ANALYSIS, DESIGN AND USE OF A FOURIER-TRANSFORM SPECTROMETER FOR NEAR INFRARED GLUCOSE ABSORPTION MEASUREMENT

by

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B.S., Mechanical Engineering
Carnegie Mellon University, 1997

Submitted to the Department of Mechanical Engineering in Partial Fulfillment of the Requirements for the Degree of

Master of Science in Mechanical Engineering
at the
Massachusetts Institute of Technology

September 1999

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ABSTRACT

Noninvasive blood glucose monitoring is a long pursued goal in clinical therapy as an invaluable tool that would aid in the treatment of diabetes. The importance of such device is marked by the market value of glucose testing devices, which was estimated to be more than $2.5 billion worldwide in 1997, and growing at 10-15% a year. In this project, a modular Fourier transform spectrometer for the near infrared wavelength region was designed and built. The work was motivated by the need for a versatile and dedicated instrument for research in the area of blood glucose noninvasive measurement. Selection and design of each element of the spectrometer is discussed, with the aim of optimizing the signal-to-noise ratio in the near infrared region. Careful analysis of sources of error aids greatly to comprehension of the limiting source of inaccuracy, which enables both instrumental and procedural optimization without the need for exhaustive experimentation. Currently, absorption of aqueous glucose solution at 5930 cm⁻¹ is being investigated. The ability to resolve milli-molar levels of aqueous glucose concentration is found to be greatly dependent on the instrumental as well as procedural factors such as the optical pathlength of the solutions. Two instrumental errors found to be significant are photodetector noise and digitization noise, the later being the current instrumental noise limitation for simple, glucose-water transmission study. Digitization noise comes from the quantization error due to the limited resolution of our 12-bit analog-to-digital converter. With the present arrangement, the achievable signal-to-noise ratio is 0.67 per mmol/L for 10-mm pathlengths and 0.18 per mmol/L for 2-mm pathlengths of aqueous glucose solutions. A few methods to improve the signal-to-noise ratio are discussed.

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ACKNOWLEDGEMENTS

The success of this thesis and project work was made possible by a number of individuals to whom I am deeply grateful. First, I would like to thank my advisor, Prof. Kamal Youcef-Toumi for giving me the opportunity to work in this new and exciting area. His confidence in this project and in my ability has been a significant source of my motivation. It has certainly been a wonderful working and learning experience for me.

I extend my special thanks to my parents and my sister for giving me the support of all kinds throughout my life. Without them, I simply would not be here. My girlfriend, Riny Kwek also deserves many thanks for her understanding and support.

I also thank my lab-mates at the Mechatronics Research Laboratory for creating a friendly work environment. Bernardo Aumond and Ossamah El Rifai have been especially helpful with the mechatronics-related questions I had every now and then. I also thank Dr. Colin J.H. Brenan and Prof. Ian W. Hunter at the Biomechanics Lab for their invaluable inputs on many aspects regarding the project plan and the spectrometer design. Dr. Brenan’s willingness to share his excellent knowledge on optics in general and on Fourier transform spectroscopy especially is greatly appreciated.

Above all, I thank God for making the impossible possible.
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1. INTRODUCTION

For the past several years, quantitative analysis of physiological glucose concentration in aqueous media such as water, blood serum and whole blood have been of great interests [1-22]. These works stem from the need for a “bloodless” method for frequent blood glucose measurements required by diabetic patients. The availability of such noninvasive measurement system would greatly aid in the treatment and care of diabetes.

Among several other potential methods, near-infrared absorption spectroscopic technique is chosen for our work for reasons discussed later in the chapter. Similar to any other potential method, the major difficulty in measuring clinically relevant glucose concentration using the near-infrared absorption technique is due to the extremely weak glucose absorption signal. Most of the research works in this area have been focused on complex data processing to separate the true glucose signal from the noises present in the spectra. They have been somewhat successful for controlled experiments in vitro [1-12]. However, the signal-to-noise ratio of the raw signal for the case of noninvasive use may not be high enough for any mathematical data processing method to succeed. We believe that more effort has to be put on improving the signal-to-noise ratio of the raw signal, prior to the digital data processing stage.

The signal-to-noise ratio achievable is significantly dependent on both instrumental and procedural factors. In fact, it would be shown in this thesis that the extremely weak glucose absorption signal can force the well-known high sensitivity of the currently available commercial Fourier-transform spectrometers to operate to their limitations. Thus, comprehension of the limiting instrumental source(s) of noise in glucose quantification is an important step toward realization of noninvasive blood glucose monitoring system.

The first phase of the project involves design and implementation of a modular near-infrared Fourier-transform spectrometer. The instrument provides a versatile research tool for the subsequent works in the project. Each element is designed or chosen to optimize the sensitivity for glucose absorption analysis in the near-infrared region. Identification and quantification of the significant errors are attempted, which enables
appropriate modifications to improve the signal-to-noise ratio related to glucose measurement.

Two main topics covered in this thesis:

1. Design and evaluation of a Fourier transform spectrometer for the near-infrared wavelength region.
2. Experimental sensitivity analysis of glucose absorption signals.

This chapter starts by introducing the motivation behind this project and the issues pertaining to noninvasive blood glucose monitoring. Overview of some potentially viable techniques is given, with a comparison analysis that leads to our choice of method: near infrared absorption spectroscopy.

1.1 Background and Motivation

Diabetes mellitus is a chronic metabolic disease in which there is a deficiency of, or a resistance to an effective use of insulin. This disorder, along with its associated complications, is ranked as the seventh leading cause of death in the United States in 1994 [The Public Health of Diabetes Mellitus in the United States: Surveillance Report]. In 1996, an estimated 14 million people in the United States have been diagnosed with diabetes, accounting less than 10% of the diabetes cases in the world.

Diabetes is a serious and complex disease, having the potential in affecting nearly every body organ. Some of the diabetes-induced complications include cardiovascular disease, blindness, kidney failure and lower-extremity amputations. Many of these complications can be prevented with early detection and close monitoring of blood glucose level. Studies indicate that intensive therapy or treatment to control the blood glucose concentration level would significantly prevent or delay the progression of the complications.

This creates the need for a self-testing device that could be used regularly in the patients’ homes. In the present, people with diabetes use the "finger-prick" technique to check their blood glucose levels regularly. This technique involves puncturing the tip of a
finger to obtain a drop of blood, which is then placed on a chemical-based glucose sensor. Clearly, this method is painful and inconvenient, especially for some of the diabetic patients who need to have the test done four to five times a day, which often results in patients’ reluctance to perform the necessary frequent measurements.

The aim of this project is to create the enabling technology for a continuous and noninvasive blood glucose measurement. The availability of such system would make a way for a 24-hour blood glucose monitoring device that would help achieve the ultimate goal of diabetes therapy, which is to approximate the 24-hour blood glucose profile of a normal individual.

1.2 General Aspects of Noninvasive Spectroscopic Measurements

For a non-invasive spectrometric assay, usually the skin or some other part of the body tissue is integrally probed. The metabolic information of interest is usually gained from the blood, which constitutes only a relatively small fraction of the tissue volume under investigation (figure 2-1). Several investigators have considered measuring glucose in the interstitial fluid of the subcutaneous tissue minimal-invasively, by extracting the fluid using microdialysis, suction effusion or reverse iontophoresis technique [20-22]. However, there are still some controversies regarding the relation of glucose concentration contained in the interstitial fluid and in the blood. Some groups claim that under steady state conditions, glucose concentration in the tissue is practically identical to that in the blood. However, delay of 5 to 15 minutes is observed when glucose concentration increases sharply, for instance, after meal or sugar intake. Therefore, blood may still be the best specimen for measuring glucose concentration.

As mentioned before, the signals from the blood constitutes only a small fraction of the spectrum. Furthermore, the metabolites of interest usually have low concentrations (glucose concentration in the blood is about 0.1% for normal individuals). This presents a major problem to all potential noninvasive techniques to date.
1.3 Emerging Technologies for Noninvasive Glucose Measurement

Several optical techniques for noninvasive measurement of blood or tissue glucose have been proposed. This includes near infrared absorption/diffuse reflectance, Raman scattering and polarimetry. This section gives an overview and describes the significant features of each technique.

1.3.1 Near Infrared Absorption

The underlying principle of an absorption spectroscopic technique is that when a molecule is radiated with a range frequencies (or wavelengths), it absorbs the radiation only at certain wavelengths. In the near infrared, absorption is due to the overtone and the combination vibrations of molecules. By looking at the frequency location(s) of the absorption spectrum, one can therefore deduce the molecular composition of the sample being investigated. Furthermore, its concentration can be inferred from the intensity of the absorption peak. Figure 1-1 shows a simple schematic of the absorption process. A well-known formula that imparts a linear relationship between absorbance and concentration is Beer-Lambert’s Law:

\[
A(\nu_i) = -\log_{10}\left(\frac{T_{sample}(\nu_i)}{T_{reference}(\nu_i)}\right) = \alpha dc
\]  

(1-1)

where \(T\) is the transmission spectrum, \(\alpha\) is the absorptivity, which is a property of the sample, \(l\) is the pathlength and \(c\) is the concentration. However, this relationship does not always hold. For example, when there is a substantial light scattering due to sample, the pathlength is no longer clearly defined. Furthermore, the validity of this relationship seems to depend on the level of concentration as well [23]. However, with proper calibration over the relevant concentrations, absorption method would still be a valid method.
Figure 1-1. Schematic of absorption method

Near-infrared refers to light radiation in the wavelength region between 700 to $2500\,nm$. For noninvasive applications, this wavelength range has the advantage of being able to probe more deeply into tissue compared to the other wavelengths such as the visible, the ultraviolet and the mid-infrared. At these other wavelength regions, water (the main component of blood and tissue) and other chromophores absorb too strongly, thereby not permitting much radiation to pass through.

