

Compensation of effect of field instability by reference deconvolution with phase reconstruction

Takahiro Iijima¹, K. Takegoshi^{*}

Department of Chemistry, Kyoto University, Kyoto 606-8502, Japan

Received 31 August 2007; revised 19 December 2007

Available online 25 December 2007

Abstract

A compensation method based on reference deconvolution is developed to obtain high-resolution NMR spectra under an unstable magnetic field. It is shown that the applicability of the original deconvolution method is limited for small fluctuation, and a process what may be called phase reconstruction is proposed to compensate large field fluctuation. We demonstrate the method using a probe with a coil that can generate a fluctuation field artificially. A high-resolution ¹H NMR spectrum of ethylbenzene was obtained under the unstable field after compensation with this method.

© 2007 Elsevier Inc. All rights reserved.

Keywords: High-resolution NMR; Field fluctuation; Simultaneous measurement

1. Introduction

So far, several techniques have been developed for measuring high-resolution NMR under unstable magnetic field provided by, for example, resistive and hybrid magnets [1–5]. They include an iZQC technique [1], insertion of highly conductive metal tube [2], a fluctuation-field feedback method [3,4] and a reference-deconvolution method [3,5].

Recently we have reported another method of deconvolution which uses a field-fluctuation signal [6]. In this method an electromotive force signal induced for a pickup coil wound near a sample is measured synchronously with an FID signal. The former signal is converted to an NMR phase angle, $\phi(t)$, and used for deconvolution of the latter signal. The method was demonstrated with ⁷⁹Br MAS NMR of KBr using the hybrid magnet at National Institute for Materials Science in

Japan [6]. Deconvolution using a field-fluctuation signal has also been applied for compensation of NMR signals acquired using a pulsed magnet whose excitation time is in the order of millisecond [7].

Since it is difficult for the pickup coil to measure field fluctuation at the sample exactly, the resolution achieved employing the deconvolution method with the electromotive force signal would be good enough for high-resolution NMR in solids, but not for NMR in liquids. Compensation methods suitable for high-resolution liquid-state NMR are likely to utilize a reference NMR signal.

In fact, such NMR-NMR deconvolution technique is well known as reference deconvolution and widely used for the compensation of effect of field inhomogeneity [8–12]. So far, the reference deconvolution technique has been incorporated in various NMR spectroscopy such as 2D NMR [13,14], NMR imaging [15], dynamic NMR [16,17], diffusion [18,19] and relaxation [20] experiments and NMR with novel coil design [15,21,22] and processing scheme [23]. Although reference deconvolution in the frequency domain has been proposed [24], this compensation is conveniently conducted in the time domain [8–12]; a reference NMR signal of which the spectrum is known is mea-

^{*} Corresponding author. Fax: +81 75 753 4000.

E-mail address: takeyan@kuchem.kyoto-u.ac.jp (K. Takegoshi).

¹ Present address: Department of Molecular Structure, Institute for Molecular Science, Okazaki 444-8585, Japan.

sured and components of field inhomogeneity in an observation NMR signal is removed by deconvolving the latter signal with ratio of the experimental and “ideal” reference signals.

Since reference deconvolution is recognized as a correction of the NMR phase angle $\phi(t)$ for each point of the FID signal, effect of field instability can also be compensated by this method. Such application of reference deconvolution for compensation of field fluctuation of resistive and hybrid magnets have been recently reported from Nijmegen High-Field Magnet Laboratory in Netherlands [3] and National High Magnetic Field Laboratory in USA [5]. For instance, Bentum et al. [3] have shown a high-resolution ^{27}Al solid-state MAS NMR spectrum of a mineral sample under fluctuating field of a 24 T hybrid magnet by measuring simultaneously the signals of ^{27}Al NMR and reference ^{2}D NMR of liquid D_2O , where two samples are kept in different holder. It is envisaged that this scheme can directly be utilized for acquiring high-resolution liquids NMR under fluctuation field. Indeed, Gan et al. [5] have presented a high-resolution ^1H NMR spectrum of ethanol measured with a 25 T resistive magnet. However, as we will show below on the basis of a result of computer simulation, the original method is not always able to compensate effect of field fluctuation. Because of this, Bentum et al. [3] applied the feedback method to compensate large and fast field fluctuation of the hybrid magnet, and the reference deconvolution method was used for the removal of remaining small drift.

In this paper, we firstly touch upon the deconvolution method of Ref. [3] and examine a reason for the method to fail to compensate large field fluctuation. Then, we propose a process what may be called “phase reconstruction” to ameliorate the original deconvolution method. We demonstrate this method with a conventional stable superconducting magnet (14 T) and a probe attaching a coil wound around it to generate a fluctuating field (~ 0.1 mT) at the position of a sample. A high-resolution ^1H NMR spectrum of ethylbenzene measured under such fluctuating field with deconvolution using ^2H NMR signal of deuterated benzene will be presented.

