

Influence of Boundary Condition on Multiple Exponential Diffusion Phase Transition

L. Lin¹, and J. Zhong^{1,2}

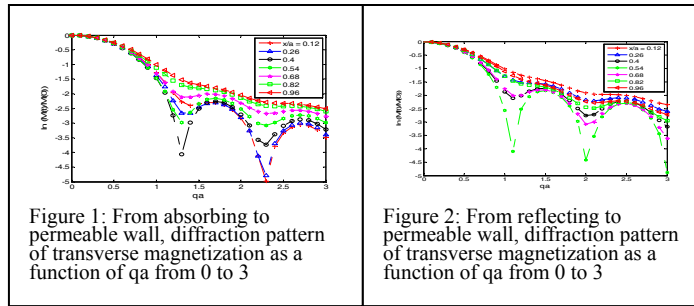
¹Department of Physics and Astronomy, University of Rochester, Rochester, NY, United States, ²Department of Imaging Sciences, University of Rochester, Rochester, NY, United States

Introduction: The diffusion phase transition from single to multiple exponential decays can be induced by variations of tissue interfaces in addition to changes in cellular geometry, size, or intracellular and extracellular compartments. We quantified the multi-exponential diffusion behavior of water molecules between two mixing boundary conditions, absorbing (reflecting) and permeable walls, evaluated with the local magnetization from the Brownian motion within pure (1) absorbing, (2) reflecting, and (3) variably permeable¹ boundary conditions. Though the water nucleus diffusion signal acquired from PGSE², OGSE³ and d-PFG^{4,5} have been shown to be useful to predict the micro-scale tissue size and structure, the permeability, relaxation rate, and mechanism of interaction between the detected molecule and the tissue surface of interests plays a crucial role to determine the accurate estimation from the signal measured to the dimension and properties of the cellular and sub-cellular structure. In this study, we look into the variations of surface relaxation rate and diffraction pattern revealing fractional pools of the phase transition from mono-exponential to bi- and tri-exponential diffusion signals for a better understanding of the relationship between the type of correlation interfaces and the measured slow, intermediate, and fast diffusion coefficients.

Theory: The particle diffusing close to the wall can be described from the Fick's second law $\partial P/\partial t = \nabla(D\nabla P)$ with boundary conditions: (1) absorbing $P(0, t) = P(a, t) = 0$ (2) reflecting $\nabla P(0, t) = \nabla P(a, t) = 0$ (3) permeable walls $D\nabla P(a, t) = -MP(a, t)$, $D\nabla P(0, t) = MP(0, t)$ (4) side-absorb, side-permeable walls $P(0, t) = 0$, $D\nabla P(a, t) = -MP(a, t)$ (5) side-reflect, side-permeable walls $\nabla P(0, t) = 0$, $D\nabla P(a, t) = -MP(a, t)$. Here, P is the conditional probability, M is the permeability, and the initial condition at $t=0$ is assumed to be $P(x, x', 0) = \delta(x - x')$. To derive the normalized echo from each of the interface, we calculated the diffusion propagator under the influence from a narrow pulse gradient assumption that the diffusion signal for a displacement from x to x' , to the baseline spin echo is $E(q, \Delta)/E(q, t) = \iint \rho(x)P(x, x', \Delta) \exp(i2\pi q(x' - x)) dx dx' / \iint \rho(x)P(x, x', \Delta) dx dx'$. The eigenfunctions constructing the propagator between mixing interfaces can be expressed as (4) $\sin(\alpha_n x/a)$, with roots $\alpha_n = \beta_n a$ satisfying $\tan(\beta_n a) = -\beta_n D/M$ and (5) $\cos(\alpha_n' x/a)$, $\tan(\beta_n' a) = M/D\beta_n'$. The echo amplitudes from the mixing walls are compared with particles within the pure interfaces

of the orthogonal sets (1) $u_n = \sin(\frac{n\pi x}{a})$ (2) $\cos(\frac{n\pi x}{a})$ (3) $\cos(\gamma_n x) + \frac{M}{D\gamma_n} \sin(\gamma_n x)$, γ_n are the roots of $\tan(\gamma_n a) = 2(\frac{M}{D})\gamma_n/(\gamma_n^2 - (\frac{M}{D})^2)$. The condition probability and spin echo between the absorbing and

permeable walls can be written as $P(x, x', t) = \sum_{n=1}^{\infty} \frac{2}{a} ((\sin(\frac{\alpha_n x}{a}) \sin(\frac{\alpha_n x'}{a})) / (1 - \frac{\cos \alpha_n \sin \alpha_n}{\alpha_n})) \exp(-(\frac{\alpha_n}{a})^2 Dt)$ and