However, besides absorption, scattering also plays an important role, especially in a turbid media such as human tissue [24]. Scattering is mainly caused by discontinuities in the refractive index of tissue on the microscopic level. Although this occurrence complicates the analysis of the absorption signal, it enables radiation to be reflected back to the surface and detected. This provides the basis of diffuse reflectance technique, where thick sample can be analyzed. This process is depicted in figure 1-2. In this technique, the specular reflection (reflection due to the surface) is omitted, since it does not provide useful information on the underlying tissue and blood.
1.3.2 Raman Scattering

Raman scattering spectroscopy has been utilized over the past thirty years mainly by physicists and chemists. The inherent difficulty of this method is that its signals are very weak, having an intensity of about $10^{-3}$ of the Rayleigh scattered light intensity. Only recently, with the replacement of slow photomultiplier tubes with faster CCD arrays and the manufacture of higher power near infrared laser diodes, has the technology become available to allow researchers to consider the possibility of tissue diagnosis and blood chemicals analysis in vivo and in real time [13-16].

The phenomenon of Raman scattering is observed when a monochromatic light is incident upon an optically transparent (negligible absorption) media. A small portion of the light is scattered inelastically, exhibiting frequency shifts, which are associated with transitions between rotational, vibrational and electronic levels [25]. For in vivo tissue studies, a laser in the near-infrared region is usually used as an excitation source to minimize fluorescence background signal. A significant advantage of Raman technique over near-infrared absorption technique is that its spectrum has distinct and pronounced peaks, easing the task of separating signals/peaks of interest from other interfering signals. The primary problem of this method, however, is the inherent weakness of Raman signal, creating the need for high excitation power and relatively long signal...
collection time in order to get an acceptably clean spectrum. Photothermal damage of the tissue is of great concern for in vivo measurements using this technique.

1.3.3 Polarimetry

The rotation of linearly polarized light by optically active substances has been used for many years to measure substance concentration in solutions [26]. The concept behind this technique is that the amount of rotation of polarized light by an optically active substance depends on the thickness of the layer traversed by the light [18].

For polarimetry to be used as a noninvasive method, the signal must be able to pass from the source, through the body, and to a detector, without total depolarization of the beam. Since the skin possesses high scattering coefficients, maintaining polarization information in a beam passing through a thick piece of tissue including skin (for eg. a finger) would not be possible. Therefore, several investigators have suggested the aqueous humor of the eye as the media for glucose measurement [17,18].

There are several problems with this approach. First, the signal size is small. The angle of rotation for a 1 mm thick tissue, which is the average width of the anterior chamber of a human eye, would be in the order of $4 \times 10^{-5}$ degree per 1 mg/dl increment in glucose concentration [18]. Second, other optically active substances contribute to the signals, increasing or decreasing the polarization angle, thus questioning the specificity. Third, there is a time lag between blood and aqueous humor glucose concentrations during periods of rapidly shifting blood glucose concentrations. Other problems include corneal rotation and eye motion artifacts, which can produce significant measurement errors.

1.4 Method Comparison

Comparison of the methods discussed above would be based on three aspects: signal-to-noise ratio, specificity and practical considerations such as instrumentation and procedural feasibility. The result is tabulated below.
<table>
<thead>
<tr>
<th></th>
<th>NIR Absorption</th>
<th>Raman</th>
<th>Polarimetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specificity</td>
<td>moderate</td>
<td>high</td>
<td>low</td>
</tr>
<tr>
<td>SNR</td>
<td>relatively high</td>
<td>low</td>
<td>low</td>
</tr>
<tr>
<td>Practicality</td>
<td>high</td>
<td>low</td>
<td>moderate</td>
</tr>
</tbody>
</table>

Table 1-1. Methods comparison

Specificity is defined as the ability to distinguish signal due to a certain substance from interference due to others. In this regard, Raman technique is superior. Its spectrum consists of sharp peaks with well-defined features. Polarimetry on the other hand, cannot distinguish glucose signal from others present in the sample. The near-infrared absorption method falls between the two in this aspect. The absorption peaks in this wavelength are usually broad and featureless, creating difficulties in separating more than one interfering signals by conventional peak-detection scheme. However, by use of multivariate technique of partial least-squares (PLS) analysis and other data processing schemes, glucose concentrations in the presence of other substances can be determined [1-12].

The signal-to-noise ratio would amount to the sensitivity achievable, and thus the success of the technique. This is discussed in greater detail on chapter 3. In this regard, the absorption method is superior to Raman technique. To get an acceptable signal-to-noise ratio, acquisition time of more than 5 minutes and with a much higher radiation power is necessary for Raman method to get a comparable accuracy of glucose determination using the absorption technique with 1-2 minutes acquisition time [14].

Instrumentation and procedural practicality needs to be taken into consideration as well. The ultimate goal of this work is to create a system that can monitor glucose level as frequent as possible, preferably continuously, 24 hours a day. In addition, cost is a significant factor. These issues create a constraint as to how complex the system can be. In addition to the spectrometer, Raman spectroscopy requires a high-power, stabilized laser source and a high-end detector, possibly nitrogen- or thermoelectrically cooled. In contrast, the near infrared absorption technique uses a tungsten-halogen lamp as its source, and may only require a stabilized detector operating at room temperature [12]. This greatly reduces both cost and system complexity.
The choice or the required sampling sites falls onto procedural practicality issue. The need for an anterior chamber of the eye as a sampling site, polarimetric technique prohibits a 24-hour, continuous monitoring. This is an important issue considering that 50% of hypoglycaemia occur during the sleep [27]. Due to these reasons, the near infrared absorption technique stands as the most appropriate technique to be considered for noninvasive blood glucose monitoring to date.
2. SPECTROMETER DESIGN AND IMPLEMENTATION

One possible means of decomposing a light into its spectrum is by use of a dispersive method. Dispersive spectrometers use gratings or prisms to disperse the light into a spectrum of its component wavelengths. A slit is then used to select which narrow "slice" of them is allowed to strike the detector. A schematic representation of a grating-based spectrometer is shown in figure 2-1.

![Schematic of a spectrometer](image)

Figure 2-1. Dispersive Spectrometer

An alternative way is by use of interferometric techniques. A schematic of a typical spectrometer utilizing a Michelson interferometer is shown in figure 2-2.
Figure 2-2. A schematic of a Michelson interferometer-based Fourier transform Spectrometer

2.1 Overview of Fourier Transform Spectrometer Design

A white light from a tungsten halogen source is collected and collimated by a concave mirror and a pair of focusing and collimating lenses, L1 and L2. A variable aperture A1 acts as a spatial filter to limit the radiation power density when needed. A variable aperture A2 is used to limit the amount of divergence of the light entering the interferometer. The interferometer is of Michelson type, comprising a beamsplitter and two perpendicular plane mirrors, M1 and M2. M1 moves linearly in the axis as indicated in the diagram, which produces a variable path difference between the two beams reflected off of the two mirrors. The recombined beam is then focused onto the sample by means of a focusing lens L3 and onto the detector with the focusing lens L5. Although not necessary, lens L4 is used to collimate the light before it reaches the detector focusing lens to ensure a sufficiently small spot (1mm diameter maximum) arriving at the detector. The detector measures the interferogram, which is stored in the computer. This signal is then Fourier-transformed to obtain the spectrum.
In a dispersive system incorporating a grating and an exit slit, only one spectral element is sampled by the detector at a time. In contrast, in Fourier transform spectroscopy, one examines all wavelengths arriving at the detector simultaneously, which results in higher throughputs, and thus potentially higher signal-to-noise ratios. Another advantage of interferometric technique is its spectral stability due to the use of a helium-neon laser for the data acquisition sampling clock (discussed in section 2.1.5). Data can be acquired at very precise path differences, even if there are some jitters in the velocity of the moving mirror. This enables accurate signal averaging, which can greatly improves the signal-to-noise ratio.

In theory, all spectrometers can show an improved signal-to-noise ratio if spectra are averaged. However, this relies on the fact that the spectra can be exactly superimposed. Any displacement error between spectra can cause band shapes to be distorted, and as a result, the signal-to-noise ratio will fail to improve. Scanning monochromators are subject to mechanical wear and jitter [38], which may cause significant displacement errors.

From the literature and the previous preliminary experiments, it has been realized that signals due to the blood glucose variations in the physiological range are weak. Furthermore, in the noninvasive application, there is further loss of signal due to scattering. As a result, realization of accurate blood glucose quantification would likely be limited by the amount of signal-to-noise ratio achievable. Due to these reasons we choose the higher throughput and the higher SNR interferometric technique.

A modular Fourier transform spectrometer for the near infrared was designed and built to provide a versatile research instrument in the area of noninvasive blood glucose measurement. Great emphasis was placed to ensure that each element (figure 2-3) was designed or chosen to provide the maximum signal-to-noise ratio for the near-infrared absorption studies. In this chapter, a systematic, step-by-step approach to the determination of all spectrometer design variables is presented. Explanations from both mathematical and physical viewpoints are given whenever possible.
2.1.1 Light Source

Spectrometer design starts from the resolution requirement and the operating wavelength range. For noninvasive blood glucose measurement, a wavelength range between 5000 to 15000 cm$^{-1}$ has been shown to be worth investigating [1-12]. In this case, the use of a simple and inexpensive tungsten-halogen lamp would be sufficient. It provides a smooth, continuous output over the range of 300 nm to 2000 nm$^1$.

The next thing to consider is the resolution required. Since the spectra in this range are broad and overlapping, a resolution of 30 cm$^{-1}$ would be sufficient. With these design requirements, we proceed to determine the rest of the system's parameters as given in the following sections.

2.1.2 Detector and Focusing Optics

The type and size of the detector is chosen so as to minimize the Noise Equivalent Power over the wavelength of interest. NEP represents the incident power required to generate a response equal to the noise level of the detector system (to give SNR equal to one) within a specific bandwidth [29]. It is expressed as the noise current at a specified frequency in units of $(A/\sqrt{Hz})$ divided by the responsivity in $(A/W)$, with the resulting units of $(W.Hz^{-1/2})$. Responsivity corresponds to the amount of current produced with a given radiation power. A better detector has a smaller NEP number since this means that it gives a higher SNR for a certain incident power. In addition to the noise due to the detector element, the NEP value used for the calculation should also include noise due to the detector preamplifier circuit.