2. Theory

2.1. NMR signal under fluctuation field

A fluctuating magnetic field $B(t)$ can be expressed by

$$B(t) = B_0 + f(t)B_z, \quad (1)$$

with $B_0 \gg B_z$. B_0 and $f(t)B_z$ represent a static field of the order of several tens of tesla and a fluctuating field, respectively. B_z is a field having a component parallel to B_0 and $f(t)$ is a dimensionless function of time expressing fluctuation ($-1 \leq f(t) \leq 1$). When we measure single-scan NMR of an I spin under the magnetic field $B(t)$, the resulting FID signal $g_I(t)$ may be represented as [6]

$$g_I(t) = \sum_j a_I^j \exp[-i(\Delta\omega_I^j t + (1 + \sigma_j)\gamma_I F(t) + \phi_{I0}^j)] \\ \times \exp(-t/T_{2I}^j) \sim \sum_j a_I^j \exp[-i(\Delta\omega_I^j t + \gamma_I F(t) + \phi_{I0}^j)] \\ \times \exp(-t/T_{2I}^j), \quad (2)$$

with $\Delta\omega_I^j = \gamma_I B_0 \sigma_j$, a_I^j , ϕ_{I0}^j , T_{2I}^j and σ_j are, respectively, a signal intensity, an initial phase, a spin–spin relaxation time and a chemical shift for the j th spectral component of I -spin NMR. γ_I is a gyromagnetic ratio of the I spin. $F(t)$, the term caused by the fluctuating field, can be given by

$$F(t) = B_z \int_0^t f(t') dt'. \quad (3)$$

The chemical shift caused by fluctuating magnetic field, $\sigma_j \gamma_I F(t)$, is dropped in Eq. (2).

2.2. Examination of the original deconvolution method

In reference deconvolution method, NMR of a reference S -spin which has only one signal-component is measured synchronously with that of the I spin in order to remove $F(t)$ in Eq. (2). The FID signal for such an S -spin system may be written as

$$g_S(t) = a_S \exp[-i(\Delta\omega_S t + \gamma_S F(t) + \phi_{S0})] \exp(-t/T_{2S}), \quad (4)$$

where a_S , $\Delta\omega_S$, γ_S , ϕ_{S0} and T_{2S}^S have similar meanings as those in Eq. (2). Because the interaction of I or S spin with external magnetic field is different only by its gyromagnetic ratio, Bentum et al. [3] have introduced a correction function $c(t)$ as

$$c(t) = \left(\frac{g_S^{\text{ref}}(t) \times W(t)}{g_S(t)} \right)^{\gamma_I/\gamma_S}. \quad (5)$$

g_S^{ref} , representing resonance-offset for the S -spin signal, may be $\exp[-i\Delta\omega_S^{\text{ref}} t]$ and $W(t)$ is a weighting function to express the T_2 decay. In an ideal case of $\Delta\omega_S^{\text{ref}} = \Delta\omega_S$, $W(t) = \exp(-t/T_{2S})$ and $\phi_{S0} = 0$, $c(t)$ becomes

$$c(t) = (\exp[i\gamma_S F(t)]/a_S)^{\gamma_I/\gamma_S} \\ = \exp[i\gamma_I F(t)]/a_S^{\gamma_I/\gamma_S}, \quad (6)$$

and high resolution I spin NMR can be obtained by deconvoluting $g_I(t)$ with $c(t)$ as,

$$g_I^{\text{comp}}(t) = g_I(t)c(t) \\ = \sum_j (a_I^j/a_S^{\gamma_I/\gamma_S}) \exp[-i(\Delta\omega_I^j t + \phi_{I0}^j)] \exp(-t/T_{2I}^j), \quad (7)$$

which is free from field fluctuation.

To appreciate the applicability of this scheme, we undertook computer simulation and the results are schematically shown in Fig. 1. For simplicity, we assumed that each of I - (^1H) and S -spin (^2H) NMR has single spectral component on resonance ($\Delta\omega_I^j = \Delta\omega_S = 0$). The initial phases, ϕ_{I0}^j and

ϕ_{S0} , are also assumed as 0° . Thus deviance of FID signals ($g_I(t)$ and $g_S(t)$) from single exponential decay curve is due to field fluctuation ($\gamma_I F(t)$ and $\gamma_S F(t)$, respectively). The correction function $c(t)$ for the ideal condition with $W(t) = \exp(-t/T_{2S})$ is a signal without decay (Fig. 1(d)). For small field fluctuation (Fig. 1(i)), it is found that $g_I(t)$ is successfully compensated by deconvolution with $c(t)$, resulting in $g_I^{\text{comp}}(t)$ with single exponential curve as shown in Fig. 1(i-e). For large fluctuation case (Fig. 1(ii)), however, this scheme fails to compensate the fluctuation com-

ponent and the deconvoluted signal becomes a nicked curve (Fig. 1(ii-e)).

The reason of the failure is explained as follows. Suppose we have $\exp[i\gamma_S F(t)] = 0.5 + 0.5i$. We then have $\gamma_S F(t) = 45^\circ + 360^\circ \times n$, leading to $\gamma_I F(t) = \gamma_I/\gamma_S (45^\circ + 360^\circ \times n)$. The failure in Fig. 1 is due to the naive assumption of $n = 0$, which is good for the smaller fluctuation (the left column in Fig. 1) but not for the larger one (the right column).

