**NMR Notes for Future Students**

**Chapters:**

**1 – Setting up, extracting signal, and maximizing signal**

**2 – Running the LabVIEW**

**3 – Future Work**

**Chapter 1**

**Setting Up**

When connecting the main PCB to the PXI chassis, power supply, and amplifier, be sure that all cords are properly connected. After completing setup, if you do not see the pulses (near vertical lines that go to 1.3V), then cords are not properly connected. It is possible that if this happens, there is something wrong with the PCB. Only check this if you have modified the PCB in some way or exhausted all other options, but in this case, it can be helpful to resolder all components in the duplexer, being sure to not leave much extra solder paste. You can also look at the calibration on the pi filter in this case.

If the power supply doesn’t read 24V, ~1A be sure that you are on the right channel and the channel is set to be able to supply 24V, ~1A. If it is set up correctly and that is not occurring, there is a short somewhere. That can either be due to bad connection (disconnect and reconnect all wires) or a blown component on the PCB (good luck).

**Finding Signal**

Once you see the pulses, then you can start finding the signal. First, be sure that there is a sample in the magnet and that the coil is encompassing the sample – if that is not the case, you won’t see any signal. For the large magnet, start at 27.6 MHz and for the small magnet start at 24.2 MHz. You will want to check frequencies above this if it is cold and frequencies below this if it is warm. Start by going up/down by 0.01 or 0.02 MHz. As long as you are in somewhat normal temperature ranges, you should see signal by +/- 0.15 MHz from the start. If you start to see spin echoes inbetween the pulses then you can move on to maximizing signal. If you go through that range both above and below the starting point, there are some steps you can take.

First, double check that your coil is set up properly and is in the middle of the coil PCB. Check that the solder pads are not bent or twisted any way. Ensure that the coil is encompassing your sample. Ensure that your sample is in the strongest point of the magnet (usually this will be the center of the magnet, but for the large magnet this is not the case, there is a faint sharpie mark on the tray). If all else fails, you need to calibrate the impedance matching board. When doing this, it is vital to use the same cord and coil that you use for measurement (more info on this is in the HardwareX paper). If after all of these steps, you can’t find a signal, step away and do something else for a little bit – you probably did something wrong. If you are working with a new PCB, the pi-filter calibration capacitors might be wrong or you are using the wrong PCB with the wrong magnet.

**Maximizing Signal**

Maximizing signal can be pretty tough. Jake was able to achieve >400mV consistently. The hardware the group used between Jake leaving and myself arriving changed and ever since I have been here, 250mV has been considered good. I have tried to figure out what happened between his departure and my arrival that caused this dip, but to no avail. I have ruled out amplifiers, filters, general troubleshooting, and PCB components.

**Things that Mess up Signal**

If the magnet is too close to ferromagnetic objects or other magnets, it will mess with the homogeneity of the magnet and result in much less signal. Raise the magnet off the desk or put it in our makeshift Faraday cage

Try messing with the orientation of the coil slightly by pushing it up or down a little bit. It should be in-between the two solder pads on the coil PCB, but sometimes pushing it up or down can help achieve better signal

Fine-tune the Larmor frequency to find where signal is maximized

Double checking impedance matching calibration can drastically improve signal quality, this should be done once a week at least, it is a very quick process

Double checking pi filter calibration should only be done if nothing else works, but it can possibly be helpful

**Chapter 2**

**LabVIEW Code**

With LabVIEW, there are two different screens you can look at, the front panel and the block diagram. The front panel is used to monitor and adjust the way the code runs while the block diagram houses the code. It is helpful to take some time to understand what everything on the block diagram does. I won’t explain individual functions because I think that is best for you to explore. In general, the LabVIEW code does several things:

1. Creates a sine waveform, a custom pulsed waveform, and an oscilloscope instance
2. Uses the oscilloscope to collect data
3. Find peaks (spin echoes) – this process is done pretty inefficiently and goes through the dataset index by index for each spin echo to find the local maxima of a subset of indices
4. Take those peaks and place them into an array that then gets plotted on the front panel for the current scan
5. 1-4 are repeated for each scan
6. The average of the peaks are taken and stored into an array, plotted on the front panel, and saved as a csv file

**Running the LabVIEW**

In order to use LabVIEW, there are a few things you need to do:

* Be sure that the pulse file on the front panel is the one you want
* Be sure that the “Write output to file” button is on/off as needed
* Update the Larmor Frequency and the number of scans as needed

After these steps, the front panel is ready. There are also a few things you need to do on the block diagram:

* Depending on the specific iteration of the code, you may need to specify where the file is being saved

Now, the code is ready to be ran. There are a few issues that may arise. If you don’t see a nice decay curve, check to be sure you are using the pulse sequence and the LabVIEW code that you need to be using. If you change pulse sequences, you will need to change the indices of the peak-finding algorithm.

Additionally, if you run into an error of the oscilloscope not finding data, you can either go to the PXI chassis and exchange the sine waveform connections and the pulse waveform connections, or you can go into the block diagram and switch which device is connected to the sine waveform and the pulse waveform. Just swap them with each other. This may need to be repeated twice because on semi-rare occasions, it doesn’t work properly. This error is caused by the switch on the main PCB never switching due to it receiving the sine waveform rather than the pulse waveform. After fixing that, the code should run just fine

**Chapter 3**

There are several long-term goals of NMR that will need to be explored soon. In my thesis, we only looked at using copper contaminated water and utilizing an ML model on that copper data to predict the amount of copper in creeks. In reality, there will be multiple contaminants in creek water at any given time. There are a few ways this problem can be approached:

* Train the ML model on various types of contaminants. Since each contaminant will have a different magnetic moment, different amounts of different contaminants will affect the relationship between T2 time and contaminant concentration differently. Each contaminant will have a linear relationship between 1/T2, but the coefficient for that relationship will vary. Because of this, 1/T2 is a function of multiple different lines. This can be looked at with ML or mathematically. 1/T2 = mx + nz kind of equation would describe this where m and n are slopes and x and z are different contaminant concentrations
* Instead of using single exponential fitting to create a fitted T2 curve, resulting in a T2 time, look at using multiple exponential fits (sum of more than one exponential). Since we have multiple contaminants, this should able to create an exponential for each contaminant. This will allow us to distinguish contaminants.
* See how these ideas can compliment each other. We aren’t looking at different substances containing Hydrogen – we are just looking at how different paramagnetic materials can affect the NMR response of Hydrogen, it is possible that the multi-exponential fit might not be very helpful. However, even if it doesn’t provide an answer on its own, it could still provide parameters for an ML model and could be useful and combined into the first idea here.

Another long-term idea is the introduction of ligands to our system. Since we are limited to looking at Hydrogen and paramagnetic materials that affect Hydrogen compounds, there are only so many things we can measure. The idea of a ligand is to introduce a foreign compound containing Hydrogen that can be used to bond with other contaminants. This will give us a way to measure things we couldn’t measure otherwise. Additionally, these ligands are often designed to only bond for short periods of time, so they will eventually un-bond and allow us to separate out the ligand again. Implementing this in a flow-through system would be quite difficult, but it is something to consider in the future. The previous idea of distinguishing multiple contaminants is much more important than this idea, however.