---

$^1$ Wavenumber (cm$^{-1}$) = 1/Wavelength (cm)
Two factors which contribute to detector NEP figure are the detector element area and the operating temperature. Detectors with smaller area usually generate lower noise, and thus lower NEP. However, a smaller area means that less radiation power can be collected in a given time (lower throughput). The NEP value also decreases as lower operating temperature is used. Therefore, selection of a photodetector should include considerations of its responsive wavelength range, size, operating temperature (hence, the type of cooler) and of course, cost.

For our purposes, a 1-mm-diameter extended Indium Gallium Arsenide (InGaAs) detector, with a two-stage thermoelectric cooler, was chosen to be the most appropriate. The detector is responsive over the range of 800\(nm\) to 2600\(nm\). Maintaining the operating temperature at \(-40^\circ C\) with the thermoelectric cooler improves its response stability and reduces its noise value by almost two orders of magnitude [28].

The area of the detector and the "speed" of the focusing lens will determine the throughput of the detection system (detector and its focusing lens L5), which for low-resolution measurements, dictate the achievable throughput of the system. Throughput is defined as:

\[
\Theta = A\Omega
\]  
(2-1)

where \(A\) is the projected area, which in this case, the detector area, and \(\Omega\) is the solid angle formed by the focusing or the collimating optics. For a lens with a focal length \(f\) and a beam radius \(r\),

\[
\Omega = 2\pi a^2 = 2\pi \tan^{-2} \left( \frac{r}{f} \right)
\]  
(2-2)

Assuming use of an \(f/2\) lens, the detector throughput is calculated to be 0.00296\(cm^2\) \(\text{steradians}\). Readers are referred to section 2.2.2 for explanation on lens' speed and \(f\)-number. With this, the rest of the system parameter that optimizes the throughput (and hence the signal-to-noise ratio) can be determined.
2.1.3 Spectrometer Collimating Optics

Practically, the beam that enters the interferometer would not be perfectly collimated. Therefore, an aperture has to be introduced that would limit the angle of divergence, which creates another limit on system throughput. However, this is necessary in order for the intended resolution to be achieved. For a spectral resolving power $R$, which is defined as:

$$R = \frac{\nu_{\text{max}}}{\Delta \nu}$$  \hspace{1cm} (2-3)

where $\nu_{\text{max}}$ is the maximum wavenumber observed and $\Delta \nu$ is the spectral resolution, the angle of divergence is limited to:

$$\theta = \tan^{-1}\left(\frac{a}{f}\right) \leq \sqrt{\frac{2}{R}}$$  \hspace{1cm} (2-4)

where $a$ is the radius of the aperture and $f$ is the focal length of the collimating lens.

The rest of the system parameters are calculated such that the system throughput is limited by detector throughput. This is to ensure that maximum signal can be collected in a given time.

$$\Theta_c \geq \Theta_D$$  \hspace{1cm} (2-5)

where $\Theta_c$ and $\Theta_D$ is the throughput of the collimating system and the detection system respectively.

Using maximum speed of collimating lens imposed by the maximum divergence angle, we combine equations 2-1, 2-2 and 2-5 to obtain:
\[ a \geq \frac{1}{2\pi} \sqrt{R\Omega_D} \]  

(2-6)

For \( \nu_{\text{max}} = 15000 \text{cm}^{-1} \) and \( \Delta \nu = 30 \text{cm}^{-1} \), \( R \) is equal to 500, which limits the maximum speed of the collimating lens to \( f/7.9 \). With detector throughput of 0.00296 cm\(^2\)sr as calculated before, equation 2-6 gives a minimum aperture of 0.19 cm. Using a collimating lens with a focal length of 15 cm, the maximum aperture for this resolving power is given by equation 2-4 to be 0.95 cm.

This margin suggests that throughput of the system can still be improved by increasing the throughput of the detection system. This can be accomplished in two ways: using a larger detector area, or a faster lens. However, detectors which have larger area usually have higher NEP, which would reduce the SNR. The speed of the lens is usually limited by the amount of aberrations that can be tolerated. For very demanding applications, use of mirrors instead of lenses would be advantageous, since they eliminate the chromatic aberrations.

![Figure 2-4. Maximum and minimum aperture radius as imposed by throughput and divergence conditions](image-url)
Figure 2-4 shows how the maximum aperture allowable by the divergence condition and the minimum aperture to match the detector throughput are related as a function of resolving power. Using \( f = 15\text{cm} \) and \( \Theta_D = 0.00296\text{cm}^2\text{sr} \), the two conditions meet at \( R \sim 2500 \). Beyond this, the detector throughput or the focal length of the collimating lens has to be increased to hold the conditions.

2.1.4 Interferometer and Motion Control

One of the advantages of a Michelson interferometer-based spectrometer over a dispersive type is that the resolution achievable is determined by the amount of mirror scan distance, which is easily programmable.

\[
\Delta \nu = \frac{1}{\Delta x}
\]  
\[\text{(2-7)}\]

\( \Delta x \) is the amount of retardation\(^2\) required for \( \Delta \nu \) resolution. For a single-sided interferogram, the distance of the mirror scan is \( \frac{\Delta x}{2} \). Our spectrometer is designed for a resolution of 30\(\text{cm}^{-1} \), which requires a minimum travel of 0.33\(\text{mm} \) for a double-sided interferogram.

Closed-loop control of position and velocity of the motion is achieved by incorporating another Michelson interferometer. The need for a fine and an accurate feedback signal for maintaining constant velocity over the scan distance is discussed in detail in section 3.2.3.1 and 3.2.3.2. A plane-polarized HeNe laser of 632.8\(\text{nm} \) wavelength is used as the source. As the mirror moves in one direction, the recombined beams in the interferometer would be a sinusoid with frequency \( f \) proportional to the mirror velocity:

\[
f = 2v_{\text{laser}} \nu
\]  
\[\text{(2-8)}\]

where \( \nu \) is the velocity of the mirror.

\(^2\) Retardation = optical path length difference = 2 \times \text{scan distance}
Although this signal can be used to deduce the velocity, it is not yet appropriate for inferring position information as it lacks direction information. The following passage describes a technique to come around this problem. A $\lambda/4$ retarder placed after a polarizer causes the beam entering the interferometer to be circularly polarized. As a result, any two orthogonal fields will have 90 degree phase between them. A polarizing beamsplitter then splits the output beam into two orthogonal fields, each detected by a silicon photodetector. The phase between these two signals can be used to deduce direction, and therefore the position of the mirror. Schmitt triggers are then used to digitize the signals as inputs to the encoder interface of the motion controller board. Drawing of circuit is included in appendix 8.

As in the case of the HeNe laser, the speed of the moving mirror would determine the frequency modulation of the main signal, which is the white light interferogram. Since the noise of the detector and its preamplifier depends on frequency of modulation, care should be taken in choosing the velocity of the moving mirror. In addition, bandwidth of both the detector and the preamplifier should also be considered, so as not to operate in the region where signal amplitude is significantly attenuated or where the
phase shift is non-linear. In our case, \( v \) is equal to 0.132 cm/sec, thus modulating the 15803 cm\(^{-1}\) HeNe laser signal at 4172 Hz.

2.1.5 Sampling and Data Acquisition

Accurate and repeatable sampling with respect to the mirror position is important for accurate interferogram averaging. Two methods can be used to accomplish this. The first is to sample the interferogram at regular time intervals with the mirror velocity carefully controlled. The second method is to use the signal from one of the silicon photodetectors as a reference signal. Since it corresponds to the mirror position with a much greater precision, the second method is implemented in our system.

The next thing to determine is the frequency of the timing signal, that is the number of sampling points per period of the sine wave. It is usually advantageous to sample at a frequency significantly higher than the Nyquist frequency, to prevent higher frequency noise to be folded back into the spectrum. In our spectrometer, four points are sampled for each period of the cosine wave. Following the Nyquist criterion, the minimum wavelength that can be analyzed without aliasing is therefore 316.4 nm.

To implement this, we had two choices. First, we could utilize the in-quadrature sinusoidal signals from laser detector 1 and 2 shown in figure 2-5. The second method was to use signal from just one detector, and discretizing it into four levels, and thus creating four clock signals for each period. The first method seemed to be more practical since the four signals already existed due to the 90-degree phase difference. However, it turned out that the positional error was not acceptable. This was because the phase difference between the two signals was not exactly at 90-degree, which probably was due to optics nonlinearity and manufacturing tolerances of the polarizers and the retarders. Therefore, the second method was implemented in our system.

Furthermore, although the HeNe laser produced a very high frequency-stability, it did not provide a stable enough signal as seen by the laser detectors. There is a low-frequency amplitude variation of as much as 5%. This maybe due to laser power source fluctuations and temperature changes causing variable responsivity of the unstabilized laser detectors. Thus, a novel circuit was built to overcome this, whose design is
presented in detail in appendix 1. The result is an extremely accurate and repeatable
timing signal that is synchronized with the mirror position. Readers are referred to section
3.2.3.3 for a more detail discussion on the data sampling design issues.

2.1.6 Data Processing

Each measurement consists of a double-sided, 4001 interferogram points based on
averaging a number of scans. A triangular apodization function and 6000 points as zero-
fillings were applied to each interferogram. The averaged interferograms were then
Fourier transformed to produce a spectrum with 15.8\text{cm}^{-1} point spacing. Due to zero-
fillings, the final point spacing was 6.3\text{cm}^{-1}. The program code is included in appendix 7.
All data processings were done in Matlab.

There are two possible averaging techniques to improve the signal-to-noise ratio:
time-domain averaging and spectral-domain averaging. In time-domain method,
interferogram points at each retardation location are summed up, and the averaged value
is Fourier transformed to produce the spectrum. This technique relies heavily on
sampling location consistency for all scans. In spectral-domain method, Fourier
transformation is performed for each interferogram (for each scan). Because of this, this
method involves much more computation.