2.3. Reference deconvolution with phase reconstruction

For proper conversion, we propose reconstruction of the phase folded in $\pm 180^\circ$. To apply this, we firstly extract the phase part from the S-spin FID signal of Eq. (4) by the following calculation:

$$g_S^{\text{fr}}(t) = g_S(t) / \sqrt{g_S(t)g_S^*(t)} = \exp[-i(\Delta\omega_S t + \gamma_S F(t) + \phi_{S0})], \quad (8)$$

where $g_S^*(t)$ is the complex conjugate of $g_S(t)$. Note that the weighting function $W(t)$ is replaced by $\sqrt{g_S(t)g_S^*(t)}$. Then the phase angle of S-spin NMR, $\phi(t)$, is obtained by

$$\phi(t) = \tan^{-1} \frac{\text{Im}\{g_S^{\text{fr}}(t)\}}{\text{Re}\{g_S^{\text{fr}}(t)\}}. \quad (9)$$

Although $\phi(t)$ estimated in Eq. (9) lies in the range from -180° to 180° , we can easily reconstruct $\phi(t)$ to retrieve the true angle $\xi(t)$ (Fig. 2),

$$\xi(t) = \text{Reconst}\{\phi(t)\}. \quad (10)$$

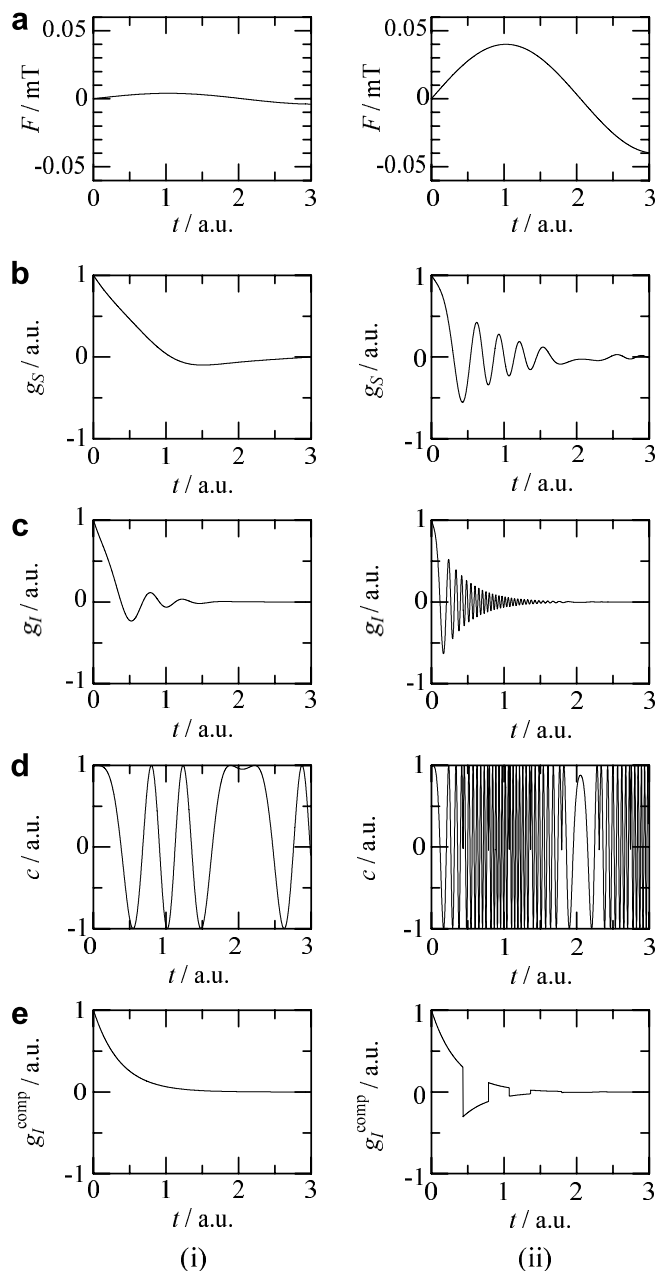


Fig. 1. Schematic diagram of compensation of effect of field instability on NMR signals by the method of Ref. [3]; (a), (b), (c), (d) and (e) show, respectively, the time dependences of $F(t)$, $g_S(t)$, $g_I(t)$, $c(t)$ and $g_I^{\text{comp}}(t)$ (see text). (i) and (ii) depict the cases of small and large field fluctuation, respectively.

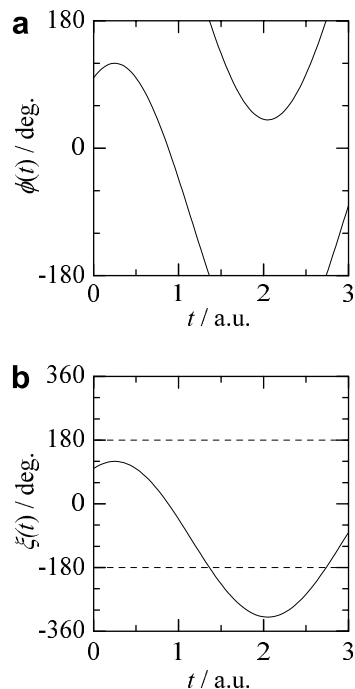


Fig. 2. Schematic diagram illustrating the phase reconstruction; (a) and (b) show, respectively, the experimentally obtainable phase angle $\phi(t)$ that lies within -180° to 180° and the phase $\xi(t)$ reconstructed from $\phi(t)$.

