COMPARISON OF FTIR APODIZATION FUNCTIONS USING MODELED AND MEASURED SPECTRAL DATA

Scott Egbert & Cody Carpenter

Mechanical Engineering Department
Brigham Young University
Provo, Utah 84602
scott.egbert@byu.edu
wcodycarp@byu.edu

ABSTRACT

Fourier transform infrared spectrophotometers utilize Fourier transformations to obtain high-fidelity spectral light measurements. This work highlights the mathematical background of FTIR spectroscopy, focusing on physical limitations in taking measurements using an FTIR. A modeled spectrum is generated in order to evaluate what a theoretical FTIR would measure under the given conditions. The effect of apodization functions and FTIR mirror path length are investigated. The results from the apodized models, along with measurements taken by an FTIR under similar conditions, are compared back to the original model. Boxcar apodization with the longest maximum mirror path length were shown to yield the best results.

NOMENCLATURE

ν Wavenumber (cm⁻¹)
I(δ) Interferogram
B(ν) Spectrum
A(δ) Apodization Function
δ Optical Path Distance
L Maximum Mirror Path Length

INTRODUCTION

Fourier transform infrared (FTIR) spectroscopy is a technique used to measure spectral emission in great detail. These measurements have applications in material identification, thin film analysis, and radiative property calculation. This work will focus on FTIR measurements applied to combustion systems where gas temperature and species concentration are important parameters to be measured. Unique in its application of the Fourier transform, the FTIR utilizes a device called a Michelson interferometer, shown in Figure 1, to generate the Fourier transformation of light spectrum. A beam splitter reflects half of the incident light off of a fixed mirror, and the other half off of a reciprocating mirror. The beams of light are then recombined at the beam splitter, constructively and destructively interfering as a function of the path length difference that the two beams traveled and the wavelengths that compose them.

Figure 1: Schematic diagram of a Michelson interferometer, as contained in an FTIR. Image from Fourier Transform Infrared Spectrometry by Griffiths and Haseth.

The result of this interference creates a signal at the detector called an interferogram, I(δ), which is a function of δ, the optical path difference between the moving and fixed mirror. An example of an interferogram is shown in Figure 2. Note the strong constructive peak at zero mirror path difference, where all wavelengths of light constructively interfere. The symmetry of the interferogram also creates unique opportunities in their measurement. This fact will not be discussed in depth in this
work, as focus will be placed on the mathematical foundation of their signal processing.

Examination of the interferogram alone does not yield much insight into the underlying spectra. The information contained in the interferogram is unlocked via the Fourier transform of \( I(\delta) \). As shown in Equation 1, the spectra incident on the Michelson interferometer, \( B(\nu) \), is obtained by taking the Fourier transform of the intensity measured by the detector \(^1\).

\[
B(\nu) = \int_{-\infty}^{\infty} A(\delta) I(\delta) \cos(2\pi\nu\delta) \, d\delta \quad (1)
\]

As can be seen, the theoretical integration range of the Fourier transform is from negative to positive infinity, physically corresponding to the interferometer mirror moving to an infinite path length difference. Intuitively it is not possible for the mirror to travel an infinite length, leading to a maximum mirror path length, \( L \).

When the integral is reduced to this finite range, the sharp discontinuity in the interferogram data produces undesirable ripples in the Fourier transform of the data, similar to those seen in Gibb’s phenomenon. This sharp discontinuity is known as a boxcar function, as it is mathematically the same as multiplying the interferogram data with a square wave, as shown in Equation 2.

\[
A_{\text{boxcar}}(\delta) = \begin{cases} 
1, & |\delta| \leq L \\ 
0, & |\delta| > L 
\end{cases} \quad (2)
\]

This is equivalent to convolving the measured spectra with the Fourier transform of the boxcar function \(^3\).

In order to reduce the magnitude of these ripples, the data can be multiplied by functions which smooth the transition at the limits of the mirror movement. Examples of these examined in this study are the triangular, and Happ-Genzel functions, shown in Equations 3 and 4 \(^1\).

\[
A_{\text{triangle}}(\delta) = \begin{cases} 
1 - \frac{|\delta|}{L}, & |\delta| \leq L \\ 
0, & |\delta| > L 
\end{cases} \quad (3)
\]

\[
A_{\text{Happ-Genzel}}(\delta) = \begin{cases} 
0.54 + 0.46 \cos\left(\frac{\pi|\delta|}{L}\right), & |\delta| \leq L \\ 
0, & |\delta| > L 
\end{cases} \quad (4)
\]

These three functions are known as apodization functions. Graphically, these apodization equations can be seen in Figure 3 applied for maximum symmetrical path length of 8 cm.

The improvement in reducing the ripples in the transformed data comes at the cost of shortening and broadening the transformed peaks \(^1\).

Additional details of the FTIR can be found in *Fourier Transform Infrared Spectrometry* by Griffiths and Haseth \(^1\).

