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Spectral resolution enhancement by chemical shift imaging

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Abstract

Three-dimensional chemical shift imaging (3D CSI) with appropriate data postprocessing can be used as a tool to improve spectral resolution in samples where large susceptibility differences and limited shim capabilities prevent good sample shimming. Data postprocessing is reduced to the realignment of individual 3D voxel spectra. As a result, the line broadening due to the field inhomogeneity over the sample's volume is reduced to the broadening by inhomogeneity within individual voxels. We compared this method with the resolution enhancement by window multiplication. We demonstrated, theoretically and experimentally, that in the presence of large, lower-order gradients, 3D CSI achieves better resolution enhancement with smaller sensitivity losses. An application of the method to a simple biological system is presented as well.

Keywords: Chemical shift imaging; Resolution-enhancement filtering; Spectroscopic resolution; Signal-to-noise ratio; Magnetic field inhomogeneity

1. Introduction

In high-resolution NMR spectroscopy of liquids, the main challenge is to minimize the effects of field inhomogeneity that lead toward losses of spectral resolution and sensitivity. In a homogeneous sample, the principal source of the field inhomogeneity is macroscopic field variation over the sample volume. Even in an initially homogeneous field and with a homogeneous sample, the susceptibility effects introduce the field inhomogeneity if the sample is not spherical or cylindrical [1–3]. Magic angle sample spinning is an elegant method to eliminate susceptibility effects, but it is limited to small and robust samples only. Another common method for resolution enhancement is the multiplication of time domain data by suitable window function, which, in turn, degrades signal-to-noise ratio (SNR). Therefore, additional methods for line narrowing, with minimal deterioration of SNR, are highly desirable.

Chemical shift imaging (CSI) is a technique that enables the acquisition of spectra from individual volume elements (voxels) of the sample [4]. CSI could be rather time-consuming because it requires many phase-encoding steps to achieve spatial resolution. The sensitivity losses, proportional to the spatial resolution, restrict the use of CSI only to cases with favorable SNR. CSI is complemented by other spatially selective spectral methods that minimize sensitivity losses by recording spectra from larger voxels (e.g., VSE [5] and CARVE [6]). However, they are also prone to the magnetic field inhomogeneity line broadening.

Resolution enhancement by CSI is based on the simple fact that the variability of the field within a voxel is much smaller than across the whole sample volume [7,8]. Individual voxel spectra have narrower lines but are shifted relatively to each other [9]. When voxel spectra are realigned, a spectrum with significantly narrower lines compared with a total volume 1D spectrum may be obtained. The alignment shifts calculated for individual voxels are proportional to the magnetic field variations (inhomogeneities) in the sample and can be used for mapping the static magnetic field. This approach was already implemented for mapping metabolites in human brain where voxels of a high-resolution chemical shift image were coadded to obtain better spectral resolution in a low-resolution chemical shift image at the cost of reduced SNR [10]. However, a decrease of the SNR (peak signal/RMS noise) is not proportional to a decrease of the voxel's volume but is, in general, lower due to higher magnetic filed homogeneity within smaller voxels [11].

The aim of our work was to show theoretically and experimentally that by proper manipulation of CSI signals, a

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total volume spectrum of comparable resolution and SNR to a resolution-enhanced 1D spectrum filtered by a window function multiplication [12] can be obtained in the same experimental time.

2. Theory

In a homogeneous magnetic field, the FID of a liquid with a single line at resonance frequency ω_0 decays exponentially with relaxation time T_2

$$S_L(t) = A\exp\left(t\left[\frac{1}{T_2} + \imath\omega_0\right]\right). \quad (1)$$

Fourier transformation from time to the frequency domain produces the Lorentzian absorption line

$$S_L(\omega) = AT_2\frac{1}{1+(\omega-\omega_0)^2T_2^2}, \quad (2)$$

with a line width at half-height $LW_\omega = 2/T_2$ or $LW_\nu = 1/(\pi T_2)$ and the resonance intensity $S_L(\omega_0) = AT_2$. Resonance frequencies follow local magnetic field induction $B(\vec{r})$, and in an inhomogeneous magnetic field, they become dependent on the spatial coordinate $\vec{r}$. Then, the signal from the whole volume V is

$$S(t)\frac{A}{V}\int_V \exp\left(t\left[-\frac{1}{T_2} + \imath\gamma B(\vec{r})\right]\right)\mathrm{d}V. \quad (3)$$

For $B(\vec{r})$=constant, Eq. (3) reduces to Eq. (1). For the arbitrary distribution of the magnetic field, the influence of gradients on the total volume signal can be approximated by a separate influence on the average resonance frequency, via frequency shift $\Delta\omega_0$, and on line width, via apparent relaxation rate T_2*

$$S(t,V,G_V) = A\exp\left(t\left[-\frac{1}{T_2^*(V,G_V)} + \imath(\omega_0 + \Delta\omega_0(V,G_V))\right]\right). \quad (4)$$

Arguments V and G indicate that the line width and the line position both depend on the sample volume and overall field inhomogeneity.