The proper I -spin phase angle is obtained from $\xi(t)$ as

$$\begin{aligned}\psi(t) &= \frac{\gamma_I}{\gamma_S} \xi(t) \\ &= \Delta\omega' t + \gamma_I F(t) + \phi'_0.\end{aligned}\quad (11)$$

The correction signal in our scheme becomes

$$h(t) = \exp[-i\psi(t)],\quad (12)$$

and the effect of field fluctuation on I -spin NMR is compensated by deconvoluting $g_I(t)$ with this signal as,

$$\begin{aligned}g_I^{\text{comp}}(t) &= g_I(t)h^*(t) \\ &= \sum_j a_j^I \exp[-i(\Delta\omega_I^{jj} t + \phi_{I0}^{jj})] \exp(-t/T_{2I}^j),\end{aligned}\quad (13)$$

where $\Delta\omega_I^{jj} = \Delta\omega_I^j - \Delta\omega'$ and $\phi_{I0}^{jj} = \phi_{I0}^j - \phi'_0$.

Note here that not only the field fluctuation term $\gamma_S F(t)$ but the resonance offset term $\Delta\omega_S t$ equivalently contribute to the S -spin phase angle ($\phi(t)$ or $\xi(t)$). Since the offset term increases linearly with increasing time, phase reconstruction will be needed even for small $\Delta\omega_S$. In the scheme of Ref. [3], this corresponds to the case of $\Delta\omega_S^{\text{ref}} \neq \Delta\omega_S$ in Eq. (5). Note also that ambiguity of choosing $W(t)$ in Eq. (5) is removed in our method. Finally, it is pointed out that phase reconstruction is not needed for compensation using homonuclear species, because a scaling factor for conversion of the phase γ_I/γ_S (Eq. (5) or (11)) is one in such a case. More exactly, phase reconstruction is unnecessary when $\gamma_I/\gamma_S = n$ ($n = 1, 2, 3, \dots$).

3. Experimental

All of NMR measurement was performed in a JASTEC 14.1 T wide-bore magnet with stable magnetic field whose homogeneity was adjusted using a 17-channel matrix shim. Neither ^2H NMR lock nor sample spinning were used. A JEOL narrow-bore HX NMR probe was modified to equip with a coil made of a 0.435 mm ϕ Cu wire wound around a shielding tube of the probe to generate a fluctuation field. The coil of 43 mm ϕ i.d. spread to 60 mm length with ca. 120 turns. The field created with this additional coil is 1 mT for 0.54 A. The coil-wound probe head was covered with a 49 mm ϕ i.d. aluminum tube of 3 mm thickness in order to reduce mutual inductance between the coil and an RT shim coil.

A JEOL ECA-based dual spectrometer having two frequency synthesizers, transmitters, receivers and AD converters was constructed for simultaneous measurement of ^1H and ^2H NMR. Resonant frequencies were 600.136 MHz for proton and 92.125 MHz for deuterium. A sample was prepared by admixing ca. 0.1 ml of 99% ethylbenzene and 1 g of 99.6% deuterated benzene (benzene- d_6) in a 5 mm ϕ o.d. glass sample tube. The pulse sequence used is shown in Fig. 3. The width of excitation pulse and dwell time of acquisition of the FID signal were 20 μs and 8 μs , respectively, for both channels, and 32 k data points were acquired synchronously. The fluctuation field applied

for the sample starts at time τ_f before rf pulse irradiation. The wave of the fluctuation field was fabricated by summing up many waves with different amplitude, frequency ranging 1–700 Hz, and phase. The function $f(t)$ was not random but periodic with cycle of ca. 20 ms. Various τ_f values around 100 ms were used for accumulation of FID signals to remove effect of this periodicity. The maximum amplitude of $f(t)B_z$ was about ± 0.1 mT. Typical time-dependence of $f(t)$ will be seen in Fig. 5.

The cancellation of field fluctuation by our scheme was performed with Eqs. (2)–(4) and (8)–(13) using a home-written FORTRAN program. An apodization with the Lorentzian line broadening of 2 Hz was employed for the FID data prior to Fourier transform. For comparison, the deconvolution calculation by the method of Bentum et al. [3] was also conducted using Eqs. (2)–(7).

4. Results and discussion

Fig. 4(a) shows the FID signals of (i) ^1H and (ii) ^2H measured under the static homogeneous field of 14.1 T, and Fig. 4(b) shows the corresponding FT spectra. 0 ppm of the spectra coincides to the observed frequency (600.136 MHz for ^1H and 92.125 MHz for ^2H). The ^2H NMR spectrum of benzene- d_6 (Fig. 4(b-ii)) exhibits a single peak at ca. -0.7 ppm. On the other hand, the ^1H NMR spectrum of ethylbenzene consists of four peaks as shown in Fig. 4(b-i). The peaks at -6.9 ppm, -5.5 ppm and doublet peak at -0.88 and -0.76 ppm can be attributed to the proton signals of methyl, methine and phenyl groups, respectively. Although each of these peaks can split into multiplet owing to J coupling, such multiplet was not observed in our measurement. This is ascribed to the poor shimming without sample spinning and NMR lock.

