

MAR07-2006-007340

Abstract for an Invited Paper
for the MAR07 Meeting of
the American Physical Society

Molecular Dynamics Underlie the Nature of MRI Signals: The NMR Shutter-Speed

CHARLES S. SPRINGER, JR., Oregon Health & Science University

Motions of the spin-bearing molecules can have profound effects on the very nature (the exponentiality) of the macroscopic NMR signal. Quantitative mechanistic protocols often involve varying the equilibrium molecular kinetics (usually by temperature change) relative to the “NMR time-scale” (SS^{-1}), usually ill-defined as the absolute difference of resonance frequencies $|\Delta\omega|$ in sites between which spins are exchanged. This holds true for the equilibrium water molecule exchange between tissue compartments and distinct populations. However, *in vivo* studies must [by regulation] be isothermal, and the tissue $^1\text{H}_2\text{O}$ MRI signals remain essentially isochronous [$\Delta\omega = 0$]. In NMR, an equilibrium process is manifest in the context of its “exchange condition.” It only “appears” to be fast or slow by comparison of its actual rate constant with its *system* “shutterspeed” (SS). [A nonzero $\Delta\omega$ is the first, but not only, SS: its dimension is reciprocal time.] The process kinetics can be measured only if its NMR condition is varied at least partway between the fast- and slow exchange limits. In an isothermal study with no catalyst, this can be accomplished only by varying the pertinent SS. An MRI contrast reagent (CR) increases the laboratory frame $^1\text{H}_2\text{O}$ relaxation rate constant, $R_i [\equiv (T_i)^{-1}; i = 1,2]$. For an isochronous exchange process, the SS is the intrinsic $|\Delta R_i|$ for the sites. In quantitative dynamic-contrast-enhanced (DCE) studies, analytical pharmacokinetic modeling is accomplished on region-of-interest (ROI) or pixel by pixel $^1\text{H}_2\text{O}$ signal time-courses following bolus CR injections. Accounting for the equilibrium transendothelial and transcytolemmal water interchange processes (a three-site exchange situation) is crucial for modeling accuracy: the relevant SS values vary during the CR bolus passage. This is so for DCE studies of cancer, multiple sclerosis, and myocardial blood flow variation. It is necessary for the successful discrimination of malignant and benign breast and prostate lesions. One can expect a SS for almost any NMR experiment. This includes diffusion weighted and rotating-frame longitudinal relaxation of *in vivo* $^1\text{H}_2\text{O}$ signals. In these latter cases, the pertinent SS can be manipulated solely by adjustment of pulse sequence parameters, leading to completely non-invasive protocols.