6/10

Experiment 1: Fourier Transform Analysis of Oscillating Chemical Reactions

Introduction

A mathematical operation used to interconvert data in the time and frequency domains, the Fourier transform is applied most widely in NMR and IR spectroscopy. Although completing essentially similar tasks, the use of an actual Fourier-transform instrument over older spectrometers, which are based on steady-state measurements, saves an appreciable amount of time.

Experiment

The Belousov-Zhabotinskii Reaction:

$$3BrO_3 + 5CH_2(CO_2H) + 3H^+ \rightarrow 3BrCH(CO_2H)_2 + 4CO_2 + 5H_2O + 2HCO_2H$$

The interesting aspect of this oscillating reaction is the ability to monitor the progress of the reaction due to a coupling of color and oxidation state changes. The addition of ferroin indicator causes the solution to alternate between red and blue instead of yellow and clear. A specific wavelength of light is used to detect/record changes in color. This data is later "transformed" to obtain the reaction period from oscillation time via conversion of time domain data to frequency domain data by Fourier method.

Experimental outlined by Eastman et. al. is followed. A He-Ne laser is used as a light source, a radiometer as a detector, and a voltmeter as a digitizer. A computer will also be utilized to assist in displaying and plotting the data collected.

The following reactants are combined: 4.3g malonic acid, 1.6g potassium bromate, 0.1626g cerric ammonium nitrate, and 2mL ferroin indicator in 135mL water. The reaction is initiated by the addition of 12.5mL concentrated sulfuric acid. Stir vigorously to prevent spatial periodicity.

Indicator is blue in an oxidizing solution and red in a reducing solution. The laser

is set at 632.8nm and is more readily absorbed by the blue solution.

Following data collection, extraneous elements, such as "noise" due to scattering of light by gaseous CO_2 in solution and other previously determined stochastic processes which litter the spectrum with high-frequency components, are removed by subtracting any that fall above a decided base line noise level.

The following equations are used in calculation of inverse Fourier transformation to arrive at reaction period.

$$g(f) = c \int_{-\infty}^{+\infty} e^{-i2\pi ft} f(t)dt$$

At discrete times:

$$g(f_m) = c \_ e^{-i2\pi f_m t_n} f(t_n) = \_ e^{-i2\pi mn/N} f(t_n)$$

The data will be analyzed with the aid of a computer program.