Fig. 4(c) and (d) show the FID signals measured under fluctuating magnetic field using the pulse sequence in Fig. 3 and the corresponding FT spectrum, respectively. The FID signals of the I (Fig. 4(c-i)) and the S spin

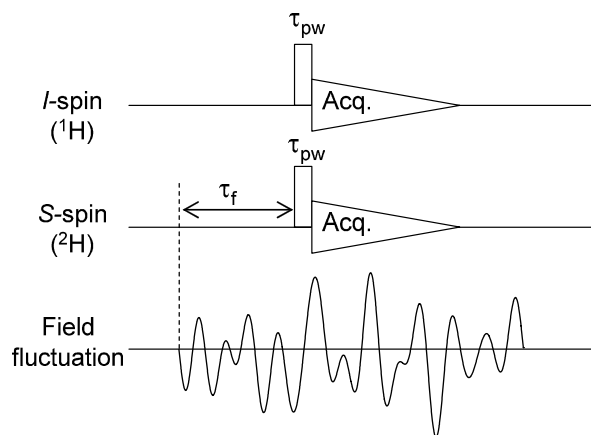


Fig. 3. Pulse sequence used in this study. Fluctuation field applied in the bore of a 14.1 T magnet starts at time τ_f before irradiating rf pulses. NMR measurements of I - and S -spin are performed synchronously.

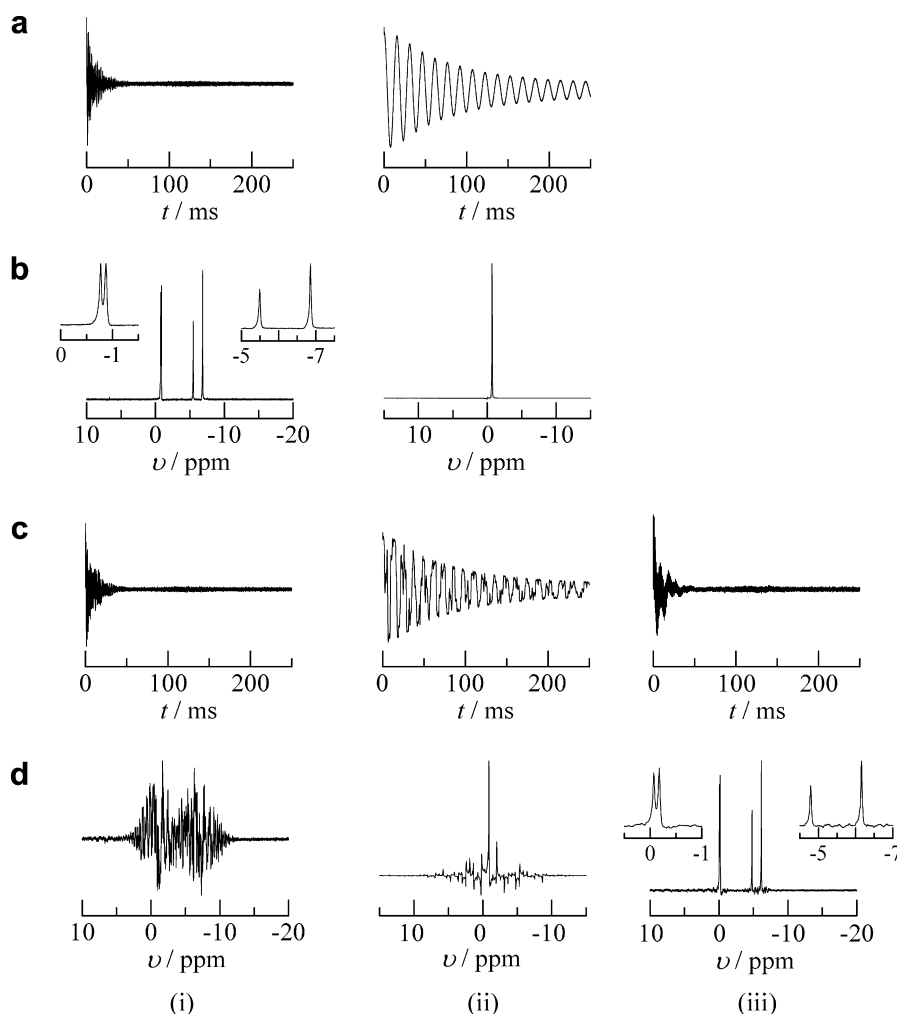


Fig. 4. Time-domain NMR signals (a, c) and corresponding FT spectra (b, d, respectively). The NMR signals in (a, b) and (c, d) were measured under static and fluctuating magnetic field, respectively; (i) and (ii) show, respectively, ^1H NMR of ethylbenzene and ^2H NMR of benzene- d_6 that were measured synchronously; (iii) shows ^1H NMR of ethylbenzene compensated by the present phase reconstruction method. Insets in (b-i) and (d-iii) are close-up of their spectra.

