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Composite pulse combinations for chirp excitation

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ABSTRACT

Composite pulses are the efficient method for broadband excitation to get control of the limitations of high field NMR, such as resonance offset effects with constraints on rf power that leads to signal intensity distortion. Phase-modulated chirp pulses are used as ordered composite pulse sequences in this paper as **CHORUS** sequence in a high-field NMR spectrometer (BRUKER 750 MHz) for broadband excitation. The composite pulse sequence applies chirp pulses with the forward and the reverse sweep mechanisms. A single excitation pulse combines adiabatic and non-adiabatic rotation, explained as a three-phase rotation, which leaves the magnetizing vectors to a non-uniform phase dispersion as a function of the offset frequency. One adiabatic refocusing pulse of the double sweep rate after the excitation pulse cannot satisfactorily compensate for the phase dispersion. Hence, composite self-refocussing **CHORUS** excitation pulse, with forward, reverse, and their combinations are used to remove the non-uniform phase dispersion generated due to offset resonance frequency. Four such combinations of composite pulses are produced with analytical explanation in this paper. MATLAB simulation results and experimental verification on the BRUKER 750 MHz NMR spectrometer of the composite pulses are also presented in this paper.

1. Introduction

Broadband excitation for wide chemical shift nuclei like ^{19}F, where the chemical shift can range over 600 ppm, is problematic as NMR signal intensity degrades towards the edges of full spectral width due to the resonance offset effect. Such nuclei require excitation of different spectra regions, at a field of 1 GHz, the target bandwidth is 50 kHz for excitation of entire 200 ppm ^{13}C chemical shifts. Because of the limited power availability of radiofrequency in pulsed excitation, signal intensity and phases distort for resonance offset effect and degrade the accuracy of signal integration. Research has been done to establish different pulse techniques for broadband excitation and inversion over time to reduce the phase variation as a function of resonance offset. Some of these methods are optimal control techniques for pulse design [1–5], Rotating frame approximation method [6], adiabatic pulses [7–11], Polychromatic pulse technique [12], composite adiabatic pulses [13–17] etc. The method of composite pulses inevitably proves their efficacy in controlling the problems, as mentioned earlier. Research on producing various conventional composite pulses has developed [18–24]. Composite pulses are the sequence of closely spaced RF pulses, efficient to excite and invert the bulk magnetization over the broad spectral range and refocus the magnetization to eliminate the phase distortion as a function of the offset resonance frequency. Composite pulses, which are the sequence of ordered chirped-pulse for the application on ultra-broadband resonance frequency range, i.e., **CHORUS** are less sensitive to the degradation of the signal intensity over the full spectral range [25,26].

The main focus of this paper is an analytical explanation of the composite pulse **CHORUS** for broadband excitation, where the chirp pulses of different sweep rates are applied for excitation and refocussing of the magnetization. In [27] an analytical explanation for the forward sweep **CHORUS** sequence for chirp excitation is provided. Whereas this paper emphasizes the reverse sweep **CHORUS** sequence and the combination of both. Other analytical explanations are also present for broadband excitation and inversion using the chirp mechanism in [28,29], but this paper explains it differently. The composite adiabatic pulse sequence, **CHORUS**, is based on the phase modulation scheme, which has a chirp excitation pulse component that rotates the bulk magnetization to the equator from the north pole. The chirp excitation pulse produces a three-stage rotation to bring the magnetization to the equator, but it has some non-uniform phases, depending on the resonance offset. The inversion chirp pulse with the double sweep rate can remove the phase dispersion and refocus the non-uniform

Abbreviations: CHORUS, CHirped ORdered Ultrabroadband Spectroscopy.

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