interval with permeability in the order of 0.1, 0.3 to 5 Ma/D from $b=0$ to $5ms/\mu m^2$ using the Levenberg-Marquardt algorithm performed in Matlab (MathWorks, Natick, MA). (1) A homogeneous diffusion coefficient D_{1h} satisfying $S(t) = S_0 \exp(-bD_{1h})$, (2) two diffusion pools $f_s, (1-f_s) D_{2s}, D_{2f}$, from $S(t) = S_0 (f_s \exp(-bD_{2s}) + (1-f_s) \exp(-bD_{2f}))$, and (3) intermediate diffusion included three phase pools, $f_s, f_i, (1-f_s-f_i) D_{3s}, D_{3i}, D_{3f}$ are derived according to the above boundary conditions and relaxation rates. The proton propagator, local transverse magnetization, and the spin echo amplitude are calculated between interfaces and numerically simulated from summing over the eigenfunctions with eigenvalues (1)(2) $(n\pi/a)^2 D$ (3) $\gamma_n^2 D$ (4) $\beta_n^2 D$ (5) $\beta_n'^2 D$ satisfying the reflecting/absorbing, permeable, and mixed interfaces in the time dependent exponential decay factor $e^{-\lambda_n t}$.

Results and Discussion: Figure 1 shows the transverse magnetization from $x=0$ (absorbing interface) to the permeable barrier at $x=a$ ($Ma/D = 2$). The magnetization minimum can occur at qa larger than 1.21 and at location close to the wall. Figure 2 shows the diffraction pattern observed between the reflecting and permeable interfaces. The diffraction minimum shifts to $qa \sim 1$ which decreases close to either of the reflecting or permeable walls different from the oscillation near the absorbing walls. Figure 3 shows the spin echo amplitude in three different ranges. A mono-exponential model derived D/D_0 smaller than 0.1 is identified at $f < 0.5$. At $f > 0.5$, a transition occurs into two pools, slow and fast diffusion, shown in Fig. 4. A larger deviation of diffusion coefficient between absorbing and permeable walls is observed compared to the deviation between permeable walls and permeable/reflecting walls. The diffusion coefficients provide not only the information of compartment size and structure, but also the estimation of the water-tissue interaction and relaxation rates. **References:** [1] A.L. Sukstanskii *et al.*, J. Magn. Reson. 170:56(2004) [2] J.E. Tanner and E.O. Stejskal J. Chem. Phys. 49:1768(1968) [3] Junzhong Xu *et al.*, Magn Reson. Med. 61:828 (2009) [4] Martin A. Koch *et al.*, Magn. Reson. Med. 60:90(2008) [5] Noam Shemesh *et al.*, J. Magn. Reson. 200:214(2009)

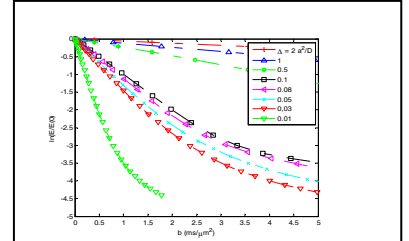


Figure3: The normalized echo amplitude from $b=0$ to $5\mu m^2/ms$ reveals three different signal decay ranges for the molecule propagating at the region between permeable and absorbing walls.

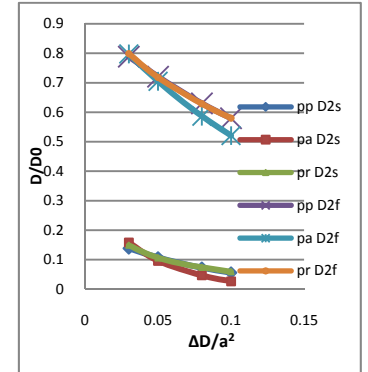


Figure4: The interface slow D2s and fast D2f diffusion coefficients derived from the echo amplitude between permeable walls (pp), permeable absorbing walls (pa), and permeable reflecting walls (pr).

$$S(q, \Delta) =$$

$$\sum_{n=1}^{\infty} \frac{2}{a^2} \frac{I_s(q)I_s(-q)}{1 - \frac{\cos \alpha_n \sin \alpha_n}{\alpha_n}} \exp\left(-\left(\frac{\alpha_n}{a}\right)^2 Dt\right),$$

where $I_s(q)$ is the Fourier

transformation quantity of the eigenfunction $\sin(\frac{\alpha_n x}{a})$.

Methods: The bulk diffusion coefficient D_0 is assumed to be $2\mu m^2/ms$ for diffusion measurable time $\Delta = f a^2/D$ ranging from short to long, $f=0.01$ to 2. The ratio of spin echo amplitude is fitted for each of the diffusion time