + h_e \sum_{e=1}^{12} Z_i^e) \tag{6}$$

where Z_i is the pixel registration of the *i*th pixel of a 3D image with $Z_i = 0$ for void and $Z_i = 1$ for solid grain. Z_i^s (Z_i^c or Z_i^e) are the 6 (8 or 12) sided (corner or edge) neighboring pixels of Z_i, and h_s, h_c and h_e are the constant probabilities of random walkers in pixel Z_i jumping into sided, corner and edge pixels, respectively.

RESULTS

Standard Geometrical Benchmarks

The validity of the NMR simulation program with updated killing probability and smoothed surface area evaluation is first verified by performing tests on standard geometries and comparing the simulated results with the theoretical ones. The consistency between simulation and theoretical results ensures the reliability of performing the simulation on realistic pore spaces, where the porous structures are highly irregular and the pore sizes are multiple-scale.

The simulation results (Table 1) show significant improvement of pore space surface area evaluation and better consistency between the predicted and theoretical T2s than the previous version of NMR simulations. It is obvious that while the previous program works well on cubic pore space consisting of planar surfaces, it fails to correctly evaluate the surface area of spherical and irregular pores which are dominant in most rock samples.

Application on Digital Rock Images

The new simulation is further tested on realistic digital images of various rock types including sandstone, carbonate and tight sandstone (Table 2). The validity of NMR simulation on realistic rock samples can only be verified by matching with experimental measurements. However, the improvement of the simulation algorithm can be verified by comparing the simulation results with the previous ones. Figure 2 shows one testing result, including decaying magnetization and its corresponding T2 distribution. With more accurate killing probability realized by corrected evaluation of the pore space surface area and more physical based random walker diffusion scheme, the T2 distribution of all rock types shift rightwards, which indicates that the previous over estimated surface area is effectively corrected. The level of correction increases as the pore space becomes more tight and tortuous.

Table 1. Simulation results on standard geometrical pore space shows that the updated simulation algorithm significantly improves evaluation of surface area and T2 for spherical pores. The testing are perform on a 200^3 image with pixel size 1.0μm and surface relaxivity 3.0μm /s.

Cubic Pore						
Length(μm)	**S_{th}(μm^2)**	**$T2_{th}$(ms)**	**S_{old}(μm^2)**	**$T2_{old}$(ms)**	**S_{new}(μm^2)**	**$T2_{new}$(ms)**
10.0	600.0	555.6	600.0	543.3	564.1	605.5
20.0	2400.0	1111.1	2400.0	1117.7	2329.0	1174.6
50.0	15000.0	2777.8	15000.0	2802.9	14820.0	2923.1
100.0	60000.0	5555.6	60000.0	5672.9	59650.0	5906.9
Spherical Pore						
Radius(μm)	**S_{th}(μm^2)**	**$T2_{th}$(ms)**	**S_{old}(μm^2)**	**$T2_{old}$(ms)**	**S_{new}(μm^2)**	**$T2_{new}$(ms)**
5.0	314.2	555.6	486.0	424.0	341.0	516.5
10.0	1256.6	1111.1	1902.0	937.3	1372.0	1047.9
25.0	7854.0	2777.8	11770.0	2380.8	8539.0	2654.9
50.0	31415.9	5555.6	47070.0	4827.9	34140.0	5332.8

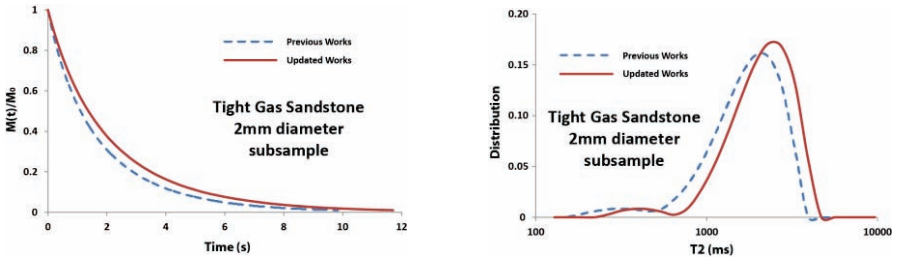

Figure 2. Comparisons of previous and updated works of NMR simulation on digital images of a 2mm diameter tight gas sandstone subsample.

Table 2. Simulation results of various rock types and scales. The surface relaxivity is taken as 4.0μm /s.

Sample	Image Size (voxel)	Voxel Size (μm)	Porosity (%)	S_{old} (μm^2)	S_{new} (μm^2)	$T2_{old}$ (ms)	$T2_{new}$ (ms)
Sandstone	300^3	8.68	14.13	1.73E-04	1.28E-04	4438.03	5722.38
Carbonate	800^3	4.93	7.82	7.19E-04	5.16E-04	869.82	1178.16
Tight gas 1	1000^3	14.30	1.99	4.42E-03	3.28E-03	3720.65	5323.14
Tight gas 2	1000^3	2.77	7.10	2.33E-04	1.67E-04	2306.66	2928.23
Tight gas 3	1000^3	1.15	6.59	2.32E-05	1.66E-05	1608.27	2111.32

More accurately simulated T2 distributions provide several important potential practical applications. The SRS is largely unknown but is needed to convert the experimental T2 distribution from time scale to length scale. Another example is to provide accurate porous surface area which is important for some surfactant experiments.

CONCLUSIONS

We propose two important updates to previous NMR simulations. One is a newly derived killing probability, based on the physical process of an ensemble of random walkers diffusing, hitting and being absorbed by a porous space solid surface, to replace the previous killing probability which fails to recognize the global irregularity of the pore shapes. The other is an optimized algorithm to increase the accuracy of porous space surface area evaluation, which was over estimated, previously. Both successfully reduce the uncertainties resulting from previous works. With the new killing probability and smoothed surface area evaluation, the NMR simulation can be reliably matched with experimental measurements and thus, provides a more accurate surface relaxivity strength and surface-to-volume ratio. Based on these improvements, NMR simulations can be extended to images with different saturation stages. Families of T2 distributions under various saturations can be simulated to calibrate NMR well logging data and to obtain more accurate estimates of irreducible water saturation.

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