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Elimination of digital and analog artefacts from time-domain signals

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ABSTRACT

A method is described for the elimination of artefacts that arise in time-domain signals because of the presence of digital and analogous filters. Such artefacts are mostly located at the beginning of the free-induction decay (FID). The procedure introduced here is particularly important if at least one signal component decays rather quickly, i.e. if there is only a small number of data containing this component (as for solid-state ^{1}H or ^{2}H FIDs). The method is able to restore the original signal by deconvolution of the spectrometer output from the transfer function of the spectrometer console. The transfer function is connected to the filter characteristics. Experimental estimation of this function is demonstrated. The estimation applies differentiation of the output signal in the case of a step-like input. This kind of input could be realized either by very slowly decaying FID or by digitizer overflow. The results are discussed with respect to the best approximation of original FID.

1. Introduction

The analysis of time-domain NMR signals of solids requires accuracy particularly for the first data points due to the short transversal relaxation. This involves, for example, the estimation of the relative contents of rigid (crystalline) and mobile components from the proton FID shape of polymers [1,2], as well as investigations of FID shape for confirmation of theoretical models [3].

Obstacles in the way of accurate data arise for two different reasons: (i) ring down of rf oscillations in the probe circuit following an rf pulse, which urges the operator to insert a delay between the end of the pulse and the start of data acquisition, and (ii) distortion of the initially sharp voltage jump in the preamplifier immediately after the receiver gate has been opened. For minimizing ring-down disturbances, the electronic optimization of the probe and appropriate experimental setup [4] enables the use of shorter pre-acquisition delays.

However, this paper deals with the second problem. An example is shown in Fig. 1. Spurious oscillations, as well as a signal shift, which do not belong to the NMR signal, are observed. The frequency spectrum of the voltage jump at the beginning of the original signal contains intense components at high frequencies which are suppressed during passing analog electronics and digital signal processing because the bandwidth of any device is finite. Moreover, filters are used to minimize noise. Thus, the artefacts are concentrated at the beginning of the signal for which FID analysis might be particularly sensitive.

This initial distortion can be reduced but not completely eliminated by choosing maximum receiver bandwidth and maximum frequency range corresponding to a minimum dwell time. However the consequence would be noise enhancement. Use of spin echo sequences (solid echo, magic sandwich echo) seems to overcome both pre-acquisition data loss and the jump-distortion problem. Conversely, echo intensity and shape depends on molecular mobility. This means that the relative amount of components with different mobility might deviate from those in the original FID. Even if calibration experiments can help, it is preferable to obtain signals which are as similar as possible to the original FID before passing the spectrometer.

If all experimental possibilities of reducing the initial distortions are exhausted and these distortions still perturb the data analysis, the question arises if there will be a possibility for numerical correction. In this paper, a procedure is given in which the initial distortions can be removed if they depend linearly on signal amplitude. This method uses deconvolution of the spectrometer output from spectrometer transfer function. Possible ways for the estimation of the transfer function are described and discussed.

The procedure introduced in the present paper is analogous to a method by which linear artefacts in the frequency domain can be removed [5,6]. However, the estimation of the transfer function is completely different in both methods. Furthermore it should be mentioned that in FT spectroscopy, initial distortions of the FID only play a minor role because they affect frequency regions close to the Nyquist frequency which are of no relevance when the sampling rate can be properly chosen.

2. Signal distortions and linear response theory

In the following analysis, the spectrometer is considered a black

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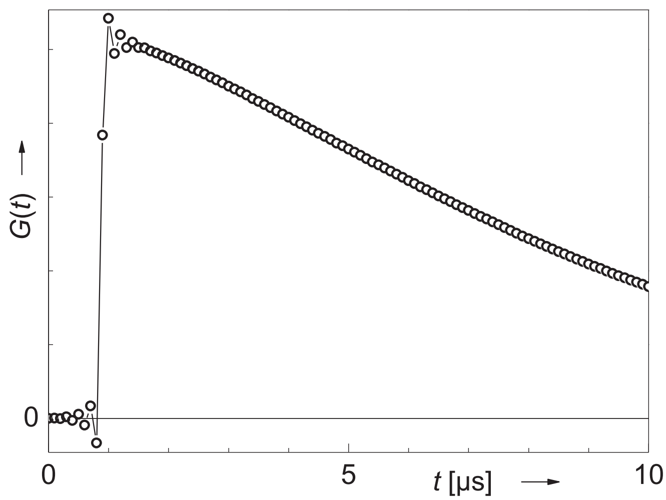

Fig. 1. Distorted spectrometer output: Proton FID of polyethylene obtained by AVANCE III (Bruker Biospin) at 200 MHz, sampling interval: 0.1 μs.

box; input $F(t)$ represents the original FID and response $G(t)$ is the spectrometer output. Using the symbol $\widehat{D}$ as the operator of signal deformation, the distortions can be classified with respect to their relationship to the strength of the input signal (besides irregular perturbations like noise):

$$F(t) \overset{\widehat{D}}{\Longrightarrow} G(t) = G_0(t) + G_l(t) + G_h(t) \tag{1}$$

