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NMR Sensitivity to floor vibration

Yuval Ben-Dov^a, Roland Kappel^b, Peter Heiland^a and Srinivasan Rajan^c

^aIDE, 68 Mazzeo Drive, Randolph, MA 02368, USA

^bIntegrated Dynamics Engineering GmbH, Karl-Liebkecht Str. 30, D-65479 Raunheim,
Germany

^cNovartis Institutes for BioMedical Research, 250 Massachusetts Avenue, Building #600
Room # 6C-172, Cambridge, MA 02139, USA
roland.kappel@ideworld.com

Nuclear magnetic resonance (NMR) is widely used in the determination of molecular structures in solution. Floor vibrations interfere with the NMR measurements and are coupled with the signal of interest. To minimize the effect of floor vibrations, NMR spectrometers are typically installed on a solid floor with minimal structurally induced vibrations. However, in some cases this is not possible, and the tool is exposed to structural vibrations. We study the NMR sensitivity to floor vibrations. A Bruker 500MHz installed on IDE active isolation platform is used. By exciting the platform in a controlled manner we can measure the noise as observed in the NMR spectrum due to the platform vibrations. The sensitivity highly depends on the excitation frequency, and is not well reflected in a typical requirements specification. Revised requirements are presented for the floor vibration both for a tool installed as is, and for a tool on top of our isolation platform.

1 Introduction

Nuclear Magnetic Resonance (NMR) spectroscopy is routinely used to study chemical and biological properties of matters [1]. Floor vibrations induce noise which interfere with the signal of interest. To minimize the noise due to vibration, an NMR spectrometer is typically installed on a solid floor with minimal structural induced vibrations. However, in some case this is not a practical option, and the NMR spectrometer need to be installed on a floor that exhibits higher floor vibrations. In such a case the use of a vibration isolation system can significantly improve the SNR of the instrument.

In this paper we examine the sensitivity of an NMR spectrometer to floor vibrations. Our goal is to specify the requirements for floor vibration on a potential site, and help to determine whether an active vibration isolation system is required and sufficient. We will also compare those requirements with the instrument manufacturer's specifications.

All measurements reported in this paper are performed on a Bruker AVANCE 500MHz NMR spectrometer. The spectrometer was installed on top of Total Magnet Suspension (TMS), an active vibration isolation platform which was developed specifically for this application by Integrated Dynamics Engineering (IDE). More details about the TMS platform are given in the appendix.

2 Methods

We performed our measurements at different vibration levels. The NMR spectrometer is installed on top of an active vibration isolation platform (IDE's TMS), that can also be used to induce higher level of vibrations by injecting noise signal to the motors. There are six degrees of motion in the system, defined as X, Y, Z translations and the rotations around each axis. We studied the sensitivity to vibration in the three principal axes (X, Y and Z, where Z is defined as the vertical axis). Our measurements consist of two parts:

- NMR spectrum scans of a known standard at different vibration levels, and
- Vibration measurements to correlate with each scan.

2.1 NMR Scans

A 1% $CHCl_3$ in acetone-d6 sealed standard sample was used for all measurements. A single scan without spin-

ning the sample was performed following a 90° flip pulse, 1H NMR detection. Sampled 16k complex points, at operating frequency of 500.13 MHz. Sweep width was 1001.603 Hz and acquisition time of 16 seconds. Example of NMR scan results obtained with the active isolation system on and off are shown in figure 1, and on larger scale (excluding the center line) on figure 2.

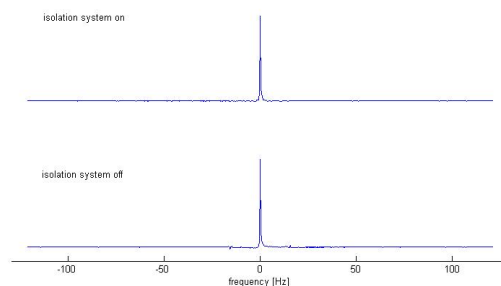


Figure 1: Example NMR scan results as measured with IDE's TMS isolation system on and off.

