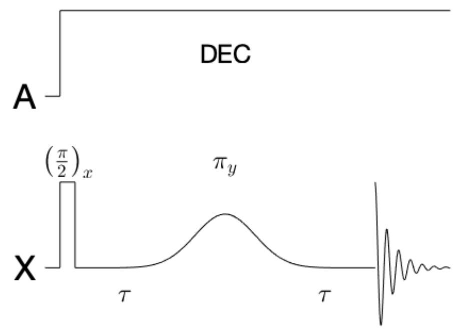
October 2021 NMR Topic of the Month: Pulse Sequence Diagrams



What is a pulse sequence diagram?

A pulse sequence diagram is a cartoon plot of the spectroscopically important elements of a pulse sequence versus time. The diagram provides a graphical view of the experiment, which facilitates expressing the elements of an experiment in a platform-independent way. There is rarely any attempt to keep the diagram to scale, instead elements of more "interest" are given more prominence. The cartoon is separated into rows, one for each frequency of interest.

Pulses are shown as idealized shapes for the pulse (the gaussian shape and small rectangle above) being used and may have a flip angle (the π and $\pi/2$ above) and sometimes phase (the x and y above) indicated. Blocks of sequence for which the exact rf (radiofrequency) profile and timing are less important but accomplish a goal are often shown as large, labeled boxes (the DEC, for decoupling, above). The squiggle is a representation of a FID (Free Induction Decay), and indicates which frequency is being detected and where.

The taus (τ) below the diagram indicate timing, here indicating that there is an equal amount of time before and after the π pulse. Often dashed lines are dropped through the diagram to show where the timing of important elements match up and/or repeated elements in the sequence.

What does this sequence do?

1. It turns off the coupling between the A spins and the X spins.
   Decoupling is the application of rf for specifically this purpose. In this sequence the decoupling during the echo and acquisition means that the A spins will not play a (significant) role in the result.
2. It refocuses some of the X spins, allowing them to be detected.
   Consider two uncoupled X spins (1 and 2) the initial product operator would be $I_{1z} + I_{2z}$, which following the $\pi/2$ pulse would be $-I_{1y} - I_{2y}$. These magnetizations then evolve under their chemical shifts for a time τ, for which product operator would be $-I_{1y}cos(\omega_1\tau) + I_{1x}sin(\omega_1\tau) - I_{2y}cos(\omega_2\tau) + I_{2x}sin(\omega_2\tau)$. Next, only the #1 X spin sees the π pulse, so the product operator is $-I_{1y}cos(\omega_1\tau) - I_{1x}sin(\omega_1\tau) - I_{2y}cos(\omega_2\tau) + I_{2x}sin(\omega_2\tau)$. The final evolution time then produces a product operator of $-I_{1y} - I_{2y}cos(2\omega_2\tau) + I_{2x}sin(2\omega_2\tau)$, so only the #1 X spin has returned to where it was just after the initial $\pi/2$ pulse.

How do I view a sequence diagram in the software?

On a Varian system: either type "dps" on the command line or click the "Sequence Diagram" button with the Acquire tab selected. On a Bruker system: click the "Graphical display of pulse program" button in the PULSEPROG tab.

References

1. Pulse Fourier transform NMR: R.R. Ernst and W.A. Anderson, *Rev. Sci. Instrum.* **37**, 93 (1966).
2. Gaussian pulses in high-resolution NMR: C. Bauer, R. Freeman, T. Frenkiel, J. Keeler, and A.J. Shaka, *J. Magn. Reson.* **58**, 442 (1984).
3. Spin echo: E.L. Hahn, *Phys. Rev.* **80**, 580 (1950).