

good.

8.5/10

Pre-lab- Experiment 1: Fourier Transform Analysis of Oscillating Chemical Reactions

Introduction: The Fourier Transform (FT) is an operation that can convert a function in terms of time to one in terms of frequency. This is done by taking the integral of the product of the function and a complex exponential. The most significant application of the Fourier Transform is in NMR and IR spectroscopy. Instead of having to scan for intensity over all frequencies, one can simply scan the object at a certain wavelength and record the intensity over time. This plot can be converted to intensity over a frequency range by FT.

In the BZ reaction, the Fourier Transform takes the plot of absorbency vs. time and converts it to absorbency vs. frequency. This data can be truncated by adjusting the frequency range, then inverse transformed back into absorbency vs. time. This results in a much clearer periodic function from which the period of oscillation can be more clearly observed. The BZ reaction concerns the bromination of malonic acid, during which Ce(III) is oxidized into Ce(IV). This oxidation-reduction couple allows the oscillation of the reaction, for Ce(IV) oxidizes $\text{BrCH}(\text{CO}_2\text{H})_2$, creating Ce(III) and reversing the reaction. A ferroin indicator added to the solution is blue in an oxidizing solution and red in a reducing solution (with respect to Ce(III) and Ce(IV)). A radiometer measures absorbency of the light source through the solution, creating an intensity plot reflective of what color the solution is. One complete cycle of the color change is the period of the reaction.

Experimental: The reaction mixture contains malonic acid, potassium bromate ceric ammonium nitrate, and the ferroin indicator. Since the reaction initiates with H^+ ions, concentrated sulfuric acid is added to beaker. At this point, data points of the absorbency are taken. The light source is a He-Ne laser at 632.8nm. This output is more strongly absorbed by the blue (oxidizing) solution, meaning the peaks of the absorbency plot correspond to lower absorbency of the solution, which occurs during the reduction of Ce(IV). The reaction mixture is stirred throughout the experiment because the oscillating reaction can also oscillate spatially, not just temporally. This means the reaction will become polar, with oxidization of Ce(III) in one area and the reduction in the opposing area. This will disrupt the absorbency readings, so the reaction must be kept homogeneous.

Once the data is collected, it is put through an FFT program to create the frequency plot. The data is truncated to eliminate the interference create by adverse reflections of the light beam. The frequency spectrum should reveal periodic characteristics at low frequency, having random peaks at much higher frequencies. These peaks are ignored and the overall intensity is reduced to account for stochastic processes (creation of CO_2 bubbles). This data is inverted back to data in the time domain, creating a clearer plot without as much noise.

Error Analysis: The data obtained relies on the absorption of light by the radiometer. The beam, however, is subject to interruptions by reflective or absorptive

good. but show reaction next? times quantities.

how many data points? what time interval?

What will you determine from these plots?

What will you do to prevent these errors? i.e., will you take several measurements with slightly changed conditions, and then choose best? Also, outside light sources, too much, or too little steering?

properties of molecules other than the ferroin indicator. The carbon dioxide created is released as a gas, creating bubbles in the solution. These cause random peaks and valleys because they affect the strength of the beam. Another factor affecting the absorption could be reflective properties of the glass surface of the beaker.

The uncertainty in the measurements arise in taking so many data points within a short period of time. The program most likely has an uncertainty in the ms or tenth of a ms, resulting in about 0.1-1% uncertainty. Once the data is truncated, the intensity error is reduced significantly; however, the time error still remains. When determining the reaction period, the interval will have an error corresponding to the error in each time value.

$$h(t) = A \quad |t| < T_0$$

$$h(t) = 0 \quad |t| > T_0$$

Will you calculate an average for your result, or just report one value? also, mention calculation standard deviation for values where it is appropriate.

$$A e^{-i2\pi f t} \quad \int_{-T_0}^{T_0} A \cos 2\pi f t dt \quad \int_{-T_0}^{T_0} A \sin 2\pi f t dt$$

$$= \frac{A}{2\pi f} \left[\sin 2\pi f t \right]_{-T_0}^{T_0} + i \frac{A}{2\pi f} \left[\cos 2\pi f t \right]_{-T_0}^{T_0}$$

$$\frac{A \sin 2\pi f T_0}{\pi f} \quad \checkmark$$