The satellite that are seen on either side of the main peak on figure 2 represents an actual splitting of the main signal by the naturally occurring ^{13}C in the $CHCl_3$. The value of this $^1H/^{13}C$ one bond coupling is $\sim 212Hz$. The natural abundance of ^{13}C is 1.1%. Thus, the satellite on either side represents an internal marker at 0.55% amplitude of the main signal. Based on that peak we normalized the data to obtain concentration in [%].

2.2 Vibrations Level

At each direction (X, Y & Z) NMR scans were performed with the active vibration cancellation turned off in that direction (in the TMS), and with added noise injected to the motor in the axis of interest. The data thus consists of NMR and accelerometer measurements at two different vibration levels at each axis. We also collected the same data when the vibration isolation platform is on and off in all axes, for reference.

For each scan the vibrations level on the platform was measured by a seismic accelerometer at the direction of interest. Vibration measurements were performed roughly at the same time as the NMR scans, however those measurements were not synchronized. The signal acquired is scaled to units of $[mm/sec^2]$, and power spectral density (PSD) is calculated.

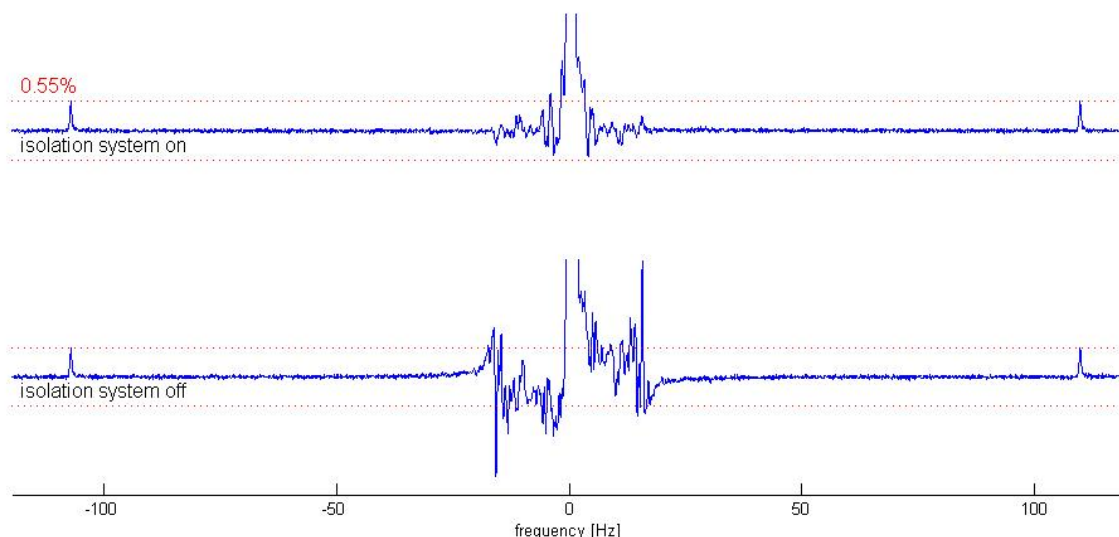


Figure 2: Example NMR scan results as measured with IDE's TMS isolation system on and off - zoom in. The dotted lines represent the marker level at $\pm 0.55\%$ for reference.

2.3 Estimate Sensitivity

The next step is to estimate the sensitivity of the NMR spectrometer to vibrations. We assume that the NMR sensitivity is linear (double the vibrations level and you get twice the noise), and is frequency dependent. Thus, at each frequency (f), the NMR noise (N_{NMR}) can be represented as $N_{NMR}(f) = \alpha(f) \cdot a(f) + \beta(f)$

where $a(f)$ is the acceleration at frequency f , $\beta(f)$ is noise at that frequency which is not due to vibrations and thus is not expected to change when we change the vibrations level. $\alpha(f)$ is the NMR sensitivity to vibrations at frequency f , and it has the unit of $[\%/(mm/sec^2)]$.

To enhance the quality of our measurement we reduced the frequency resolution to 2 Hz, allowing averaging of more data points.

