The Agilent NMR System

DirectDigital Receiver

Technical Overview

Advantage Statement

The DirectDigital Receiver in Agilent NMR (and MRI) systems delivers greater accuracy and better signal-to-noise with demanding samples.

High Fidelity FID

In an ideal NMR experiment, the sample would be excited with an infinitely short RF pulse and the spectrometer would begin receiving accurate NMR signal immediately thereafter. Since, in this ideal case, the first data point would be captured at the exact time NMR precession starts, the resultant data set would have no frequency dependent phase shift across the spectra. Furthermore, because the amplitude of the first and subsequent data points would be accurately recorded, the resultant spectra after a Fourier Transform would have a flat baseline with accurate line shapes and integrals.

The reality is different. Pulses are not infinitely short and we need to gate the receiver to protect it from being overdriven by the large RF pulse used for excitation, and for some time thereafter for the voltages associated with that pulse to decay. Some information is inevitably lost before we can open the receiver gate and start to gather information on the NMR response.

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Unfortunately, the first part of the NMR response we do collect can also be distorted by charge-up characteristics of the analog or digital filters used in the signal path. Traditional digital filters that multiply the first point of the incoming FID by zero are particularly pernicious in this respect, as they produce FIDs with significant distortions, that is, the FID starts at zero, not at its full undistorted intensity. The large group delay associated with traditional digital filters also greatly complicates data processing. It is equivalent to many (60 or more) times 360 degrees of phase shift across the resultant spectra.

Agilent's DirectDigital Receiver solves these problems by using exceptionally high sampling rates (80 MHz), to capture the early NMR responses accurately, coupled with Time Corrected Digital Filters that not only eliminate the large group delay inherent in traditional digital filters, but also correct for precession during the finite RF pulse and necessary receiver gating periods. FIDs from the Agilent NMR system achieve an unprecedented level of accuracy and produce spectra with flat baselines, accurate line shapes, and no frequency dependent phase shift using only a simple Fourier Transform for data processing, exactly as theory would predict for an FID that has been acquired without distortion.

Increased Dynamic Range and Signal-to-Noise

If we think back to the concept of our ideal NMR experiment, we would digitally sample the NMR signal as close to the receiver coil as possible with minimal electronics in the signal path to add noise and distortion.

In practice, however, because NMR signals resonate at frequencies of hundreds of MHz, and only create an analog signal in the receiver coil at microvolt levels, some electronics are necessary to both lower the frequency and amplify the voltage of the signals to the point where they can be captured by an ADC. Keep in mind that the signal coming from the receiver coil in the probe is a simple voltage versus time, that is, the fid is real, not complex or in quadrature, and has full signal-to-noise.

For many years however, NMR spectrometers have relied on super-heterodyne techniques to lower the frequency of the NMR signal so that the center of the spectrum, the carrier, was converted to base band or DC (0 Hz). That was done so the ADCs available at that time could conveniently digitize the incoming data. With a base band receiver, quadrature phase detection (two reference signals and two ADCs) was used in order to reconstruct which signals (and noise) were above and below the carrier in the original signal at the probe. The use of quadrature phase detection thus regained the root two signal-to-noise lost during the down conversion process. It also allowed the transmitter to be conveniently placed in the center of the spectrum. (Simply using two ADCs to sample the same data would accomplish nothing.) While quadrature phase detection, its associated artifacts, and dual ADCs were once a necessary evil, today there is a much better way to design a receiver that preserves full signal-to-noise, and over a much wider range of samples.

The Agilent DirectDigital Receiver features Direct Detection, achieved by sampling or digitizing the NMR response directly at the 20 MHz IF frequency with a single 80 MHz ADC. This eliminates several analog mixing and amplification stages associated with traditional base band receivers and quadrature phase detection. With the DirectDigital receiver, the need for quadrature detection and its associated artifacts is eliminated.

By capturing the NMR signal closer to the source, one not only gets a more accurate signal, but also a signal with less noise from analog receiver stages. To understand the advantages of this design, consider two systems equipped with identical probes. The first uses a traditional base band quadrature receiver with two ADCs and the other a new DirectDigital receiver. Under conditions typically used to measure signal-to-noise, for example, high receiver gain, signal-to-noise is entirely determined by the probe and the preamp. Hence the two systems we are considering would give identical results with the Ethyl Benzene signal-to-noise sample.

With a high dynamic range sample, however, such as the gasoline sample shown in Figure 1, we start to see some real differences in performance between the two systems. The higher dynamic range sample requires a lower gain setting to accommodate the larger signals associated with it. At these lower spectrometer gain settings, noise from the probe and preamp are no longer the dominate noise sources. Now the fewer analog stages (and especially analog mixing stages) involved in the DirectDigital Receiver show a real advantage. Fewer analog stages mean fewer analog noise sources. (Many spectroscopists may associate dynamic range with ADC resolution, and quantization error, but given the massive oversampling rates available with today's very high-speed ADCs, quantization error can be reduced to the point where analog noise sources determine signal-to-noise even at low spectrometer gain settings.)

The improvement in signal-to-noise and baseline performance with DirectDigital detection is clearly evident in the gasoline sample spectra shown in Figure 1.

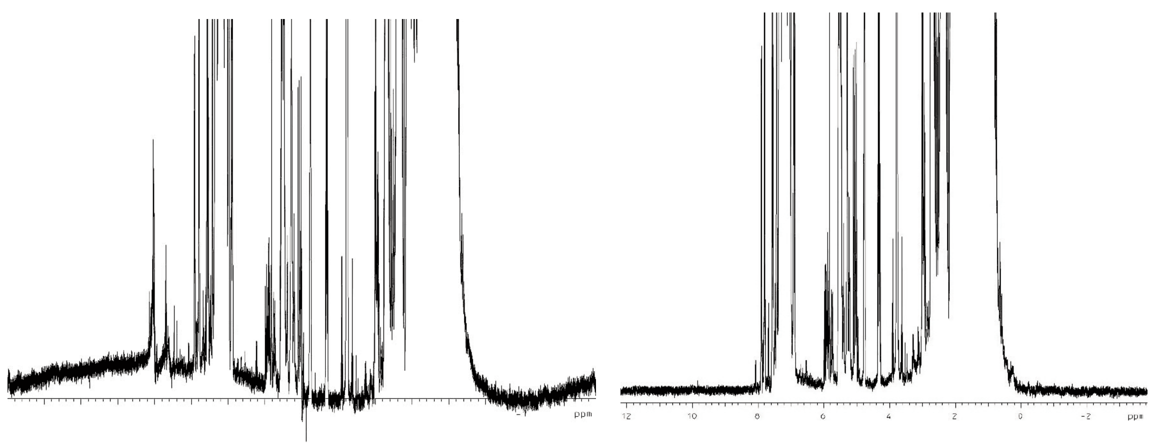

Figure 1. Comparison of spectra of a 30% gasoline sample in CDCl3 acquired at 500 MHz on an Agilent NMR System (right) and a similar system with a traditional quadrature-based base band receiver.

Greater accuracy, simpler data processing and better signal-to-noise come from doing things right in the NMR detection pathway. Direct Detection, 80 MHz sampling and patented Time-Corrected Digital Filters are all features unique to the Agilent NMR (and MRI) systems.

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