P93 Bipolar double-PFG NMR Reveals Pore Morphology in Randomly Oriented Cylindrical Compartments and in Spherical Yeast Cells

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Diffusion NMR is the most important methodology for non-invasively characterizing pore morphology. Scenarios such as diffusion in spheres or in locally anisotropic but randomly oriented compartments are extremely difficult to characterize using conventional single-PFG (s-PFG) MR. The angular double-PFG [1] (d-PFG) methodology at long mixing times (t_m) offers a novel means to overcome this limitation, since it provides quantitatively different angular dependencies for spheres and randomly oriented cylinders [2]: a flat angular dependence is expected for spheres, while a modulated bell-shaped function is expected for locally anisotropic but randomly oriented pores [2]. Another advantage of angular d-PFG is that it can be conducted at low q-values [3]. Here, we used controlled randomly oriented cylindrical pores, in which the inner diameter (ID) and compartment shape are known a-priori. S-PFG and long t_m angular d-PFG experiments were performed. Scanning electron microscope images confirmed that the specimen is indeed comprised of completely randomly oriented cylindrical microtubes. The line width of the water resonance in these pores was $\sim 0.5\,\mathrm{kHz}$, a manifestation of large susceptibility artifacts. Conventional s-PFG experiments surprisingly showed direction-dependant signal decay, clearly unexpected for randomly oriented compartments. However, when we employed bipolar gradients in the s-PFG sequence (bp-s-PFG), an isotropic decay was observed, as expected. The angular d-PFG experiments yielded inverted angular dependencies, from which microstructural information could not be obtained; therefore, we implemented a d-PFG NMR sequence with bipolar gradients (bp-d-PFG). The angular bp-d-PFG NMR yielded the expected [2] modulated bell-shaped function, providing insights that could not be inferred from s-PFG methodologies. First, the presence of restricted diffusion was easily inferred, since the non-flat angular dependencies are only observed when restricted diffusion occurs. Second, we could infer on the eccentricity of the pores, a fact we could not infer from s-PFG experiments. To demonstrate that spherical pores yield a flat angular dependence in long t_{m} angular d-PFG experiments, we used a suspension of fixed spherical yeast cells. Indeed, a flat angular dependence was observed, unequivocally characterizing the pores as spherical. Very accurate pore size measurements were also obtained using these approaches for both specimens. The bp-d-PFG methodology offers a new quantitative means for characterizing pore morphology, including pore size and shape. Applying bipolar gradients clearly eliminates the significant susceptibility artifact. Therefore, bp-d-PFG NMR may emerge as the method of choice for non-invasive characterization of heterogeneous specimens characterized by compartment shape anisotropy.

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