Theoretically, both methods would give the exact same result:

\[
\mathfrak{S}\left(\frac{1}{N} \sum_{i=1}^{N} I_i(t)\right) = \frac{1}{N} \sum_{i=1}^{N} \mathfrak{S}\{I_i(t)\} \quad (2-9)
\]

where \(\mathfrak{S}\) is the Fourier transformation operator, \(I_i(t)\) is the interferogram at scan \(i\) and \(N\)
is the number of scans. This is because Fourier transformation is a linear operation. In
practice, however, the resulting spectra may not be the same. The spectral-domain
method is potentially more accurate, since timing signal drifts in-between scans are
neglected. A good example of this type of error is the positional sampling error due to
temperature change discussed in section 3.2.3.3.
2.2 Overview of Hardware Implementation

2.2.1 Structure

The system is built on a 0.9 X 0.6m optical breadboard with modular opto-mechanical structure for assemblies. A photograph of the system is included in appendix 5. A few criteria which were important in choosing the opto-mechanical bench and mounts included flexibility, ruggedness and precision. Other factors included size and compatibility with products from other manufacturers. *Microbench* from SPINDLER & HOYER met our criteria. It allowed us to assemble our system with great ease and precision. The system is placed on an air-damped vibration isolator, making it insensitive to mechanical shocks and vibrations.

2.2.2 Optics

In this section, discussions will include the selections of lenses, mirrors and beamsplitters. Lenses are used for focusing and collimating purposes in our system, due to the simplicity and ease of alignment. Selecting the type of lenses involves determination of size, shape, material and focal length.

First, the material and coating of lens needs to be determined, because they may limit the available forms/shapes available. The material is chosen that will produce the highest transmission over the wavelength range of interest. On the practical side, durability, cost and maintenance requirements should also be considered. For our spectrometer, lenses made of calcium fluoride are found to be the most appropriate due to its high transmission, low refractive index and a relatively low cost. Calcium fluoride has a useful transmission over the spectral range between 200nm and 8000nm, with more than 90% transmission over the near infrared [30]. The low refractive index (~1.43 over the near infrared) means that it may be used without an anti-reflection coating.

Next, the speed and size of the lens has to be determined. Speed of the lens is defined as:
where D is the lens diameter and f is the focal length [38]. Note that the diameter here refers to the effective diameter, which in most cases is smaller than the true diameter due to presence of a stop or aperture. In selecting the lens speed and diameter, two things need to be considered are the throughput and the aberrations. The higher the speed, the higher the aberrations would be. As a rule of thumb, the f-number should be more than 4 for simple lens forms such as a plano-convex. Aberrations are discussed in detail in any optics textbook [39].

Our collimating and focusing optics L1-L4 in figure 2-2 have 25.4mm diameters and 150mm focal lengths. This imposes a maximum speed of 0.17 or an f-number of 5.9. Except for L1, where it collects light from the source, the full diameter is never used, due to the presence of an aperture. For the detector focusing lens L5, a focal length of 50mm is used. For the setup as in figure 2-2, this may seem unnecessary, because the throughput is always conserved throughout the system. However, for the noninvasive application, where diffuse reflectance technique is used, the spectrometer would be uncoupled with the detector and its focusing optics. The diffuse reflected signal would be of much lower density, thus the use of a higher lens speed is well justified.

Mirror selection is somewhat easier, especially since we are only concerned about plane mirrors. Considerations include percent reflectance, size, durability, surface finish and cost. For our low-resolution interferometer, silver-coated plane mirrors with 1/10 flatness are more than sufficient. They provide >97% reflectance throughout the near-infrared range.

Beamsplitter is an important element in interferometric systems. Discussion on different types of beamsplitters used in Fourier transform spectroscopy is satisfactorily done by Bell [31]. There is a significant potential loss of radiation power due to the beamsplitter in any Michelson interferometer design. The beamsplitter efficiency \( \xi_{bs} \) is determined by both reflectance, \( R_{bs} \) and transmittance, \( T_{bs} \), values of the beamsplitter:

\[
\xi_{bs} = 2R_{bs}T_{bs}
\] (2-11)
For an ideal case where $R_{bs} = T_{bs} = 0.5$, the maximum efficiency is 50%. The loss is due to the half of in-coming radiation being returned back to the source.

Our system incorporates a non-polarizing beamsplitter cube made of optical glass material. This low-cost beamsplitter provides ~35% transmittance and ~60% reflectance at 1600nm (OptoSigma Corporation). The cube design allows stable and easy mounting.

### 2.2.3 Linear Actuator for Interferometer

A photograph of the interferometer system is included in appendix 4. The michelson interferometer is constructed from two plane surface mirrors and a broad-band cube beam splitter. One mirror is fixed on a micrometer-driven translation stage, and the other is mounted on a flexure, driven by a voice-coil actuator. Figure 2-6 shows the schematic of the actuator-mirror assembly.

![Figure 2-6. Schematic of the linear actuator assembly.](image)

---

---
The actuator and the flexures come together as a unit supplied by *Link Dynamic Systems Corporation* (model V203). The flexure assembly enables a smooth motion due to almost negligible friction. The stiffness provided by the flexures also makes the system more stable, and thus less susceptible to environmental conditions and easier to control.

In our configuration, the mirrors are put off-axis to permit both the main radiation and the HeNe laser to travel on the same optical axis. This is important to ensure that sampling positional errors are minimized. This is discussed in detail in appendix 2. In this appendix, an alternative method is presented, which makes use of a retro-reflector to guide the laser for a 180-degree turn. Detail calculation is presented.

**2.2.4 Computer Interface**

Data is acquired with a 12-bit A/D converter (PCI-MIO-16E-1, National Instruments). It provides 8 differential analog input channels, 2 analog output channels, 8 digital inputs/outputs and 2 24-bit up/down counter/timers. The maximum data acquisition rate is $1.25\text{MHz}$. The differential input configuration is of importance for our purposes, since it significantly reduces picked up noise and increases common-mode rejection.

Data acquisition is started at the first interferogram centerburst after the user start-command. This is accomplished by using an analog trigger with a voltage level specified through the software. Gaussian noise of 0.5 LSB-$rms$ is generally applied to improve the resolution and the signal-to-noise ratio.

Servo control of the moving mirror is accomplished digitally using a motion controller board with an on-board DSP (digital signal processor) (PCI-FlexMotion, National Instruments). A PID closed-loop algorithm is implemented, with a trapezoidal velocity profile. Both motion control and data acquisition systems are operating under LabView. Its user-friendliness enables fast development time.
3. PERFORMANCE EVALUATION AND ERROR ANALYSIS

In this section, we attempt to analyze the instrumental sources of errors in the manner in which they affect the results of quantitative works for the near-infrared aqueous glucose absorption. The inherent weakness of clinically-relevant glucose absorption signal coupled with sub-millimolar accuracy required for the ultimate noninvasive application have imposed an enormous instrumental sensitivity requirement.

As with any other instrument, each subsystem produces its own errors. It is therefore important to analyze each element, and quantify the signal-to-noise ratio achievable in that element. Identification of the limiting source(s) of errors would enable justifiable approach(s) in improving the system as a whole.

Before we begin, it is important to note the nature of operation:

1. Interferometer is used in a "rapid-scan" manner, where each wavenumber is modulated in the audio-frequency range.
2. A minimum of 20 averaged-scans (10 seconds in time) for each measurement is generally used.
3. Operation is in the near-infrared wavelength region between $5000\, cm^{-1}$ and $15000\, cm^{-1}$.
4. Resolution intended is larger than $20\, cm^{-1}$.

The first two notes deal with the manner and duration in which each measurement is taken, which will influence the way noise is captured by the instrument. For example, rapid-scan interferometers are less prone to slow variations of source intensity than the slow-scan or the stepped-scan interferometers. The advantages and disadvantages of the fast-scan and the slow-scan methods are discussed in detail by Griffiths [23].

In the near-infrared region, the absorption peaks are usually broad and featureless. In most cases, a resolution of $30\, cm^{-1}$ will suffice. However, the shorter waves in the
near-infrared means that timing signal accuracy and motion straightness requirements are more demanding.

In any error analysis attempt, performance, which in our case is defined as signal-to-noise ratio should be categorized into two [32]:

1. accuracy
2. repeatability

Accuracy measures the deviation from the "ideal" case (what it should be), whereas repeatability measures the ability to reproduce the same results over and over again. There are two dimensions that we deal with in spectroscopic measurements: wavelength and intensity. For measurements using a Fourier transform spectrometer, wavelength is usually the only dimension that matters for accuracy. The main reason simply is that there is no way of quantifying universally the intensity of the signal measured by Fourier transform spectrometers. The efficiency, the throughput and the gain due to the electronics, among other things, would be different between various instruments, and they all contribute to the intensity of the spectrum.

Repeatability, on the other hand, is very important in both dimensions, especially in quantitative absorption applications based on ratiowing single-beam spectra. Most of current FT-spectrometers, including ours, employ single-beam measurement technique. This means that the absorption plot is produced by ratiowing the sample and the reference spectra taken at different times (usually back-to-back). Ideally, the tranmission spectrum \( T \) of a sample referenced to itself should be a flat line at zero, or the 100% line \( \frac{T_A}{T_B}, A = B \) is equal to 1. In this case, the signal-to-noise ratio is infinity. More on this is in section 3.2.

3.1 Wavelength Accuracy

We test our instrument's wavelength accuracy simply by observing the transmission spectra of a narrow band filter and an HeNe laser to within the specified resolution. The resulting spectra are shown in figure 3-1.
Figure 3-1. Wavelength accuracy of a 632.8\textit{nm} HeNe laser (top) and a 1600\textit{nm} bandpass filter (bottom)

The resulting spectrum of the helium-neon laser should indicate that the spectrometer's wavelength accuracy is excellent. It confirms very well to the laser wavelength specification, 632.8\textit{nm}. The lower plot shows a spectrum of a narrow-band filter, which according to the specification provided by the manufacturer, has a center wavelength of 1600\textit{nm} $\pm$ 20\%. The resulting center wavelength as indicated in the diagram is still well within the tolerance. Note that these two spectra were taken using only 1 scan (no averaging was performed).