(Fig. 4(c-ii)) correspond to $g_I(t)$ in Eq. (2) and $g_S(t)$ in Eq. (4), respectively. The ^2H spectrum of Fig. 4(d-ii) consists of the original strong peak at ca. -0.7 ppm and many spike peaks around it with different intensity and phase. The spike peaks can be attributed to the frequency components of field fluctuation applied to the sample. The effect of field fluctuation on the ^1H NMR spectrum is large as shown in Fig. 4(d-i) and it is difficult to guess the original spectrum from this spectrum. Using simultaneously measured data of ^1H (Fig. 4(c-i)) and ^2H (Fig. 4(c-ii)) FID signals, the calculation of compensation was performed according to Eqs. (2)–(4) and (8)–(13). Fig. 4(iii) shows the result of compensation. The ^1H NMR spectrum of ethylbenzene with four peaks, that is similar to the original spectrum of Fig. 4(b-i), was obtained successfully. The peak positions before (Fig. 4(b-i)) and after (Fig. 4(d-iii)) compensation differ about 0.7 ppm. This is ascribed to the deconvolution, because the original peak of the ^2H NMR spectrum (Fig. 4(b-ii)) was ca. -0.7 ppm off the resonance (see Eq. (13)). Signal to noise ratio of the spectrum after compensa-

tion was somewhat decreased. This may be caused by invasion of noise from the ^2H signal and also that rises when the fluctuation field is generated artificially by the external coil.

Fig. 5(a) and (b) show time dependences of applied field fluctuation $f(t)$ and the S -spin phase angle $\phi(t)$ obtained from the S -spin FID signal, respectively. The reconstructed S -spin phase angle $\xi(t)$ is also shown in Fig. 5(b). Fig. 5(c)–(e) show their enlarged view. The phase angle $\phi(t)$ lies within -180° to 180° as described in the previous section. It is notable that $\phi(t)$ is a discontinuous function of time because of the limitation of $\pm 180^\circ$. After phase reconstruction, the phase angle $\xi(t)$ became continuous curve.

In Fig. 5, a gradual decrease component of $\xi(t)$ with increasing t is due to $\Delta\omega_S t$ and the residual fluctuating component is to $\gamma_S F(t)$ (see Eqs. (8)–(10)). Unfortunately, with the fluctuation field larger than that we used in this paper ($\sim \pm 0.1$ mT), the magnetic field created by the external coil interacted with the RT shim coil by mutual induction, leading to spectral broadening caused by field inhomogeneity.

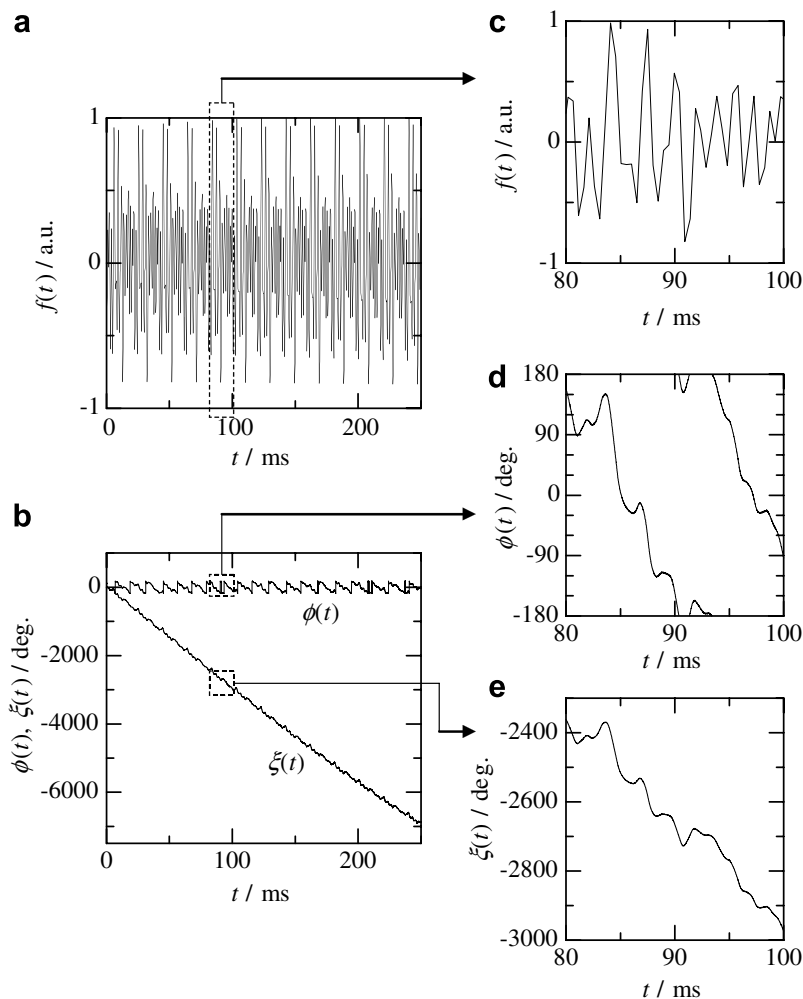


Fig. 5. Time dependence of (a) applied field fluctuation $f(t)$ and (b) phase angles, $\phi(t)$ and $\zeta(t)$. (c), (d) and (e) show, respectively, time dependence of $f(t)$, $\phi(t)$ and $\zeta(t)$ in the range of $t = 80$ – 100 ms.

