Coherent Integration of Cross Relaxation and Magnetization Transfer in a Coupled Two-Spin Model of a Paramagnetic Complex in Water Solution.

Challenges exist in the development of MR contrast materials that may be facilitated by accurate modeling of the relaxation process. Conventional mathematical models, such as by Meiboom, consider the T_1 relaxation from proton-proton interactions and from proton-electron coupling separately, and incoherently combine them in a weighted summation. Analysis of the spin coupling or coherence effects between these interactions, however, is appropriate.

The developed model is similar to that of Koenig (*Mag. Reson. Med*., 30:685, 1993), however it considers proton-electron coupling with the contrast media, rather than proton coupling with protons bound within proteins. In this model, dipolar relaxation of a paramagnetic complex in water solution is described by a set of coupled macroscopic equations of motion for the net magnetic moment of water protons and unpaired electrons. These are formed by a coherent sum of interfacial and bulk contributions from both of these spin reservoirs. Only after these derivative contributions are in place does the model perform the integration that describes the dephasing and realignment characteristics of relaxation.

Preliminary results of a phantom study are presented comparing this model with conventional methods. Included in the discussion are meaningful parameters related to chemical exchange and the effective transition probability rate associated with internal unpaired electron reservoir coupling.