**METHODS AND APPROACH**

To evaluate the effects of mirror path length limitations and apodization functions on FTIR measurements, theoretical combustion gas emissions were evaluated as though they were measured using an FTIR. The modeled spectrum used, shown in Figure 4, corresponds to a gas temperature of 1371 K, optical path length of 58 cm, total pressure of 0.844 atm, \( \text{H}_{2}O \) concentration of 16.12% and \( \text{CO}_2 \) concentration of 8.06%. Spectral gas data was obtained using a derivative of the HITEMP 2010 database \(^4\). These modeled conditions correspond to conditions measured in a 75 kW natural gas burner flow reactor \(^5\).
The Fourier transform of the spectral data file was taken per Equation 5 to obtain the theoretical interferogram corresponding to the modeled spectra\textsuperscript{1}.

\[ I(\delta) = \int_{-\infty}^{\infty} B(\nu) \cos(2\pi \nu \delta) d\nu \]  (5)

This interferogram represents what would be measured by an FTIR with an infinitely long mirror path length. To represent the limitations inherent to FTIR measurements, apodization functions were applied at maximum mirror path lengths of 4, 8, and 16 cm. The interferogram shown in Figure 2 corresponds to a boxcar apodization for a maximum path length of 8 cm. Apodization functions corresponding to a maximum mirror path length of 8 cm are shown in Figure 3.

After multiplying the interferogram by the apodizing function, the Fourier transform of the interferogram was taken to obtain the apodized gas spectrum.

Spectral emissions data was measured using a Thermo Scientific Nicolet 6700 FTIR under conditions matching those used to generate the modeled spectrum. The FTIR operated with a mirror path length of 8 cm and the measured interferogram was processed using the boxcar apodization\textsuperscript{5}. Given the limitations of the measured spectral data inherent to FTIR spectroscopy, it is assumed that modeled data best represents the spectra present under the given conditions. Therefore, both measured and apodized data will be compared to the original modeled data.

The original model and measured data were then compared to the apodized model results for the three mirror path lengths and three apodization functions.

**RESULTS**

Spectral results were grouped by maximum mirror path length. Original model and measured results are identical for all three conditions. Results for 4, 8, and 16 cm are shown in Figures 5, 6, and 7 respectively.

It can be seen that the agreement between apodized spectra and the original model improves as the maximum path length increases. This improvement corresponds to the apodized data approaching the theoretically infinite interferogram, one which contains all frequency information relevant to the spectrum. This is especially apparent when evaluating the separate modeled emission peaks shown. None of the theoretical 4 cm apodizations are able to resolve the distinct peaks. All of the 16 cm
apodizations successfully resolve both peaks. At 8 cm, the boxcar apodization is able to resolve the two peaks while the Happ-Genzel and triangle functions are not. This agrees with the theoretical assessment that the boxcar apodization function is preferable for resolving peaks.

Comparable to the decreased peak resolution, the clipping of peak height caused by the triangle, and to a lesser extent the Happ-Genzel, apodization functions can be seen in all three plots. For a given maximum mirror path length, the boxcar apodization best represents the modeled spectral peak height. As discussed previously, this comes with the tradeoff of small ripples near the troughs of the boxcar data. These ripples are much less pronounced in the Happ-Genzel and triangle apodized data.

The fidelity of the measured data best compares to the 4 and 8 cm maximum path length modeled data. This is based on the resolution of the distinct modeled peaks as well as the broadening of the spectrum. This agrees with the specifications of the FTIR as having an 8 cm mirror path length.

It was noted that the integrated intensity of the original spectra is equal to the integrated intensity of the apodized spectra (error across the entire measured spectrum less than 0.001%). This is the case for all three apodization functions. Similarly, the error in the integrated intensity between the measured and modeled spectrum is 0.66%. The decrease in peak height is balanced with peak broadening.

Due to the comparable integrated areas and general trends across all maximum mirror path lengths, the boxcar function is the recommended apodization function when using an FTIR. This is because of the improved ability of the boxcar function to resolve peaks and peak heights. For long path lengths, the selection of the apodization function becomes less important.

CONCLUSIONS

The mathematical foundations of the Fourier transform infrared spectrophotometer were discussed. Mirror path length limitations presented while taking physical measurements were explored. The Fourier transform was applied to modeled spectral data comparable to the behavior of a Michelson interferometer in an FTIR. Path length limitations were explored by applying different apodization functions and evaluating the effect on resultant spectral data.

It was found that longer maximum mirror path lengths resulted in better apodized modeled data. Of the apodization functions explored, the boxcar apodization was best able to resolve peaks, and peak heights for all maximum mirror path lengths. Boxcar apodization also produced more ripples in the spectral troughs. Happ-Genzel and triangle functions perform opposite to the boxcar, poorly resolving peaks and peak height, though ripples are significantly reduced.

The apodized modeled data represents the discrepancy between the measured and original modeled data well. It was shown that the measured data agrees best with the apodized data between 4 and 8 cm maximum path length. This is comparable to the maximum path length of the FTIR used to collect the data, which is listed as 8 cm.

It was found that the apodization of the modeled data had no effect on the integrated intensity of the spectrum. Similar agreement is also seen between the measured and modeled spectra, notwithstanding the similarly broadened peaks.

Given the similar agreement in integrated intensity for all apodization functions, ability to resolve peaks and peak heights is likely considered more important than the reduction of ripples in spectral troughs. Between the three apodization functions evaluated, the use of the boxcar apodization function is therefore recommended for general FTIR spectroscopic applications.

REFERENCES