\subsection*{3.2 Repeatability}

As mentioned before, most of the current spectrometers, including ours, employ single-beam measurements, which means that the absorption plot is produced by ratioing the sample and the reference spectra taken at different times. Thus, we define $SNR_{\text{root-mean-square}}$ to be:
\[ SNR_{rms} = \frac{1}{e_{rms}} \quad (3-1) \]
\[ e_{rms} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left( \frac{T_A}{T_B} - 1 \right)^2} \quad (3-2) \]

where \( N \) is the number of elements observed and \( A = B \) is the sample being measured. It is important to note that the calculated error is the "root-mean-square" error, which is usually a few times smaller than the peak-to-peak error. It needs to be accounted for if sample concentration prediction is made based solely on simple peak observation. From this point on, \( SNR_{rms} \) would be denoted just by \( SNR \).

In keeping with the convention, the absorption spectra should be defined as:

\[ A(v_i) = -\log_{10}\left( \frac{T_{\text{sample}}(v_i)}{T_{\text{reference}}(v_i)} \right) \quad (3-3) \]

where \( A(v_i) \) is the absorbance and \( T(v_i) \) is the transmittance at wavenumber \( v_i \). This conventional relationship is due to a well-known Beer's Law which imparts a linear relationship between the absorbance and the sample concentration:

\[ A(v_i) = \alpha(v_i)lc \quad (3-4) \]

where \( \alpha(v_i) \) is the absorptivity of the sample at wavenumber \( v_i \), \( l \) is the path length and \( c \) is the sample concentration.

3.2.1 Light Source

Power fluctuation refers to wavelength-independent variation that may be caused, for example, by input current variation. On the other hand, spectral variation refers to wavelength-dependent variation, causing relative energy density change across the spectrum. To access the first, we can monitor the source intensity by observing the output
voltage of the detector that is directly coupled to the light source. However, the second cannot be measured experimentally without the use of the spectrometer (which will then includes other sources of noise).

To ignore the effect of spectral variation, we put a narrow-band optical filter between the source and the detector, and measure the output voltage that represents the total light power transmitted. According to the specifications provided by the manufacturer, the filter has a center wavelength of 1600 nm and a full-width-at-half-maximum (FWHM) of 10 nm (F10-1600-4, CVI Laser Corporation). Since the energy density under consideration is now limited to 5 nm at half-maximum, the spectral variation can be neglected.

![Graph showing intensity variation as a function of time](image)

**Figure 3-2.** Source variation as a function of time

Figure 3-2 shows the result of the procedure. Only the first 0.4-second is shown to discern the ±1% 120Hz fluctuations. Although multiple scans averaging should eliminate most of this noise, further investigation may be necessary for seriously demanding applications.

The effect of light source is seldom an important discussion in absorption spectroscopy, because it has always been assumed that it provides a continuum spectrum over which the absorption takes place. The absorption peaks are sharp enough relative to
the spectral changes of the source, that baseline corrections are usually sufficient. However, for broad absorption peaks in the near-infrared region, more careful attention may need to be given to the light source stability.

3.2.2 Optics

Imperfections of focusing and collimating optics, as well as the beamsplitter would result in deviations from the "ideal" spectra. These imperfections include, but not limited to aberrations and absorption, where the significance of both varies as a function of wavelengths. Since these errors do not usually change with time (reproducible), their contribution to the SNR defined above can be considered negligible.

Another possible error in the optical elements outside the interferometer is a change in alignment. The Microbench system from the SPLINDER & HOYER we used provides a very rugged structure assembly. In addition, the instrument is placed on an air-damped vibration isolator, making it insensitive to mechanical shocks. Due to the absence of moving parts, the only possible cause of misalignment is temperature change, which may cause material expansions. For this to occur, temperature in our temperature-controlled room must change significantly. If it does happen, we should worry about other elements which may be much more sensitive to this, such as the interferometer alignment, spectral shift and positional sampling error due to material expansion (see section 3.2.3.3). Furthermore, according to Griffith [23], alignment change outside the interferometer would degrade the spectrum intensity only by a constant throughout the wavelengths. With a baseline correction algorithm, this error would be as good as zero.

3.2.3 Interferometer

This is probably the instrument subsystem that is most prone to errors and variations due to its dynamic nature. Problems can arise from:

1. Change in the alignment of interferometer components
2. Non-constant mirror velocity during data sampling
3. Sampling incoherence
In this section, each type of error would be analyzed. Comprehension of its nature and its relation to the signal-to-noise ratio achievable with respect to glucose measurements would be beneficial.

3.2.3.1 Interferometer Alignment Error

Misalignment of one of the perpendicular mirrors in the interferometer will result in the loss of spectral accuracy, with the shorter wavelength more poorly affected. We distinguish interferometer alignment errors into two types: static and dynamic errors. Static error corresponds to the slow alignment variation that is due to, for instance, temperature change. Dynamic error is caused by poor mirror drive, which means that the alignment is not maintained throughout the scan. Analytical examinations of some problems pertaining to interferometer misalignment errors are given by Griffiths [23].

A measure of how well the interferometer is aligned, the value of the interferogram signal at the centerburst, \( I(0) \) as compared to the interferogram signal value at high retardation, \( I(\infty) \) can be used.

\[
B = \frac{I(0) - I(\infty)}{I(\infty)}
\]  

(3-5)

For a well-aligned interferometer, \( B \) should be greater than 0.9 [23].

To examine the alignment stability of our spectrometer, values of interferogram peaks were measured every two minutes for a period of two hours. Figure 3-3 shows the results.
Figure 3-3. Peak intensity based on 20 averaged interferograms normalized to average value, as a function of time.

In this plot, the peak intensities are normalized to a value of their average value. The experiment was begun right after powering up all components including the light source, the HeNe laser and the actuator. Components warm-up may explain the constant decrease in stability for the first 20 minutes. However, for the rest of the experiment, the fluctuations were within 0.6%. In fact, for any two consecutive measurements, the variability was less than 0.2%. These suggest that the spectrometer had an excellent stability, both short and long terms. Note that the variations measured would also include other noises such as light source fluctuations (figure 3-2) and sampling errors (discussed later in the section) among others.

The quality of the drive mechanism of the moving mirror will determine whether the spectral resolution achievable would be attained as specified by the maximum retardation of the mirror (equation 2-7). According to Griffiths [23], for no loss of resolution, the angle variations throughout the scan should be limited to:

\[
\beta < \frac{1}{20Dv_{\text{max}}} \hspace{1cm} (3-6)
\]

Where \(D\) is the diameter of the collimated light entering the interferometer, \(v_{\text{max}}\) is the maximum wavenumber and \(\beta\) is the tilt angle in radians.
The drive mechanism that we use now (figure 2-6) is actually an improvement from an old mechanism based on ball-bearings, whose picture is included in appendix 3. To demonstrate the effect of a poor mirror drive spectra of an air background are compared, which are shown in figure 3-4.

![Figure 3-4](image)

Figure 3-4. Four consecutive spectra displaying how quality of drive mechanism affects repeatability. Two spectra were taken with a poor quality velocity control (poor control) and the other two with the best control. All spectra are taken using the ball-bearing mechanism.

These four spectra were taken using the old drive mechanism (appendix 3). The two higher intensity spectra represent two consecutive spectra taken with the best close-loop control algorithm. The lower two were taken using a slightly worse control algorithm, causing an unsteady velocity. Due to the off axis weight, this unsteady mirror velocity causes mirror tilts during the scan.
Figure 3-5. Comparison of 100% lines of different drive qualities. The current drive using flexure is superior.

As defined before, SNR achievable for a single-beam measurement is a measure of repeatability of consecutive measurements. Figure 3-5 shows three 100% lines corresponding to 6 measurements with three different configurations: ball-bearing with poor control, ball-bearing with good control and the current flexure mechanism with good control. Looking at the plots, the current configuration is much more superior. The calculated SNRs are 150, 500 and 5000. Thus the current mechanism has an SNR value an order of magnitude greater than the ball-bearing drive with a good control. All spectra were measured using 20 scans.

3.2.3.2 Nonuniform Velocity

Besides regular interval sampling, it is very important that each interferogram data point is sampled at exactly the same mirror retardation distance for every scan. Otherwise, signal averaging will not only fail to improve the signal-to-noise ratio, but it will also distort the resulting spectrum. With the use of the HeNe laser signal as reference, it seems that changes in velocity does not matter, as the timing signal is not referenced to time but directly to retardation distance. Theoretically, this is true, but not
in practice. A few things that may cause problems if mirror velocity is not maintained constant:

1. non-zero phase response of detector preamplifier
2. frequency-independent timing circuit delay
3. mirror tilt-angle increase due to off-axis weight

First, to prevent high frequency noise to be folded into the spectrum, a low-pass filter should be used. This filtering can, and is usually done by the detector preamplifier circuit, which has a bandwidth just high enough to pass the highest frequency in the modulated radiation. However, this creates a significant, non-zero phase value. If the mirror velocity is precisely constant, this does not present a problem, since all the points will be delayed by the same amount. Circuit delays also play the same role in this case, although their phases are not as functions of a frequency, but rather a constant.

For a variation of Δν in velocity and a time delay of Δt due to preamplifier phase and circuit delay, sampling error Δx can be represented by the following equation:

$$\Delta x = \Delta \nu \Delta t$$  \hspace{1cm} (3-7)

From this equation, it is clear that it is advantageous to minimize any time delay present in the system. In our system, the total time delay is approximated to be 1.5 μsec (with preamplifier gain of $10^7$). The velocity variation is observed to be within 1% (±0.5%) in the relevant range where data is being sampled (figure 3-6). The nominal steady-state velocity is 0.132cm/sec. Thus, equation 3-7 yields a sampling error of 0.02nm.

Hirschfeld [34] has suggested that the signal-to-noise ratio achievable with a positional error Δx is given by the following equation:

$$SNR = \frac{4}{v_{\text{max}} \Delta x}$$  \hspace{1cm} (3-8)

Thus, for a maximum wavenumber of 7500cm⁻¹ (as is usually in our case, with placement of a 1400nm long-wave-pass filter), the SNR due to the sampling error is calculated to be
265000. Without even considering signal averaging, this is remarkably high. Note however that the phase due to the detector amplifier is dependent on the gain being used. In most cases, the higher the gain, the lower the bandwidth, and thus the greater the time delays. However, a remedy to this is as easy as decreasing the speed of the mirror.

