2. Essential Theory for NMR Probe S/N Optimization. The basis of S/N optimization has been well understood and presented in numerous articles for more than 35 years. The primary objective is maximizing $B_1/P^{1/2}$, where is P is the rf input power at the matched port and B_1 is the average magnitude of the transverse component of the right-circulating component of the rf magnetic field generated (by input power P) within the sample. For example, for the transverse solenoid with the sample confined to the homogeneous region (about 80% of the overall length), $B_1 = B/2$, where B is the average value of the peak rf field generated by the solenoid within the sample.

Other (normally secondary) objectives often include:

1. ability to generate intense B_1 at voltages that do not lead to arcing,
2. ability to tune and match (so as to maximize $B_1/P^{1/2}$) for a wide range of conditions (samples and temperatures),
3. ability to tune and match to several frequencies simultaneously and/or sequentially,
4. use of sample coils that do not perturb the B_0 homogeneity and achieve high B_1 homogeneity though out the sample, and
5. compatibility with various space and sample handling constraints.

Excellent summaries of the essentials of NMR probe design can be found in the following:

1. FD Doty, "Probe Design and Construction," Electronic Encycl. of NMR, Wiley, 2007.
2. The ARRL Handbook.
3. FD Doty, G Entzminger, J Kulkarni, K Pamarthy, JP Staab, “RF Coil Technology for Small-Animal MRI”, NMR in Biomedicine, 20(3):304-325, 2007.
4. FD Doty, G Entzminger, and A Yang, "Magnetism in HR NMR Probe Design – Part I: General Methods," Concepts in MR, (4), Vol 10(3), 133-156, 1998.
5. PL Gorkov, EY Chekmenev, C Li, M Cotton, JJ Buffy, NJ Traaseth, G Veglia, WW Brey, “Using low-E resonators to reduce RF heating in biological samples for static solid-state NMR up to 900 MHz”, J Magn. Reson., 185:77-93, 2007.
6. PL Gorkov, WW Brey, and JR Long, “Probe Development for Biosolids NMR Spectroscopy” in Solid-State NMR Studies of Biopolymers, ed. A. E. McDermott and T. Polenova, Encycl. of Magn. Reson., John Wiley & Sons Ltd, Chichester, UK, 2010, p. 141.
7. FD Doty, "The Doty NMR S/N Applet…" Available at the Dotynmr website.

Most of the concepts and equations in these papers can be found in standard texts, but a few important equations are less commonly seen in other articles on this subject, or have sometimes been presented incorrectly, and are key to numerical optimization. They are reviewed here.

As noted above, the primary objective is to be able to calculate B_1 for a known input power. When the wavelength is large compared to the sample dimensions (the usually case in NMR), it can be shown that the mean B_1 [T] throughout the homogeneous region is given precisely by the following, which also serves to define β, a dimensionless magnetic effectiveness determined solely by the coil geometry.

$$B_1 = 0.0001\beta\sqrt{\frac{\eta_E P Q_{0L}}{f_M V_C}} \qquad [B_1 \text{ in T, from mixed units}] \qquad (2.1)$$

where η_E is the rf efficiency (fraction of power dissipated in the sample coil), the frequency f_M here is in MHz, Q_{0L} is the Q of the sample coil at f_M, and the coil's inner volume V_C is in mL. Note that the above has sometimes been presented with different definitions of η_E and Q, but the above is correct, and it is the most convenient method of calculating B_1 using standard linear circuit simulators. The various separate losses (sample, capacitors, leads, other coils, etc.) do not appear in equation (2). They are all fully accounted for in a proper calculation of the rf efficiency, which is easily done with modern circuit simulators.

Also note that magnetic filling factor does not appear in equation (1). There are alternative methods of calculating B_1 which utilize filling factor, but the above expression seems to be the best for linear circuit simulators. (We expect to present a method better suited to 3D EM simulators in a later chapter.)

It is important to keep the various Q definitions straight. Unfortunately, in most standard software, the Q of a coil (defined as R_P/X_L, where R_p is its effective parallel resistance and X_L is its reactance at f_M.) is usually denoted Q_L. Exactly the same symbol, Q_L, is also always used to denote the matched Q at a port, defined as f_0 / f_{3dB}. These two Q's are not at all the same. The first of these is typically two to three times the second, depending on many circuit details. To avoid confusion, we will use Q_{0L} for the Q of coils.

While many papers and presentations over the years may have given the impression that circuit efficiencies are generally close to unity and the main problem is maximizing Q_{0L} and β, our experience shows a different picture. The solenoid's Q_{0L} is well predicted by the following for typical NMR sample coils at RT using round Cu wire, with wire spacing similar to the wire radius:

$$Q_{0L} = \frac{7.2\, d\, l \sqrt{f_M}}{l + 0.35\, d} \qquad (2.2)$$

where d [mm] is the inside diameter of the coil and l [mm] is its overall length.

Typical values of β (where the external shield is not close) are as follows:

for the transverse solenoid with $l=d$, β~2.4;
for the transverse solenoid with $l=d/2$, β~1.5;
for a saddle coil, beta ranges from 0.9 to 1.5, depending mostly on surface coverage;
for the outer ^{1}H "DE" resonator used on many Doty MAS probes, β~1.25;
for a solenoid at the magic angle, beta is reduced by 16%.

On the other hand, with mid-sized multi-nuclear multi-tuned circuits at high fields, values of η_E are usually in the range of 0.2-0.5, and analysis of some published circuits suggests η_E was probably below 0.1 at one or more of their port frequencies. (We'll often express the efficiency as percent, but we'll append the percent sign when doing so to prevent confusion.)

Getting an accurate value for η_E from the equations attached to the schematic of a simulator also requires an accurate value for the inductance of the sample coil – with zero lead inductance. That means the lead inductance – no matter how small – must be subtracted from the measured value of the coil. Often a calculation of the coil's inductance will be more accurate than a measured value.

Many different expressions for the inductance of a solenoid have been published over the years. We are currently using the following (inputs in mm, result in nH), which fits well for coils using round wire where the surface coverage is ~0.7:

$$L = \frac{4n^2\, r_e^2\, k_{sh}}{l + 0.7 r_e} \qquad \text{[nH]} \qquad (2.3)$$

In the above, r_e [mm] is an effective radius, and k_{sh} corrects for the effect of nearby shields, as follows:

$$r_e = r_i + d_w / 10 \qquad \text{[mm]} \qquad (2.4)$$

$$k_{sh} = 1 - \frac{1}{(k_{rs} + 1.3)^2} \qquad (2.5)$$

where r_i [mm] is the inside radius of the solenoid, d_w [mm] is the wire diameter, and k_{rs} is the ratio of the shield radius to the coil radius.

Finally, for the benefit of those new to NMR, we include here a few more basic equations.

The precession frequency f_{rk} in the rotating frame in kHz is

$$f_{rk} = 1000\, \gamma'\, B_1 \qquad \text{[kHz]} \qquad (2.6)$$

where γ is the magnetogyric ratio in MHz/T (e.g., 42.5 for ^{1}H, 10.71 for ^{13}C, 4.314 for ^{15}N, …). The $\pi/2$ pulse length, pw90 or τ_{90}, in μs is given by

$$\tau_{90} = 250 / f_{rk} \qquad [\mu\text{s}] \qquad (2.7)$$

As noted at the beginning of this section, the primary objective of the circuit optimization will usually be maximizing $B_1/ P^{1/2}$, or equivalently, minimizing the product $\tau_{90}\, P^{1/2}$.