Since the removal of field inhomogeneity is beyond the scope of this method, we conducted the experiment with $B_z \sim 0.1$ mT, and $\Delta\omega_{st}$ plays an important role for $\phi(t)$ to exceed $\pm 180^\circ$. However, since both of $\gamma_S F(t)$ and $\Delta\omega_{st}$ affect $\phi(t)$ equivalently and the small off-resonance arising from drift is probable in practice, we believe that our experiment is suitable for evaluating the performance of our method applied to NMR experiments using a hybrid magnet.

We performed simultaneous measurements of ^1H and ^2H NMR for four times by setting the τ_f value in Fig. 3 to be 100, 101, 102 and 103 ms. By changing τ_f , we mimicked field fluctuation with different time-dependence. Fig. 6(a) shows the ^1H NMR spectrum of ethylbenzene accumulated after compensation with phase reconstruction. Noise appearing in the single-shot compensated spectrum in Fig. 4(c-iii) almost disappeared by accumulation. Fig. 6(b) depicts the ^1H NMR spectrum of ethylbenzene compensated not by using the phase angle $\zeta(t)$ but by $\phi(t)$; that is compensation without phase reconstruction. In addition to the original proton peaks many ghost peaks emerged. Further, it was difficult to remove those ghost

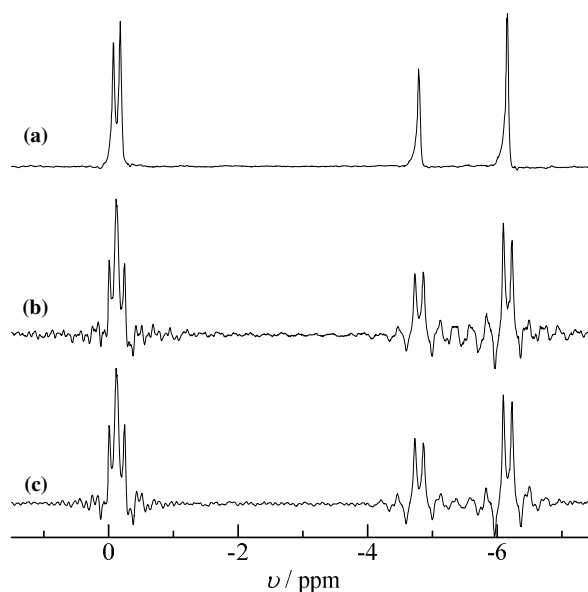


Fig. 6. ^1H NMR spectra of ethylbenzene compensated with (a) and without (b, c) phase reconstruction; (a, c) are accumulated spectra of four signals, while (b) is a single shot spectrum.

peaks by accumulation as shown in Fig. 6(c). This clearly shows that phase reconstruction is indispensable for correct compensation. Finally, it is pointed out that, in accumulation, one has to consider the relative initial phase for the *S* spin between scans. In other words, Eq. (9) should be rewritten as $\phi(t) = \tan^{-1} \text{Im}\{g_S^{\text{fr}}(t)\} / \text{Re}\{g_S^{\text{fr}}(t)\} + 360^\circ \times n$. Therefore, the deconvoluted signal should be phase corrected with the value of $360^\circ \times n \times (\gamma_I/\gamma_S)$ before accumulation. It is, however, not difficult to find a proper *n* value.

5. Conclusion

In the present work, we proposed a method for compensating effects of large field fluctuation on an NMR signal observed under an unstable magnetic field. In this method two NMR measurements, one of which is used as a reference, is performed simultaneously for deconvolution calculation. The phase angle of NMR for the reference spin is extracted and then reconstructed for proper compensation. To show the feasibility of the method we measured NMR signals under a 14.1 T static field with a probe attaching a coil to generate field fluctuation artificially. ^1H NMR of ethylbenzene was measured synchronously with reference ^2H NMR of benzene-*d*₆ under such a fluctuation field and, after compensation, the ^1H spectrum obtained under the static field was reproduced. High-resolution NMR using the present method with a hybrid or resistive magnet is in progress.

Acknowledgments

Authors thank JEOL Co. Ltd., JASTEC Co. Ltd. and Probe Laboratory Co. Ltd. in Japan for their technical supports. This work was financially supported by Special Coordination Funds for Promoting Science and Technology and by Grant-in-Aid for Scientific Research of Japan.