Since we have measurements at two levels of vibrations at each direction we can estimate α and β for each axis. For better results, the data collected while vibration isolation platform is working was also included for all axes.

3 Results

3.1 NMR Sensitivity to Vibrations (α)

The estimated NMR sensitivities to vibrations in the three principal axes are plotted in figure 3. As shown in the figure, there are two obvious observations:

- The sensitivity strongly varies with frequency and is most significant below 10 Hz.
- The sensitivities to horizontal vibrations are about 10 times higher than the one to vertical vibrations.

The horizontal sensitivities are varying from 10 to 20 $\%/(mm/sec^2)$ at 4 Hz, to 1 $\%/(mm/sec^2)$ or less at 20Hz. The vertical sensitivity in that range varies from 1 to $< 0.1 \%$ $\%/(mm/sec^2)$. At higher frequencies both signals were very low, and the estimate is less reliable.

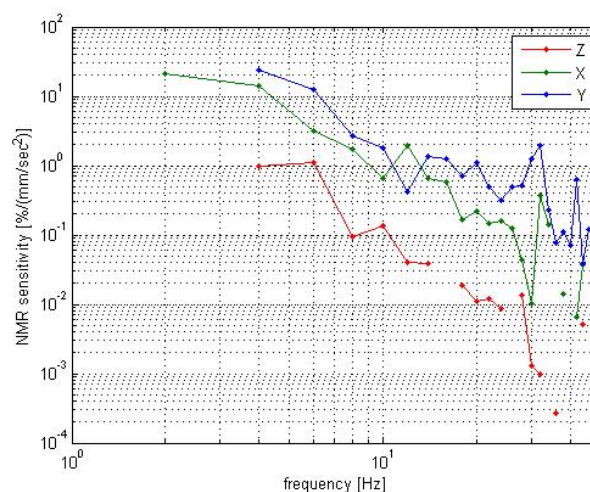


Figure 3: NMR sensitivity (α) as estimated for the three principal axes (Z is vertical)

3.2 Other NMR Noises (β)

Figure 4 shows the calculated β , which estimates the noise in the NMR scans which is not due to vibrations. Note that missing data points are due to negative calculated value, which are physically meaningless (the noises are calculated as root mean square). In this case the results are not clear, and seem to carry mostly residual noise due to vibrations. Above $\sim 20Hz$ the noises seem not to vary with frequency, and all are not significant above $\sim 10Hz$. To better estimate these noises one would need to acquire many more scans for averaging (at random order), and better synchronizing the vibration measurements with the NMR scans. However, since this was not the focus of our work we did not pursue this direction.

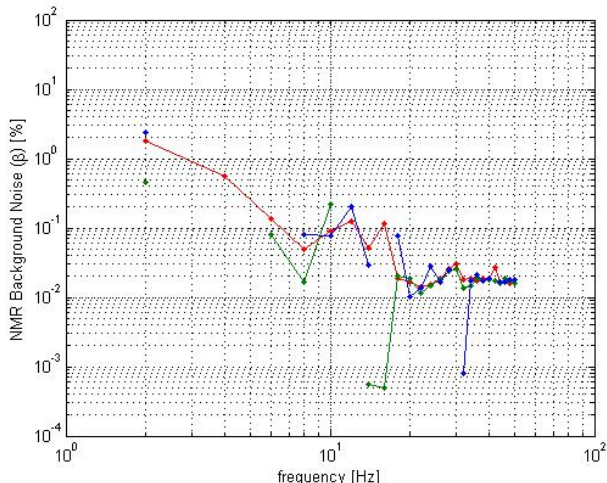


Figure 4: NMR noise which is not due to vibrations (β)

4 Conclusions

This section consists of two parts. In the first one we will discuss what is the significance of our results. In the second part we will offer an alternative set of requirements for such an NMR site based on these results.

