DOTY SCIENTIFIC

# The Resonator

NMR - MRI Newsletter

Winter 2015

## IN THIS ISSUE:



## UPCOMING CONFERENCES

TUE 15 DEC 2015 - SUN 20 DEC 2015

**The 2015 International Chemical Congress of Pacific Basin Societies (PAC CHEM™)**
**Honolulu, Hawaii, USA.**
***www.pacifichem.org***

David and Judy Doty and Laura Holte will be attending. Catch David Doty's talk on Tuesday December 15th at 4:45. "Closed-Loop MAS-DNP-NMR at 30 K for Affordable Dramatic Gains in S/N"

SUN 10 APR 2016 - FRI 15 APR 2016

**57th ENC**
**Wyndham Grand Hotel,**
**Pittsburgh, Pennsylvania**
***www.enc-conference.org***

## DEAR COLLEAGUE,

In September, Doty Scientific received a Phase II SBIR grant from NIH for Development of "Closed-Loop CryoMAS-DNP-NMR at 30 K for Affordable Dramatic Gains in S/N".

We are particularly grateful for continued orders and support from the NMR community. We would like to say Thank You.

### On a personal note ...

Many of you expressed concern for us after the "1000 year flood" in Columbia, SC, when the area received 18 to 20 inches of rain in less than 3 days in early October this year. Located on small hill, Doty Scientific was spared from any flood damage. All in all, our staff was also fortunate to have experienced little damage. We are well, and we thank you for your kind words.

Laura Holte attended the Alpine Solids NMR Conference in Chamonix France, Sept. 13-17. David and Judy Doty, and Paul Ellis attended the SEMRC in Daytona Beach, Florida, Oct 9-11. Both conferences provided the productive and enjoyable opportunity to meet with friends and colleagues, and to discuss new projects. Back in Columbia, we continue to focus intense efforts testing new advances that we will have more to say about later.

David and Judy Doty

## NEW RESONATOR NEWSLETTER FEATURE

With this issue we begin a series of articles on "Guide to Simulating NMR Probe Circuits". We will strive to keep the perfect balance between in-depth, tutorial, and detailed. We plan to present many state-of-the-art circuits of interest to researchers in liquids and solids NMR and MRI over the next several years. This series, which will include circuit simulation files ready to run *(if you have a Genesys license)*, will be fully available on our website, and a brief summary of each article will be included in the newsletter.

### With this inaugural issue:

1. Introduction - Guide to Simulating NMR Probe Circuits

2. Essential Theory for NMR Probe S/N Optimization.

   *A few equations (for $B_1$, $\beta$, $Q_{OL}$, L, pw90...) that might not be in standard repertoires – in just 3 pages! Visit dotyscientific.com*

3. RF Efficiency Calculations.

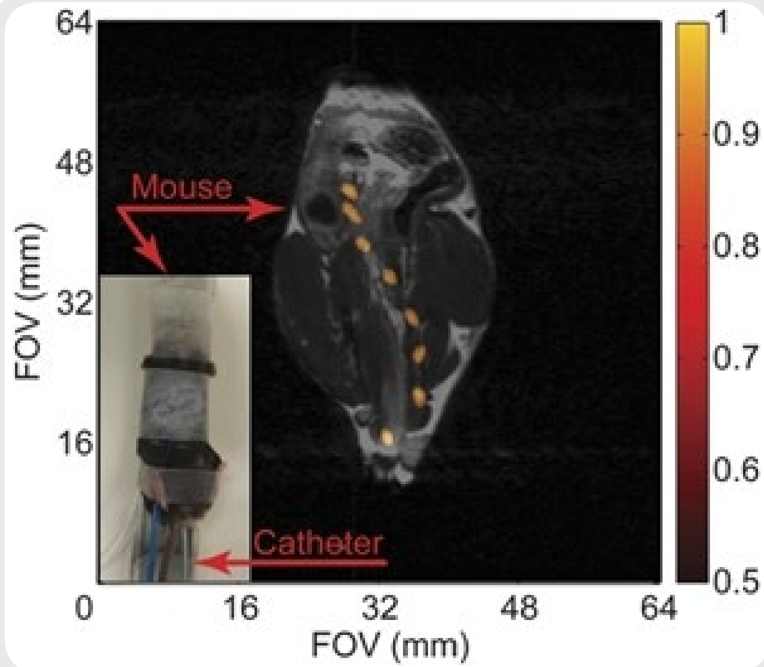
   *Basic equations and two simple single-tuned examples, one with lossless tuning components and one with real components. Circuit files: H2_130MHz_4mm_ideal.wsx; H2_130MHz_4mm.wsx. Visit dotyscientific.com*

## USER SPOTLIGHT:

### Hyperpolarized $^{29}$Si MRI at MD Anderson Cancer Center

Whiting, N. et al. Real-Time MRI-Guided Catheter Tracking Using Hyperpolarized Silicon Particles. Sci. Rep. 5, 12842; doi: 10.1038/srep12842 (2015).
*www.nature.com/articles/srep12842*

Researchers at MD Anderson Cancer Center are developing a magnetic resonance imaging-guided catheter tracking method that utilizes hyperpolarized silicon particles and a Doty dual frequency $^{1}$H/$^{29}$Si 7 T Litz volume coil for mouse. The increased signal of the silicon particles is generated via low-temperature, solid-state dynamic nuclear polarization, and the particles retain their enhanced signal for ≥40 minutes–allowing imaging experiments over extended time durations. With continued development, this method has the potential to supplement x-ray fluoroscopy and other MRI-guided catheter tracking methods as a zero-background, positive contrast agent that does not require ionizing radiation.