- G_0 is constant, i.e., it does not depend on input (e.g., ring down of probe circuit; this is beyond the scope of this paper, as mentioned above).
- G_h describes the nonlinear component of distortion (can arise from diodes and B- or C-class amplifiers); this treatment can be described by Volterra's expansion of the distortion operator.
- G_1 contains the linear component of the distortion, which is described by a linear operator D_{lin}, i.e. for arbitrary original signals $F(t)$, $F_a(t)$ and $F_b(t)$ and an arbitrary complex λ

$$\widehat{D}_{lin}\ [F_a(t) + F_b(t)] = \widehat{D}_{lin}\ F_a(t) + \widehat{D}_{lin}\ F_b(t)\widehat{D}_{lin}\ [\lambda \cdot F(t)] = \lambda \cdot \widehat{D}_{lin}\ F(t) \tag{2}$$

must be valid.

The distortions considered here are linear, as shown below. Linear distortions can be caused by the following:

- Finite bandwidth of the probe circuit, preamplifier, and if present, analog amplifier stages.
- Digital signal processing. This procedure includes oversampling followed by decimation of the number of data points. Filtering is required to avoid mirroring of remote noise into the spectral range of interest.

For a delta-function-like input, the related response $R(t)$ is known as impulse response or transfer function:

$$\widehat{D}_{lin}\ \delta(0) \equiv R(t) \tag{3}$$

The linear deformation of all other types of input signals can be described by convolution with transfer function. This is shown by writing $F(t)$ as the weighted sum of an infinite number of delta functions, shifted in time:

$$F(t) = \int_{-\infty}^{\infty} F(t')\ \delta(t - t')\ dt' \tag{4}$$

If, and only if, the linearity relationship (Eq. (2)) is valid, then the deformation operator can be moved into the integration immediately before the delta function. Therefore, we have the following:

$$\widehat{D}_{lin}\ F(t) = \widehat{D}_{lin} \int_{-\infty}^{\infty} F(t')\ \delta(t - t')\ dt' = \int_{-\infty}^{\infty} F(t')\ \widehat{D}_{lin}\delta(t - t')\ dt'$$
$$= \int_{-\infty}^{\infty} F(t')\ R(t - t')\ dt' \quad \text{or} \quad G(t) = F(t)\ *\ R(t) \tag{5}$$

The asterisk between two functions is used as the symbol of the convolution operation.

The Heaviside step function ($H(t)$=1 for t≥0 and zero for $t<0$) is another particular input shape; the corresponding response is then defined as $G_H(t)$:

$$G_H(t) \equiv H(t)*R(t) = \int_{-\infty}^{t} R(t)\ dt \tag{6}$$

Therefore, the subsequent numerical removal of linear distortions comprises the deconvolution of the spectrometer response from the transfer function. However, before the deconvolution is executed, the transfer function has to be estimated.

3. Estimation of transfer function from filter characteristics

For studying the effect of different filters on the spectrometer output, the input is assumed to be a step-exponential function:

$$F(t) = \begin{cases} \exp(-t/T_2) & \text{if } t \geq 0 \\ 0 & \text{if } t < 0 \end{cases} \tag{7}$$

Signal distortion cannot be avoided completely for a finite bandwidth of the spectrometer passband. Consequently, the type and amount of signal deformation depends on the type and width of filters used in the device. Hence the filter choice influences the signal distortions. Then, it is possible to derive the transfer function from the transfer curve of the filters.

Filters with sharp edges (extreme case: rectangular filter, see Fig. 2B) have an advantage because the signal transduction does not depend strongly on the frequency. Conversely, this produces overshooting of the signal resulting in an oscillating behavior. Smooth filters avoid overshooting but the signal transduction varies strongly with frequency; for example see Lorentzian filter (Fig. 2A). A compromise could be a "rounded-rectangle" filter (Fig. 2C).

If the passband characteristics have the Lorentz shape, the pulse response is a step followed by exponential decay:

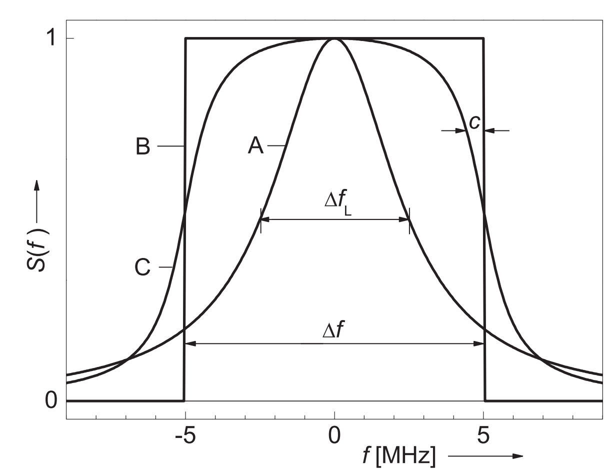

Fig. 2. Examples of passband curves: (A) Lorentzian curve, Δf_L =5 MHz; (B) rectangular passband, Δf =10 MHz; (C) rounded rectangular curve, Δf =10 MHz, rounding parameter c =0.8 MHz.