Figure 3-6. Output of frequency-to-voltage converter. The vertical axis is proportional to mirror velocity, and the horizontal axis is proportional to time.

Another possible error due to inconsistent mirror velocity is mirror tilt which is due to the off-axis weight pertaining to our mechanism design (figure 2-6). Any acceleration and deceleration in the relevant sampling range will result in mirror tilt. Thus, the velocity needs to be maintained as smooth as possible. Looking at the velocity profile in figure 3-6 above, this should not present any problem. Note that the small amplitude fluctuations present on the plot was not caused by velocity fluctuations, but rather due to noises in the frequency-to-voltage converter used to obtain this graph.

3.2.3.3 Incoherent Data Sampling

In the previous section noise caused by sampling errors due to time delays was discussed. The signal-to-noise ratio for a system limited by this type of errors is given by
equation 3-8. In this section, other factors contributing to generation of sampling errors will be given.

Figure 3-7 shows the components that are related to sampling and thus potential contributors to errors. In short, the laser interference produces a sinusoidal signal as a function of mirror B position. This signal is processed in real-time to become a suitable signal as a data sample clock by a signal processing circuit given in appendix 1. As with any other real device, this component introduces some errors. Another possible source of noise is distance variation between mirror face A and mirror face B, $\Delta d$. This variation may come from material expansion due to temperature change. Thus, positional sampling errors are caused by the following factors:

$$e_{total} = e_{process\sin g} + e_{delay} + e_{mechanical} \tag{3-9}$$

Here, $e_{delay}$ represents the error due to non-zero phase of the detector preamplifier circuit and the frequency-independent electronics delay discussed in section 3.2.3.2. Note that $e_{process\sin g}$ comes from the same signal processing circuit as $e_{delay}$.

![Diagram of data sampling procedure](image)

Figure 3-7. Schematic of data sampling procedure
To assess the errors due to the signal processing electronics, the following procedure was carried out. A/D converter was set up so that it sampled the laser interference signal, instead of the white light interferogram. The timing signal was still provided by the laser interference signal after passing through the signal processing circuit. The output from the A/D converter is then a sinusoid signal sampled four times each period, corresponding to four voltage levels. Magnitudes of errors were examined by looking at the signal variation at one of these levels. This is plotted in figure 3-8. The straight line represents an ideal case with zero variation. This voltage value is already converted to the corresponding positional error value, which makes up the vertical axis.

![Figure 3-8. Plot of positional sampling variations in nm for 250 data points.](image)

The variations as plotted above has an rms value of ~0.27nm. This value is much greater than the noise due to time delays as calculated in section 2.4.3.2, which is 0.02nm. For a maximum wavenumber of 7500cm⁻¹, according to equation 3-8, the SNR achievable due to the electronics time delay and laser signal processing is ~18000.

Let us now consider the effect of material expansion (Δd) to the SNR value. The thermal coefficient of expansion of aluminum alloys is 23×10⁻⁶/°C. Thus, for a thickness d, the positional error is given by:
\[ \Delta x = 23 \times 10^{-6} d \Delta T \] (3-10)

where \( \Delta T \) is the temperature change. Thus, for the above SNR value, with \( d = 3.5 \text{mm} \), the temperature has to be maintained within four thousandths of a degree. This is certainly an imposing requirement. However, it should be realized that compared to the two types of noises discussed previously, this noise would be of a much lower frequency. In a temperature-controlled room, there should not be a significant change in between scan. Thus, interferogram averaging can still be applied. However, for measurements longer than a minute or two, spectral-domain averaging should be considered. See section 2.1.6 for discussion on their distinctions.

3.2.4 Detector

Contrary to the popular belief, detector noise may not always be the limiting factor in a spectrum measured using a Fourier-transform spectrometer. To quantify detector noise, a good figure of merit to use is its NEP, which stands for Noise Equivalent Power. Basically, NEP measures the minimum incident power required to produce a signal-to-noise ratio of one, within a specific bandwidth [29]. Besides the noise due to the detector element, the NEP value used for the calculation should also include the noise due to the detector preamplifier circuit.

In calculating the signal-to-noise ratio of the spectrum in the detector noise-limited, Griffith [23] gives the following equation:

\[
SNR = \frac{U(v) \Theta \Delta \nu^{1/2} \xi}{NEP}
\] (3-11)

where \( U(v) \) is the spectral energy density, \( \Theta \) is the throughput of the system, \( \Delta \nu \) is time spent in collecting the data and \( \xi \) is the efficiency of the system. The numerator, excluding the time factor basically represents the signal power that falls on the detector. For a blackbody source, the term \( U(v) \), which is a function of temperature, can easily be calculated. Most of the time, however, the spectral energy density function is not easily
calculated, especially when a sample is present. Therefore, we present another more practical method of calculating the signal-to-noise ratio of a detector noise-limited case.

The relationship between the spectral density function and the measured interferogram can be represented by the following equation:

\[
S(u_i) = \sum_{l=-N/2}^{N/2} I(lh) \cos(2\pi u_i h) \tag{3-12}
\]

where \(S(u_i)\) is the spectral intensity at wavenumber \(u_i\), \(I(lh)\) is the interferogram as a function of an integer \(l\) times the sampling interval \(h\) and \(N\) is the number of points sampled.

When the source is a continuum, as is generally encountered in the near-infrared absorption studies, the interferogram signal dies out rapidly to a constant value as the mirror retardation is increased. Figure 3-9 (top) shows part of the ac-coupled interferogram of water in 1-mm cuvette, whose spectrum is depicted in figure 3-9 (bottom). The "wings" of the interferogram convey the medium and the higher resolution element of the spectrum, which most of the time, is the part of the spectrum that is of interest. Therefore, it is reasonable to use the average power at this part of the interferogram as the contributing signal in the approximation of the signal-to-noise ratio. Thus, the SNR of the interferogram for detector noise-limited case can be approximated as:

\[
SNR^i = \frac{W\sqrt{Ct}}{NEP}, W = \frac{V}{gR(u_i)} \tag{3-13}
\]

where \(W\) is the power received by the detector in watts, \(t\) is the one scan measurement time in seconds, \(C\) is the number of scans, \(V\) is the preamplifier output voltage, \(g\) is the transimpedance gain in volts/amperes and \(R(u_i)\) is the responsivity at the observed wavenumber \(u_i\). In our calculation, the spectrometer efficiency, the spectral change due .
to the presence of the sample and the throughput conditions at the time of the experiment have been accounted for.

Figure 3-9. Interferogram (top) and spectrum (bottom) of water in a 2-mm cuvette.

In going from the interferogram to the spectrum, the SNR deteriorates by the square-root of the number of interferogram points [34]. For a double-sided interferogram, the number of interferogram points is equal to twice the spectral resolution element. Therefore, signal-to-noise ratio of the 100% line upon ratioing becomes:

\[
\text{SNR}^2 \equiv \frac{W \sqrt{Ct}}{\sqrt{2\text{NEP}}} \left( \frac{\Delta \nu}{2(v_{\text{max}} - v_{\text{min}})} \right)^{1/2} \frac{\rho(v)}{\rho_{\text{mean}}} 
\]  

(3-14)

where \( \Delta \nu \) is the resolution and \( \frac{\rho(v)}{\rho_{\text{mean}}} \) is the ratio of the spectral power density at the analyzed wavenumber(s) to the average power. Two terms of \( \sqrt{2} \) appear as results of
spectral ratioing and the fact that for a double-sided interferogram, the interferogram points are twice the spectral resolution elements.

Our TE-cooled InGaAs detector has an NEP value of $0.16 \, pW / Hz^{1/2}$ and a responsivity of $\sim 1.5A / W$ at $5920 \, cm^{-1}$. The detector preamplifier circuit has three steps of gain, $10^6$, $10^7$ and $10^8$. Its NEP value depends on the gain setting, with the highest one having the lowest noise. We proceed to calculate the SNR achievable due to the detector noise for the two cases: 2-mm and 10-mm pathlength water measurements.

For the 2-mm pathlength, the lowest gain was used, resulting in a total NEP of $\sim 2 \, pW / Hz^{1/2}$. The voltage at the wings of the interferogram was observed to be $4V$. The wavenumbers being analyzed ranged from $5850 \, cm^{-1}$ to $6000 \, cm^{-1}$, with the spectral density power of $\sim 30$ times as high as the mean one. With 200 scans and $\sim 0.3$ second one-scan-time, the resulting SNR due to the detector noise was calculated to be more than $3 \times 10^6$.

The 10-mm pathlength permits only a much lower transmittance, due to water absorption. Thus, the highest gain was used, resulting in an NEP value of $\sim 0.2 \, pW / Hz^{1/2}$. With all else being equal, the SNR achievable if it was detector noise limited was calculated to be $\sim 350000$. Although there is a decrease of an order of magnitude, this SNR value is still remarkably high.

### 3.2.5 Digitization

A commonly neglected noise in the FT-IR measurement is the quantization noise due to the finite resolution of an analog-to-digital converter. Hirschfeld [34] stated the rms signal-to-noise ratio of the 100% line of two consecutively measured spectra is:

$$SNR = \sqrt{\frac{3}{2}} \left( \frac{N \Delta v}{\nu_{\text{max}} - \nu_{\text{min}}} \right)^{1/2} 2^b k \frac{\rho(v_i)}{\rho_{\text{mean}}} \left( \frac{1}{\sqrt{2}} \right)$$

where $N$ is the number of scans, $b$ is the number of bits, $k$ is the portion of the full dynamic range where it is being used, $\Delta v$ is the resolution, and $\rho$ is the spectral power.
density. A factor of $\frac{1}{\sqrt{2}}$ is placed in modification to the equation given by Hirchfeld, to account for a double-sided interferogram being used to obtain the spectrum.