4.1 Discussion

Our results show higher sensitivity at horizontal directions, and especially at lower frequencies. This is in contrast with the requirements specified by the NMR spectrometer manufacturer, which requires vibrations to be below a constant $< 0.1\text{mm}/\text{sec}^2$ for all frequencies and directions. Meeting this requirements does not ensure 'noise free' NMR scans - with $0.1\text{mm}/\text{sec}^2$ in all directions one would observe at 4 Hz noise level equivalent to more than 2.5% concentration, or five times the height of the satellite peak. However, the sensitivity at higher frequencies is significantly lower. This frequency dependency makes sense as the NMR spectrometer has also a passive vibration isolation, which acts as a mechanical low pass filter.

Less obvious is the higher sensitivity to horizontal vibrations. This could be a result of the mechanical structure of the spectrometer, along with a less affective passive isolation in these directions. In our study we did not measure the vibrations of the spectrometer magnet, but focused on the environmental requirement for the tool, which we treated as a black box.

Figure 5 shows an NMR scan while the vibration isolation system is working (red line), as well as an estimate of noise level that could be observed while meeting the original requirements specified by the instrument manufacturer (at blue). This plot illustrates why we think a better requirements specification is needed.

4.2 Proposed Requirements

The questions of interest when considering a site for an NMR spectrometer is: how much vibrations can we

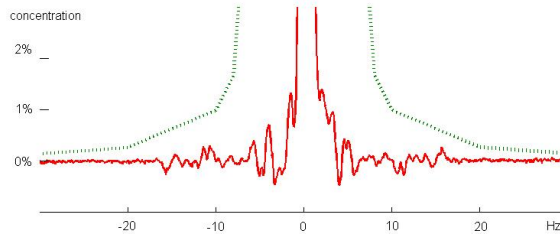


Figure 5: NMR scan while the active vibration isolation is working (in red), and an estimate to the maximum noise level that could be observed meeting the original requirement (vibrations below $0.1\text{mm}/\text{sec}^2$).

allow?

To answer this question we have to assume what noise level is acceptable, which highly depends on the application. For our calculations we will assume that noise level equivalent to concentration of 0.2% is acceptable. This number is somewhat arbitrary, and if lower (or higher) noise level is required the requirements need to be adjusted accordingly. NMR spectrometer settings can also affect the SNR, for example by adjusting the acquisition time, windowing function, and of course multiple-scan averaging.

Figures 6 and 7 present the maximum allowed floor vibrations in the vertical and horizontal directions based on our study. They also show the maximum tolerated vibrations when the NMR spectrometer is installed on our active isolated system, to help determine its benefit.

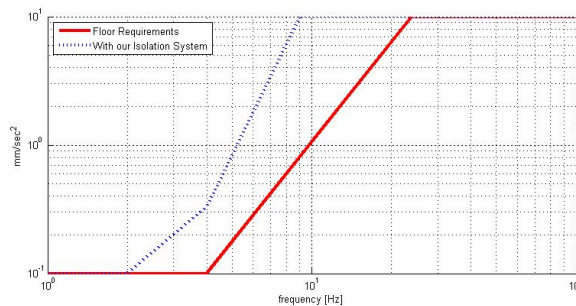


Figure 6: Proposed requirements for maximum floor vibrations in the vertical direction

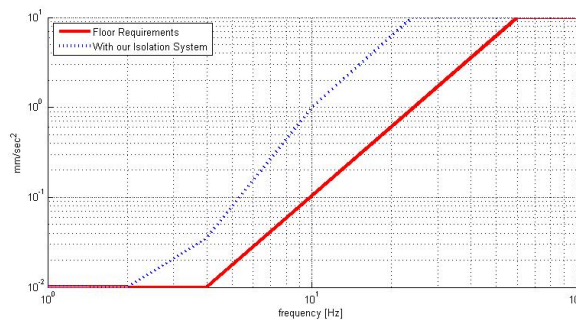


Figure 7: Proposed requirements for maximum floor vibrations in the horizontal directions

Appendix: TMS Vibration Isolation

All the tests described in this paper were performed with an NMR spectrometer installed on IDE's Total Magnet Suspension (TMS) isolation platform (see figure 9). For reference, figure 8 show the absolute vibration levels that were measured on the floor along with those measured on the TMS platform, in vertical and horizontal directions.