3D CSI discerns spectra from individual voxels, and then, the jth voxel spectrum depends on the voxel size υ and gradients G_V within the voxel

$$s_j(t,\upsilon,V,G_V) = A\frac{\upsilon}{V}\exp\left(t\left[-\frac{1}{T_{2,j}^*(\upsilon,G_V)} + \imath\left(\omega_0 + \Delta\omega_{0,j}(V,G_V)\right)\right]\right). \quad (5)$$

Plain coaddition of the voxel spectra yields the total spectrum according to Eq. (4). The resultant line is broader than individual voxel lines because distribution of the voxel resonance frequencies effectively shortens T_2*. However, if, prior to coaddition, voxel spectra are mutually shifted, each for its own alignment frequency $-\Delta\omega_{0,j}$ (V,G_V), then the shift due to the field inhomogeneity is eliminated and the resulting line width is affected only by the field variation within a voxel

$$S(t,\upsilon,G_V) = A\exp\left(t\left[-\frac{1}{T_2^*(\upsilon,G_V)} + \imath\omega_0\right]\right). \quad (6)$$

The Fourier transform of Eq. (6) yields a Lorentzian line with a line width $2/T_2$*(υ) rather than $2/T_2$*(V) as is in the 1D spectrum (Eq. (2)). Since T_2*$(\upsilon) >> T_2$*(V), appreciable narrowing can be achieved. However, resolution enhancement is always followed by sensitivity losses, and further, we focus on the SNR analysis.

2.1. Time domain SNR (SNR_t)

To establish the relationship between CSI and 1D spectra, again, we consider a homogeneous sample in an inhomogeneous magnetic field. Suppose that, immediately after the 90° excitation pulse in the standard 1D experiment, the signal from the sample has maximal amplitude $S(t=0)=A$ and a noise level σ_t. The time domain SNR for the one-pulse experiment is then simply $SNR_{t1}=A/\sigma_t$. In the 3D CSI experiment, signals $\hat{S}_j(t)$ acquired from M^3 k-space points form a 3D matrix with the dimension M^3. Inverse Fourier transformation of the k-space matrix gives the time domain signals from voxels at different positions $\vec{r}_i$

$$S_i(t) = \frac{1}{M^3}\sum_{j=1}^{M^3}\hat{S}_j(t)\exp\left(-\imath\vec{r}_i\vec{k}_j\right). \quad (7)$$

Then, the signal from the whole sample is a sum of M^3 voxel signals $S_i(t)$

$$S_\Sigma(t) = \sum_{i=1}^{M^3}S_i(t) = \frac{1}{M^3}\sum_{j=1}^{M^3}\hat{S}_j(t)\left[\sum_{i=1}^{M^3}\exp\left(-\imath\vec{r}_i\vec{k}_j\right)\right] = \frac{1}{M^3}\sum_{j=1}^{M^3}\hat{S}_j(t)M^3\delta_{j,1} = \hat{S}_1(t). \quad (8)$$

Here, the order of voxel (index i) and k-space (index j) summation is reversed, and the sum within the bracket is expressed over the discrete delta function. Similar transformation holds also for noise

$$\sigma_{t,\Sigma} = \sqrt{\sum_{i=1}^{M^3}|\sigma_{t,i}|^2} = \frac{1}{M^3}\sqrt{\sum_{j=1}^{M^3}\sum_{j'=1}^{M^3}\hat{\sigma}_j\hat{\sigma}_{j'}^*\sum_{i=1}^{M^3}\exp\left(\imath\vec{r}_i\left(\vec{k}_{j'}-\vec{k}_j\right)\right)} = \frac{1}{M_3}\sqrt{M^3\sum_{j=1}^{M^3}|\hat{\sigma}_j|^2} = \sigma_t. \quad (9)$$