“Selective radiofrequency pulses in localization sequences for in vivo MR spectroscopy“

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The thesis work was conducted under the supervision of Prof. J. Frahm of the Biomedical NMR Research Group at the Max-Planck-Institute for Biophysical Chemistry. Thesis advisors on behalf of the University of Göttingen were Prof. F. Smend and Prof. R. Pottel of the Dept. of Physics.

Background:

Radiofrequency (RF) pulses are by definition the pivotal elements of NMR pulse sequences. *Vice versa*, the effect of a particular RF pulse on the evolution of magnetization will depend on the context of the sequence. While the product operator formalism provides a general framework to describe the effect of non-selective pulses on weakly coupled spin systems, there is no consistent framework describing the effect of selective pulses in the context of MRI sequence. The excitation profile is the result of frequency dependent trajectories describing the complex interaction of nutation and precession. In spin-echo sequences, the refocusing pulse acts on a spatial distribution of transverse magnetization that may by spatially dispersed by the magnetic field gradient applied during the RF pulse. This situation is further complicated for the stimulated echo acquisition mode (STEAM), as the stimulated echo is created from a spatial distribution of transverse *and* longitudinal components. Aim of the thesis was a qualified choice of selective RF pulses for an improved definition of the localization volume for in vivo MR spectroscopy (MRS) and a critical appraisal of optimised RF pulse shapes.

Methods:

The problem was addressed by building a theoretical framework by numerical simulations and with experimental methods. All experiments were performed on a clinical MR system operating at 2 Tesla (Siemens Magnetom SP). ‘External’ RF pulse shapes employed by the pulse sequences were calculated individually by FORTRAN routines. A phase-sensitive method was developed to measure the distribution of the localized distribution of transverse magnetization along arbitrary spatial directions. This required the acquisition of a full echo after initial gradient reversal. The signal was evaluated using the scanner’s MRS evaluation tool with suitable zero-filling and phase correction. This proved a more realistic and less time consuming technique than the common approach of creating a magnitude image of the localized signal by spatial spin-warp encoding, as phase sensitivity and fully relaxed conditions were preserved.

A fourth-order Runge-Kutta algorithm was used for numerical integration of the Bloch equations during arbitrary RF pulses. A simulation tool-box was written to calculate trajectories, the frequency dependence of the Cartesian rotation matrix, spin-echoes and stimulated echoes of dispersed transverse magnetization. A comprehensive theoretical framework was established from these findings.

Results and Discussion:

The STEAM and double spin echo (or PRESS) localization sequences were described by Cartesian rotation matrices, thus accounting for the magnetic field gradients along the spatial axes. A suitable description of spoiler gradients provided a transformation of the matrix elements to four basic slice ‘profiles’. Two of these profiles are readily observable, as they correspond to the creation of transverse magnetization by ‘excitation’ of longitudinal magnetization and ‘refocusing’ of spoiled transverse magnetization. Two profiles are created in the z-component from longitudinal magnetization (‘saturation’) and from spoiled transverse magnetization (‘flipback’). These can only be observed after converting longitudinal magnetization by a read-out pulse and suitable refocusing. Excitation, refocusing, and flipback yield phase-sensitive profiles. Observation of phase coherent superposition of transverse magnetization, that is maximum signal, requires refocusing by a characteristic fraction of the slice selection gradient (*i.e.*, displacement in *k*-space in an MRI context).

These profiles (complemented by the two spoiled transverse components that are unobservable unless the whole gradient is refocused), the nine matrix components, and the nine coherence transfer paths yield equivalent descriptions of an RF pulse acting on arbitrary spin-½ magnetization. Fundamental symmetries were established for symmetric pulses between excitation and flipback by time-reversal, and between saturation and refocusing. The challenge of calculating slice profiles of spin echoes and stimulated echoes could thus be reduced to the relatively simple cases of excitation and saturation.

The flip angle dependent non-linear effects of selective RF pulses were studied on two archetypical pulse shapes: a multilobe *sinc*-shaped pulse with a large time-bandwidth product creating sharp profiles, and a monolobe *gaussian*-shaped pulse with a small time-bandwidth product. The quality of the localization depends on the slice profile, the signal strength also on refocusing. 90° excitation pulses require slightly more than 50% refocusing to obtain the maximum degree of coherence. The excitation slice profile deteriorates for flip angles exceeding 120°. Gaussian-pulses are reasonable all-purpose pulses, but MRS applications suffer from soft profiles resulting in an inferior slice definition. Sinc-pulses showed major and far extending out-of-slice excitations. These require suppression by suitable low-pass filtering.

All investigated optimized excitation pulse shapes showed out of slice-excitations of a size that prohibited their application in MRS sequences, as this requires sufficient suppression of subcutaneous fat signals. Self-refocusing pulses work similar to spin-echoes and require high RF amplitudes. They are thus unable to reduce the effective echo time (TE) regarding the evolution of coupled resonances. For symmetry reasons they must be implemented into the STEAM sequence in a back-to-back fashion. Windowed sinc-pulses are an acceptable compromise for STEAM localization in terms of slice definition, out-of-slice suppression, time-bandwidth-product and RF amplitude.

Therefore, we assessed the ability of various low-pass filters (window functions) to suppress out-of-slice excitations. For ‘short’ sinc-pulses with 3 side lobes, the Kaiser (or Bessel) window yielded optimal results. Exceptionally sharp profiles without negative excitations were obtained with a ‘long’ sinc-pulse with 6 side lobes and a triangular filter. In the standard implementation of the external sinc-pulses, only the bandwidth sinc- and gauss-functions were changed while the window functions were kept constant. This resulted in bandwidth-dependent refocusing and in deterioration of the pulse profile for low bandwidth pulses (or small voxels). Therefore, the optimized pulse shapes were implemented with a minimum bandwidth. For larger bandwidths, the shortened pulse shape was padded by zeroes and shifted to adapt the refocusing. This implementation warranted bandwidth independent profiles and refocusing.

Conclusion:

The effect of any slice-selective RF pulse on spin 1/2 magnetization in an arbitrary pulse sequence may be described in correspondence to the coherence transfer pathways by four different slice profiles and degrees of dephasing (two for symmetric pulse shapes). This concept was applied to study the volume localization of MRS sequences, but may be readily applied to MRI sequences.