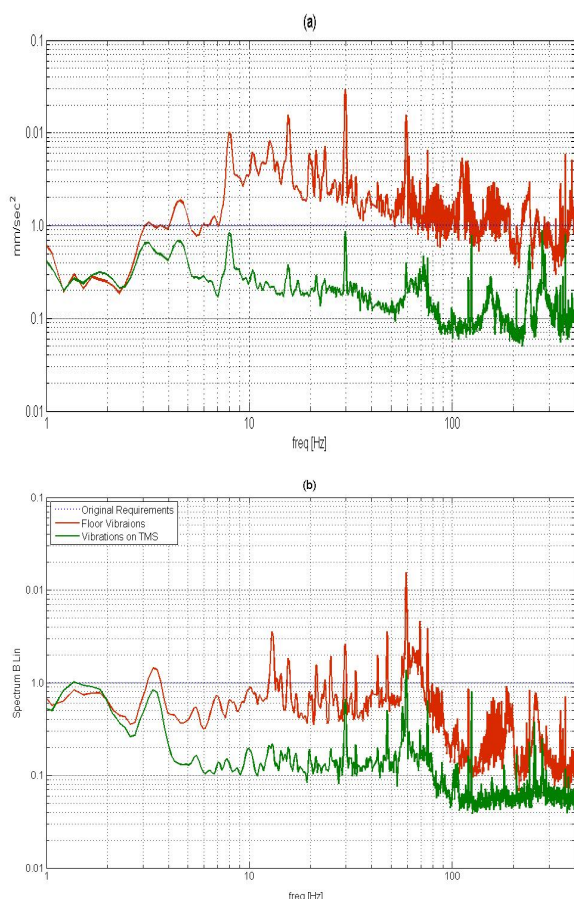


Figure 8: Absolute vibrations level on the floor and on top of the TMS platform, in vertical direction (a), and horizontal direction (b). The dotted line represent the original floor vibration requirement of $0.1\text{mm}/\text{sec}^2$. As shown, the TMS isolates floor vibrations from $\sim 2\text{HZ}$.

The TMS is based on patented technology [2]. It was developed by Integrated Dynamics Engineering to operate at strong magnetic fields, up to 5T. To minimize interference with the isolated instrument it utilizes an ultra-low ferridic materials and non-magnetic actuators and sensors, and generates zero magnetic stray field when operating. Its design utilizes a hybrid approach using inherently stiff passive isolators and a servo mechanism to minimize payload vibration. This particular feature allows for the mounting and suspension of payloads with high center of gravity locations, such as the NMR spectrometer.

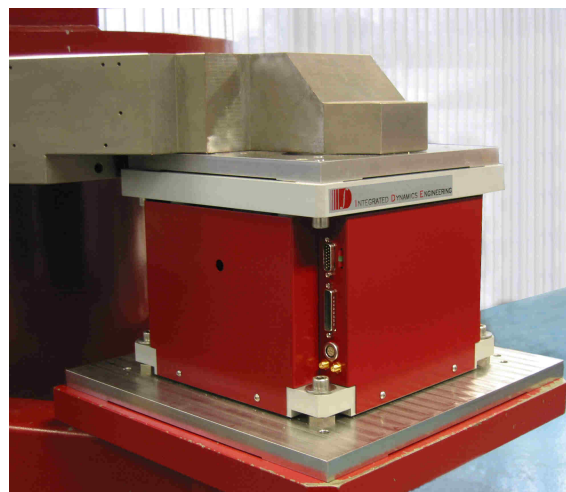


Figure 9: TMS isolator. Each isolator has actuators and sensors for vertical and horizontal directions. The platform used for the tests described in this paper consists of three isolator to provide 6 degrees of freedom (X, Y, Z and the three rotational axes).

References

- [1] J. Keller, "Understanding NMR Spectroscopy", *WILEY Publications*, (2005)
- [2] P Heiland, Apparatus and Method for Vibration-Isolating Bearing of Loads, US Patent No. 0067 583 12 (2004), Europe Patent No 001 253 346 (2001).