ELECTROMAGNETIC SIMULATION AND COMPARISON OF NMR COIL/CAPACITOR DESIGNS TO LESSEN RF HEATING THROUGH MINIMIZATION OF E/B RATIOS

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Solid state NMR is developing into a powerful technique to determine the structure of membrane proteins in a near-native environment. However, the high intensity RF electromagnetic (EM) fields required for PISEMA and other SSNMR techniques tend to heat the temperature sensitive protein samples, degrading the resulting spectra and even damaging the samples [1]. "Low-E" probes have been developed to reduce sample heating by employing a loop gap resonator (LGR) to reduce the energy deposited by the ^{1}H EM field [2]. To find out if it might be possible to reduce sample heating further by optimizing the design of the LGR, electromagnetic simulations were carried out. Six different low-*E* coil capacitor designs at 630 MHz were simulated to minimize the average *E*/*B* ratio over the sample volume, thus reducing RF-induced heating. The simulations were carried out with IE3D (Zeland, Inc., Fremont, CA), a method-of-moments electromagnetic simulation program. Because this program did not support detailed models of the commercial multilayer capacitors used in the actual LGR, we designed several versions of single layer parallel plate capacitors. The simulations indicated that the details of the capacitor design make a large difference in the average *E*/*B* ratio and therefore to the anticipated sample heating.

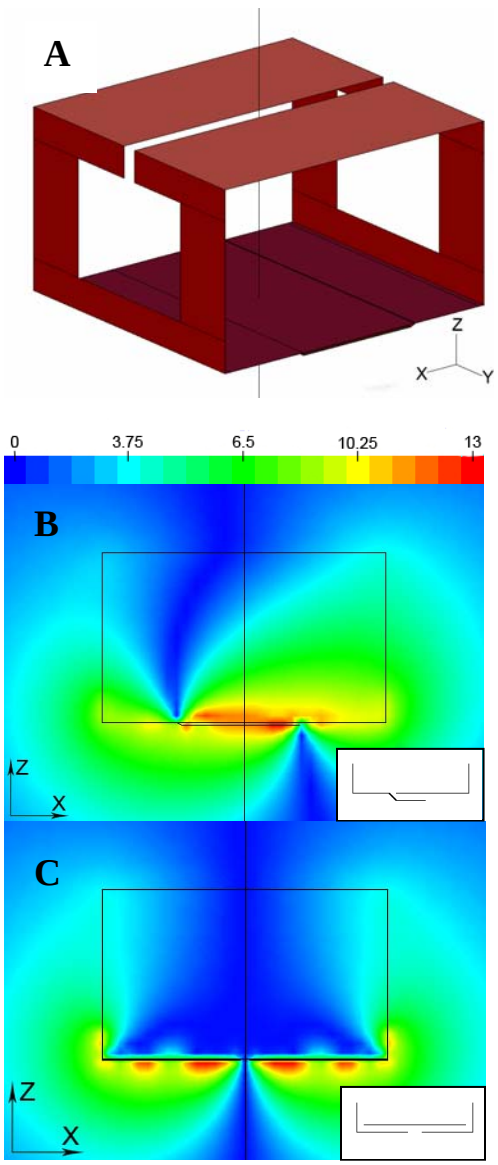


Figure 1. (A) Rendering and scalar potential plot of (B) Coil #1 and (C) Coil #2. Insets show capacitor design. Scale is in volts.

Figure 1 (A) and (B) illustrate the design and results of the first coil simulated. In operation, the LGR shown in Figure 1(A) would surround a solenoid for excitation and detection of ^{15}N or ^{31}P nuclei. The slot at the top of the LGR reduces interaction with the solenoid, and the windows in the LGR allow for sample insertion. The bottom of the structure incorporates a parallel plate capacitor. The magnitude of the scalar potential, or simply the voltage, is displayed in color plots 1 (B) and 1 (C). The electric field is simply the gradient of the scalar potential. Both LGRs are tuned to approximately 600 MHz and simulated at resonance. It's clear from Figure 1 (B) that the residual electric field in the LGR is driven by the sharp potential difference across the capacitor gap. Changes in the design of the capacitor were made to reduce the electric field while still using a parallel plate capacitor. A more satisfactory configuration is shown in Figure 1 (C), which uses effectively two gaps in series. What electric field remains is pushed to the ends of the resonator where it has little interaction with the sample. As shown in Table 1, modifying the capacitor design reduced the average *E*/*B* by a factor of two, a change that would be expected to reduce heating by a factor of four.

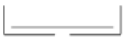
	Coil #1	 Coil #6
Avg. E (V/m)	1470	795
Avg. B(A/m)	27.3	30.2
Avg. E/B (V/A)	53.8	26.3

Table 1. Average electric and magnetic fields and E/B calculated over the sample volume for two LGR coil capacitor designs.

These simulations predict that the detailed design of the LGR can significantly affect the level of sample heating, and will form a starting point for work on an improved low-*E* resonator.

[1] Li, C. *et al.*, J. Magn. Reson., **180**, 51-57 (2006).
[2] Gor'kov, P.L. *et al.*, J. Magn. Reson. **in press**.

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