Figure, above:

Hyperpolarized $^{29}$Si particle MRI-tracking in vivo. Composite of $^{29}$Si images (co-registered with single 1H anatomical scan) showing transit of angiocatheter loaded with silicon particles through the large intestines of a live normal mouse (picture inset) over the course of 4 min. Absolute $^{29}$Si signal intensities are denoted in arbitrary units on the colored scale; greyscale denotes 1H intensities. It should be noted that $^{29}$Si MRI scans were completed with single scans (no averaging needed).

Special thanks to Pratip Bhattacharya, PhD, Dept. of Cancer Systems Imaging, Univ. Texas MD Anderson Cancer Center, Houston, TX.

## NIH/DOE/NSF WORKSHOP: ULTRA HIGH FIELD (UHF) NMR AND MRI

Tatyana Polenova and Thomas Budinger lead a seminal workshop in Bethesda, MD on November 12-13 to highlight the revolutionary-type progress that has been made in superconductor wire for UHF magnets over the past five years and the vital role UHF NMR can play in addressing hard-to-solve problems in all areas of science, particularly biochemistry, medicine, and catalysis.

It was an honor to be invited to participate in this "who's who" event of distinguished leaders giving exciting presentations on the fore-front of high-field NMR applications in their areas. From the presentations, it was clear that the technology (magnet wire, magnets, probes, consoles...) is ready to respond to the science drivers with NMR at 1.2 GHz in the near term and 1.8 GHz a decade from now – if the funding mechanisms can be found. One of the goals of this group is to put together the kind of convincing case it will take to get Congress to appropriate the budget needed over the coming decade to allow UHF NMR to provide break-through solutions for Alzheimer's disease, cancer, and other major societal health costs. This will not be easy in the current U.S. funding climate, but we are hopeful.

# GUIDE TO SIMULATING NMR PROBE CIRCUITS

**1. Introduction.** Many publications have appeared over the past four decades presenting approximate analytical solutions for many different simple NMR probe circuits. While analytical solutions of simple circuits – perhaps up to three coils, maybe a dozen capacitors, and several resistors – are clearly the place to begin, real circuits in high-field multi-nuclear probes are far more complex. They may include dozens of leads, stray capacitances, and couplings that make accurate analytical solutions impossible. Fortunately, there are several excellent numerical options for accurate solutions of real, complex NMR probe circuits. Of course, rf and microwave engineers are well versed in using these tools to solve the kinds of problems they typically encounter, but their objectives are generally rather different from those needed in NMR probe optimization. Moreover, most graduate students called upon to design a special purpose NMR probe are not electrical engineers, and there are very few good references to help them use available tools effectively to design and optimize a complex NMR rf probe circuit.

There appears to be a need within the NMR community for a tutorial-type treatment of circuit simulations using both linear circuit simulators and 3D full-wave simulators. That is the purpose of what we are beginning in the December 2015 issue of our Newsletter. Our intent is to present another chapter, usually with a circuit and solution, in each issue going forward for the next few years. We will keep a list of the topics presented in prior issues for reference, and they will be permanently available on our website, along with example simulation files, ready to run. These articles will generally not be of the style and format expected in professional journals, and they may not be like most wiki articles, summarizing material widely available in standard texts and many other on-line references. Many may be more like technical help manuals.

The first few chapters in this series are not likely to enable the novice to proceed effectively into optimization of a very complex circuit, but they will introduce the basics and show how to determine the pw90 in a simple example simulation. Subsequent issues will present additional concepts and show progressively more complex examples. Eventually we expect to have a very complete treatment of this important subject.

The software we are using for circuit simulations is Agilent-Genesys. There may be other products that are better – it just happens to be an adequate option. Two requirements that are not present in all circuit simulators are: a good graphical interface for building and modifying the schematic, and the ability to easily attach fairly complex programs to the schematic that smoothly communicate with it in both directions, as the S parameters calculated by the circuit solvers themselves are never sufficient. Thankfully, gone are the days of inputting node-list codes! All circuit simulators should give exactly the same results for the same circuit model, and all modern simulators probably have excellent graphical display capabilities for calculated results.

We've compiled a "Getting Started" guide to Genesys that is available at our website to complement the tutorials and manuals the vendor provides – and point out it's many "Gotcha's". (One of the more significant limitations of Genesys is its simple one-pass interpreter of user-written programs attached to the schematics. Another is its poor handling of error conditions – and there are others!) That guide is specifically for new users of Genesys and is completely orthogonal to this series on probe simulations, which is intended to be useful to all probe builders using any modern linear circuit simulator.

*In this issue we include only the Introduction. Please visit our website for chapters 2 and 3.*

*This series will be posted on our website and available for download, along with the Genesys circuit files presented, though a license would need to be purchased from the vendor to read or run them. The first three chapters, now available on www.dotyscientific.com:*