References

- [1] Y.Y. Lin, S. Ahn, N. Murali, W. Brey, C.R. Bowers, W.S. Warren, High-resolution >1 GHz NMR in unstable magnetic fields, *Phys. Rev. Lett.* 85 (2000) 3732.
- [2] E.E. Sigmund, V.F. Mitrovic, E.S. Calder, G.W. Thomas, H.N. Bachman, W.P. Halperin, P.L. Kuhns, A.P. Reyes, Inductive shielding of NMR phase noise, *J. Magn. Reson.* 159 (2002) 190.
- [3] P.J.M. van Bentum, J.C. Maan, J.W.M. van Os, A.P.M. Kentgens, Strategies for solid-state NMR in high-field bitter and hybrid magnets, *Chem. Phys. Lett.* 376 (2003) 338.
- [4] V. Soghomonian, M. Sabo, A. Powell, P. Murphy, R. Rosanske, T.A. Cross, H.J. Schneider-Muntau, Identification and minimization of sources of temporal instabilities in high field (>23 T) resistive magnets, *Rev. Sci. Instr.* 71 (2000) 2882.
- [5] Z. Gan, P. Gorkov, T. Cross, H.-T. Kwak, W. Brey, D. Massiot, A. Samoson, L. Butler, P. Subramanian, P. Grandinetti, Practical aspects and recent results of high resolution solid state NMR of quadrupolar nuclei using 45 T hybrid magnet, 44th Experimental NMR Conference, Savannah, GA, March 2003.
- [6] T. Iijima, K. Takegoshi, K. Hashi, T. Fujito, T. Shimizu, High-resolution NMR with resistive and hybrid magnets: Deconvolution using a field-fluctuation signal, *J. Magn. Reson.* 184 (2007) 258.
- [7] J. Haase, First ^2H NMR at 58 T, *Appl. Magn. Reson.* 27 (2004) 297.
- [8] G.A. Morris, Compensation of Instrumental imperfections by deconvolution using an internal reference signal, *J. Magn. Reson.* 80 (1988) 547.
- [9] A. Gibbs, G.A. Morris, Reference deconvolution–elimination of distortions arising from reference line truncation, *J. Magn. Reson.* 91 (1991) 77.
- [10] H. Barjat, G.A. Morris, A.G. Swanson, S. Smart, S.C.R. Williams, Reference deconvolution using multiplet reference signals, *J. Magn. Reson. A* 116 (1995) 206.
- [11] G.A. Morris, H. Barjat, T.J. Horne, Reference deconvolution methods, *Prog. Nucl. Magn. Reson. Spectr.* 31 (1997) 197.
- [12] K.R. Metz, M.M. Lam, A.G. Webb, Reference deconvolution: A simple and effective method for resolution enhancement in nuclear magnetic resonance spectroscopy, *Concept. Magn. Reson.* 12 (2000) 21.
- [13] A. Gibbs, G.A. Morris, A.G. Swanson, D. Cowburn, Suppression of t_1 noise in 2D NMR spectroscopy by reference deconvolution, *J. Magn. Reson. A* 101 (1993) 351.
- [14] T.J. Horne, G.A. Morris, Combined use of gradient-enhanced techniques and reference deconvolution for ultralow t_1 noise in 2D NMR spectroscopy, *J. Magn. Reson. A* 123 (1996) 246.
- [15] M.E. Halse, P.T. Callaghan, Imaged deconvolution: A method for extracting high-resolution NMR spectra from inhomogeneous fields, *J. Magn. Reson.* 185 (2007) 130.
- [16] P.S. Denkova, V.S. Dimitrov, Combined use of complete lineshape analysis of 1D spectra subjected to reference deconvolution and linear prediction, 2D-EXSY spectra and a double fitting method for the study of chemical exchange. Application to an eight-site exchange system, *Magn. Reson. Chem.* 37 (1999) 637.
- [17] N.G. Vassilev, V.S. Dimitrov, Dynamic NMR: combined use of 1D selective EXSY and complete lineshape analysis of spectra subjected to reference deconvolution and linear prediction or the maximum entropy method, *Magn. Reson. Chem.* 39 (2001) 607.
- [18] R. Huo, R. Wehrens, L.M.C. Buydens, Improved DOSY NMR data processing by data enhancement and combination of multivariate curve resolution with non-linear least square fitting, *J. Magn. Reson.* 169 (2004) 257.
- [19] M. Nilsson, G.A. Morris, Correction of systematic errors in CORE processing of DOSY data, *Magn. Reson. Chem.* 44 (2006) 655.
- [20] G. Mladenov, V.S. Dimitrov, Extraction of T_2 from NMR linewidths in simple spin systems by use of reference deconvolution, *Magn. Reson. Chem.* 39 (2001) 672.
- [21] T. Hou, E. MacNamara, D. Raftery, NMR analysis of multiple samples using parallel coils: improved performance using reference deconvolution and multidimensional methods, *Anal. Chim. Acta* 400 (1999) 297.
- [22] C. Massin, F. Vincent, A. Homsy, K. Ehrmann, G. Boero, P.A. Besse, A. Daridon, E. Verpoorte, N.F. de Rooij, R.S. Popovic, Planar microcoil-based microfluidic NMR probes, *J. Magn. Reson.* 164 (2003) 242.
- [23] H.T. Hu, Q.N. Van, V.A. Mandelshtam, A.J. Shaka, Reference deconvolution, phase correction, and line listing of NMR spectra by the 1D filter diagonalization method, *J. Magn. Reson.* 134 (1998) 76.
- [24] M. Goez, R. Heun, Reference deconvolution in the frequency domain, *J. Magn. Reson.* 136 (1999) 69.