To observe the effect of digitization noise to the achievable SNR of glucose-in-water measurement, $rms$ noise values between $5850 \text{ cm}^{-1}$ and $6000 \text{ cm}^{-1}$ of two ratioed water spectra for different values of $k$ were measured (by varying the radiation power entering the spectrometer). The experiment was done for two cases: 2-mm pathlength and 10-mm pathlength. Each measurement used 200 number of scans. The wavelength range was chosen because of the important presence of a glucose absorption band centered at around $5920 \text{ cm}^{-1}$ [6,7]. Figure 3-10 shows the experimental and the theoretical SNR values as functions of the fraction of the number of bits used, for the 2-mm and the 10-mm pathlength.

For the 2-mm pathlength, the experimental values consistently exceed the theoretical ones. However, linear relationship, as predicted by the theory seems to occur. This may indicate that equation 3-15 is a valid, conservative approximation. More importantly, it can be deduced that digitization noise is a significant, if not the limiting factor in these measurements under the above experimental conditions. Figure 3-10 especially shows that higher signal-to-noise ratio, and thus higher sensitivity can be gained by using a higher resolution A/D board. For the 10-mm pathlength, the experimental values follow the theoretical ones more closely. The lower signal-to-noise ratio in this case may be due to other sources of noise such as noise due to the sample itself and detector noise. Detector noise for the 10-mm pathlength case may be more crucial because light transmission is significantly reduced due to strong water absorption.
3.3 Efficiency

Efficiency of a spectrometer is an important consideration in the cases where the radiation source is weak, and thus, the limiting source of noise is usually the detector noise. For measurements based on diffuse reflectance on tissue, this is certainly important. Therefore, we attempt to assess the efficiency value of our spectrometer.

Figure 2-3 shows the functional blocks of the Fourier transform spectrometer. The efficiency value measures the loss of the radiation in the collection optics and the interferometer subsystems. Causes of radiation loss include the absorption due to the lenses and the beamsplitter, as well as the loss to the environment. The procedure to obtain the efficiency figure is described in the following paragraphs.

The radiation power emitted by the light source was directly measured by the photodetector. Energy was limited by means of placing a narrow band filter at 1600nm and a fixed-diameter aperture. A mechanical chopper was used to modulate the light at 1KHz, to optimize the detector performance. Power in Watts, $P_1$, was recorded. The light
source and the detector were then assembled back. With the same narrow band filter and the same fixed-diameter aperture, the spectrometer was operated to generate interferograms. At zero mirror retardation value (at centerburst), each interferogram value corresponded to the sum of the radiation power, $P_2$, across the wavelength components present. For an efficiency figure equal to one, this value would be equal to $P_1$. Thus, efficiency was defined as: $\xi = \frac{P_2}{P_1}$.

The assessment resulted in the efficiency value of 0.085. This value is comparable to other Fourier transform spectrometers reported [36,37]. If needs arise, the spectrometer efficiency can be improved by replacing lenses with mirrors. This eliminates the radiation loss due to the absorption by lens material.
4. MEASUREMENT OF AQUEOUS GLUCOSE SOLUTIONS:
SENSITIVITY ANALYSIS

As mentioned in the previous chapter, most of the absorption studies with FTIR spectrometers employ single-beam technique, including glucose measurements. This technique relies on the fact that in-between-measurement errors are significantly smaller than the signal changes due to the absorbing substance.

\[ |e_{\text{rms}}| < A_{\text{sample}}(\nu_i) \Rightarrow \frac{1}{\text{SNR}} < A_{\text{sample}}(\nu_i) \]  

(4-1)

where \( e_{\text{rms}} \) is the root-mean-square noise value over the relevant wavelength range and \( A_{\text{sample}}(\nu_i) \) is given by equation 4-1.

With the knowledge of the \( rms \) noise and the glucose signal intensity for a given set of experimental conditions, minimum resolution in mmol/L of glucose concentration can be calculated. However, it is important to realize that the value is an optimistic approximation due to the use of \( rms \) noise value. As a rule of thumb, the actual peak-to-peak noise value would be about four times as high. However, the actual prediction capability will also depend on the algorithm used to process the data.

4.1 Procedures

4.1.1 Experimental

Anhydrous D-glucose were dissolved in distilled water, with concentration levels: [3.3, 5.9, 9.3, 12.5, 14.3, 25.4, 45, 70, 100] mmol/L. Except for the 45, 70 and the 100mmol/L, glucose concentrations were determined by using a commercial electrode-based sensor, GLUCOMETER ELITE, manufactured by Bayer Corporation, USA. Due to the limited range of sensor, the higher concentration glucose solutions were prepared simply by using their mass-molar relation. All solutions were stored in room temperature.

First, \( rms \) noise value was assessed for each pathlength. This was accomplished by performing six measurements of pure water, each with a new solution from the
reservoir, thus producing five successive 100% lines. Noise value was calculated for wavenumbers between 5850cm⁻¹ and 6000cm⁻¹, about a third-order polynomial fit to account for the low-resolution baseline variations. Next, for each concentration level, three spectra a, b, c were measured in that order: spectra a and c corresponds to the sample spectra, referenced to the pure water spectra b to obtain the absorbance plot. Measurements were done in random with respect to the concentration. A long-wave-pass filter with a cut-off wavenumber at ~7150cm⁻¹ was used for all measurements to suppress unnecessary radiation.

4.1.2 Data Processing

Each measurement consisted of a double-sided, 4001 interferogram points based on co-adding 200 scans. A triangular apodization function and 6000 points as zero-fillings were applied to each interferogram. The averaged interferograms were then Fourier transformed to produce a spectrum with 15.8cm⁻¹ point spacing. Due to zero-fillings, the final point spacing was 6.3cm⁻¹. All data processings were done in Matlab.

To minimize the effects of low-resolution baseline variations and higher-resolution noise, digital Fourier filtering was applied to the absorbance spectra [6,10,35]. In our case, a Gaussian-shaped filter was applied, with its center location determined by the equivalent width criterion [35]. The width of the filter was determined experimentally by analyzing its effect on several absorbance spectra. Note that for an optimized filter shape, an empirical method assessing a number of locations and widths of the filter should be employed, preferably in conjunction with the algorithm used for the concentration prediction, as done by Arnold et.al. [6]. However, it would require an exhaustive experimentation and a substantial amount of computation. For our sensitivity analysis purposes, this was not necessary.

4.2 Results and Discussions

In the first-overtone region, glucose absorption peak at around 5930cm⁻¹ has been found to be the most useful for physiological glucose concentration prediction [6]. The
absorbance of a few selected solutions can be seen on figure 4-1 for the 2-mm pathlength and on figure 4-2 for the 10-mm pathlength. For visualization, absorbance plots of higher glucose concentrations are used here, since baseline variations mask the absorption peaks of the lower concentrations. After the application of a Gaussian-shaped Fourier filter, the baseline variations are greatly reduced and the absorbance features are significantly improved as shown in figure 4-3 and 4-4.

Figure 4-1. Glucose absorbance plots for 2-mm pathlength aqueous solutions.

Figure 4-2. Glucose absorbance plots for 10-mm pathlength aqueous solution.
Figure 4-3. Fourier-filtered glucose absorbance plots for 2-mm pathlength aqueous glucose solutions.

Figure 4-4. Fourier-filtered glucose absorbance plots for 10-mm pathlength aqueous glucose solutions.
To assess the correlation of the filtered spectrum and its corresponding glucose concentration, simple peak-to-peak evaluation was attempted. The filtered absorbance magnitude was calculated to be the maximum peak height at around 5935 cm\(^{-1}\) minus the midpoint of the two minimum values of the valley around 5880 cm\(^{-1}\) and around 5980 cm\(^{-1}\):

\[
A_{\text{filtered}} = S_{\text{max}}(5935 \pm 20 cm^{-1}) - \frac{(S_{\text{min}}(5880 \pm 20 cm^{-1}) + S_{\text{min}}(5980 \pm 20 cm^{-1}))}{2} \tag{4-2}
\]

Figure 4-5 and 4-6 show how this value changes as a function of glucose concentration for the 1-mm and the 10-mm pathlength respectively. For both cases, the magnitude of the absorbance seems to vary linearly with the glucose concentration. The rate of change is approximately \(2.3 \times 10^{-6}\) per mmol/L for the 2-mm pathlength, and \(1.1 \times 10^{-5}\) per mmol/L for the 10-mm pathlength. Thus, the signal increases by a factor of five in going from the short to the long pathlength. However, these are not the true absorbance values due to the application of the digital fourier filter. With careful analysis, the true absorbance value was estimated to be twice the filtered value.

![Figure 4-5](image_url)

Figure 4-5. Plot of Fourier-filtered "peak" intensity using equation 4-2 as a function of glucose concentration. (2-mm pathlength solutions).
To quantify the achievable resolution, the spectral noise has to be computed as well. The $r_{ms}$ noise value was measured to be $(2.5 \pm 0.5) \times 10^{-5}$ for the 2-mm pathlength and $(3.3 \pm 1.0) \times 10^{-5}$ for the 10-mm pathlength. Thus, taking the true absorbance value to be twice the filtered value, the signal-to-noise ratio for 1mmol/L concentration change is calculated to be 0.18 for the 2-mm pathlength and 0.67 for the 10-mm pathlength. These values can then be used to predict the achievable sensitivity or resolution with the given instrumental and experimental conditions. For example, assuming that it takes an SNR of two for an acceptable accuracy glucose concentration prediction, the resolution achievable is 11.1 mmol/L for the 2-mm pathlength and 3.0 mmol/L for the 10-mm pathlength. This relationship is described by the following equation:

$$SNR_{\text{glucose}} = \frac{A(v)}{\text{noise}_{\text{rms}}} = \frac{C}{r}$$  \hspace{1cm} (4-3)$$

where $A$ is the glucose absorbance signal for a certain mmol/L glucose change, $r$ is the achievable resolution in mmol/L and $C$ is a constant that specifies the SNR value needed for a prediction with an acceptable accuracy.
As mentioned before, Beer's Law states that the absorbance \( A(v_i) \) is a linear function of optical pathlength \( l \), sample concentration \( c \) and sample absorptivity \( \alpha \) at wavenumber \( v_i \):

\[
A(v_i) = \alpha(v_i)lc
\]  

(4-4)

It can be seen from figures 4-5 and 4-6 that the absorbance of aqueous glucose at 5935 cm\(^{-1}\) seems to vary linearly as a function of concentration. In addition, our experimental results using the two pathlengths (2\( mm \) and 10\( mm \)) suggest that the absorbance at this particular wavenumber also vary linearly with the optical pathlength, giving the glucose absorptivity \( \alpha(5935\text{cm}^{-1}) \) to be \( \sim 2.2 \times 10^{-5} \). Table 4-1 shows the summary of the results.

<table>
<thead>
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<th>Pathlength</th>
<th>( Rms ) noise</th>
<th>Filtered Absorbance per mmol/L</th>
<th>Absorbance ( 1\text{mmol/L} ) change</th>
<th>SNR for 1mmol/L change</th>
<th>Absorptivity ( \alpha(5935\text{cm}^{-1}) ) (mm mmol/L)(^{-1})</th>
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</thead>
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<tr>
<td>2( mm )</td>
<td>(2.5±0.5)( \times )10(^{-3})</td>
<td>( 2.3 \times 10^{-6} )</td>
<td>( 4.6 \times 10^{-6} )</td>
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<td>( 2.3 \times 10^{-6} )</td>
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<tr>
<td>10( mm )</td>
<td>(3.3±1.0)( \times )10(^{-3})</td>
<td>( 1.1 \times 10^{-5} )</td>
<td>( 2.2 \times 10^{-5} )</td>
<td>0.67</td>
<td>( 2.2 \times 10^{-6} )</td>
</tr>
</tbody>
</table>

Table 4-1. Summary of aqueous glucose experimental results.

It has been found that for a more accurate prediction of low glucose concentration, a more complex data processing algorithm observing a wider range of spectral range needs to be employed [1-12]. The most successful algorithm has been the partial least-squares regression analysis.

### 4.3 Improving Signal-to-Noise Ratio

In all our measurements, the SNR values are limited by the digitization noise due to the limited resolution of our 12-bit A/D converter. According to equation 3-15, an improvement of an order of magnitude would be achieved by using a 16-bit A/D
converter. Only then the noise due to the photodetector becomes significant. However, upgrading to a higher resolution board is not the only solution. Analyzing equation 3-15, a few possible alternatives become apparent. First, the number of scans can be increased to yield an improvement of $\sqrt{N}$, where $N$ is the number of scans. However, this may not be a practical solution, since long measurement time may invite other errors, such as sample degradation, temperature drifts and optical alignment changes, and all these for a modest improvement in SNR. For example, increasing the number of scans (and hence the measurement time) by a factor of 10 would improve the SNR value by a mere 3.2.

Another alternative is to reduce the number of spectral resolution elements. As for all spectroscopic measurements, maximum sensitivity is obtained by using the lowest resolution that adequately resolves the peaks of interest from the other interfering peaks [23]. It can be seen from the glucose absorbance figures above that the FWHH of glucose bands are greater than $50cm^{-1}$. Our spectrometer's resolution of $30cm^{-1}$ can sufficiently resolve glucose absorption bands, while preserving the sensitivity.

Another possible solution to our digitization noise limited problem is to increase the ratio of the observed wavenumber to the mean one $\frac{\rho(u)}{\rho_{\text{mean}}}$. We can do this by limiting the radiation by placing appropriate optical filter(s) to exclude the unnecessary wavenumbers from going to the detector and hence to the A/D converter. Improvement of an order of magnitude can be achieved this way.

Finally, when the detector noise becomes significant, two remedies should be carried out together: increasing the radiation source power and placing optical filter(s) in the same manner as above. By placing the optical filters, radiation detected would be more limited, and hence decreasing the term $W$ in equation 3-14. Increasing the radiation power would thus be needed. It is generally beneficial to increase the radiation power up to the point where sample degradation starts to become a concern.
5. CONCLUSION

In this work, sensitivity analysis of glucose concentration prediction using the near-infrared absorption technique is attempted. By comparison of the available absorption signal due to glucose in aqueous media with the noise value, the signal-to-noise ratio can be computed. This value can be used to predict the success of a certain instrumental and experimental condition.

By identification of the limiting source/s of error, one can attempt to improve the signal-to-noise ratio without exhaustive experimentation. One can also predict the SNR achievable on unfamiliar conditions by modeling the significant contributors of noise. For instance, in the case of glucose measurement in blood media, errors due to light scattering in the sample would be significant, and the radiation power arriving at the detector would be much reduced, rising the significance of detector noise. However, due to the scattering, the effective optical-pathlength would be increased. Therefore, large sample thickness, detector noise may become more significant than the digitization noise.

For the noninvasive application based on diffuse reflectance, the optical pathlength would be very limited, and the noise due to scattering and other tissue variability would probably be the limiting factors. Appropriate modeling of the available glucose signal as compared to the instrumental and sample noises should be done before attempting implementation and exhaustive experimentation.

A great deal of amount of work still needs to be done before realization of a noninvasive blood glucose monitoring device is possible. This thesis work presents the preliminary studies, and it shows that the near-infrared absorption technique is indeed feasible. The next task in this project is to apply the knowledge we gained from this work to maximize sensitivity. Experiments on more complex matrices, such as blood and tissue will be performed.
REFERENCES


30. Coherent-Ealing Catalogue


APPENDIX 1: Timing Circuit for Data Sampling

[Diagram of a timing circuit with various components such as comparators, XOR gates, and operational amplifiers.]

Schmitt Trigger

C 311

V_{in}

V_{out}

3.32k

0.75k

750k

+5
APPENDIX 2: Drive Mechanism Designs

Configuration 1:

In this design, tilts will not produce positional sampling error since the broadband light and the laser travels on the same optical path. However, tilt due to the aluminum plate and flexure deflections should be of concern, as the mirror is placed off-axis. Tilt due to plate deflection can easily be calculated as follows:

Assuming cantilevered beam with dimension: b(base) × h (height) × l length:
\[ x_{\text{max}} = \frac{Fl^3}{3EI} \quad (1) \]
\[ \phi_{\text{max}} = \frac{Fl^2}{2EI} \quad (2) \]
\[ I = \frac{1}{12}bh \quad (3) \]
\[ F = m \times a \quad (4) \]

where \( m \) is the mass of the plate and the mirrors, and \( a \) is the acceleration.

\( a \) is designed to be \( 1.6 \times 10^{-2} \text{ m/sec}^2 \). To be conservative, the mass of the plate is assumed to be concentrated at the end:

\[ m_{\text{total}} = m_{\text{mirrors}} + m_{\text{plate}} = (0.008 + 0.012)\text{Kg} \]

For an aluminum alloy, \( E \approx 8 \times 10^{10} \text{ N/m}^1 \)

Hence, for \( b = 2\text{cm}, h = 0.35\text{cm}, l = 5.3\text{cm} \), equation 1 yields a maximum deflection distance of 2.8nm. The maximum deflection angle is calculated according to equation 2 to be \( 7.9 \times 10^{-10} \text{ rad} \). These values are extremely small, and thus can be neglected. The maximum deflection angle, for instance is well within the limit imposed by equation 3-6 in chapter 3.

One issue to be concerned about is the deflection of the flexure supporting the plate during movement. Due to lack of data from the vendor and difficulties in determining it experimentally, this piece of information is not yet available. However, the system has proved to perform well to produce spectra with the specified resolution. Thus, for our current application, it is satisfactory.
Configuration 2:

Due to the geometry of the actuator and a retro-reflector or a prism, the distance between the broadband light and the laser, \( d \) would be greater than 2\( cm \).

\[ x = d \sin \varphi \]  

(5)

A typical maximum tilt of an air-bearing guide (which would be superior to a flexure) is \(~2 \times 10^{-6} \ \mu rad\). Thus, equation 5 yields a displacement of 40\( nm \). This is obviously a significant positional sampling error. Using equation 3-8, the SNR achievable due to this error is 133 for \( v_{\text{max}} \) of 7500\( cm^{-1} \). Not only does this type of error causes significant decrease in SNR value, it is also very difficult, if not impossible to compensate. This is because the noise frequency is identical to the modulation frequency of the interferogram.
APPENDIX 3: Ball-Bearing Mechanism Picture

Voice-coil actuator

Ball-bearing guide

Friction, $f$

Mirrors
APPENDIX 4: Photograph of Interferometer
APPENDIX 5: Photograph of FT-Spectrometer
### APPENDIX 6: List of Components

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<td>Rod, 200mm</td>
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<td>Lab View software</td>
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<td>68-conductor ribbon cable</td>
<td>System</td>
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<td>I/O connector w/ right angled</td>
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<td>Motion controller card</td>
<td>CB-68LPR</td>
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<td>PCI-FlexMotion-6C</td>
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<td>SH68-68-EP (1 meter)</td>
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<td>Actuator and Power Amplifier</td>
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<td>Mini shaker</td>
<td>Servo Dynamics SD 24-24 CT</td>
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<tr>
<td>Linear power amplifier</td>
<td>BEI LA13-12-000A</td>
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<td>Voice coil actuator (old mechanism)</td>
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<td>Miscellaneous</td>
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<td>Basic cleaning kit</td>
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<td>2 mm rectangular quartz cuvette</td>
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<td>10mm rectangular quartz cuvette</td>
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<td>Polyethylene cell rack</td>
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<td>Optical baseplate 0.6×0.9 meter</td>
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**Company Abbreviation:**

S&H: Spindler & Hoyer Inc.
LDS: Link Dynamic Systems Corporation
BEI: BEI Sensors and Systems Company
CVI: CVI Laser Corporation
APPENDIX 7: Program Codes

Program 1: Evaluating Spectrum Based on Time-Domain Averaging
   Note: Forward and Reverse direction is Fourier transformed separately.

function [freq, spec]=spectra(data);
scans=input('Number of scans?\n');
points=2000;
h=632.8*10^-7/8;
c=6000;
[max_val, max_ind]=max(data(c/6:c*10/6));
cur_ind=max_ind+c/6;

for k=1:scans
   if mod(k,2)==1
      yy_odd(:,k)=data(cur_ind:points:cur_ind+points);
y=data(cur_ind+c/6:cur_ind+c*10/6);
      [max_val, max_ind]=max(y);
cur_ind=cur_ind+c/6+max_ind;
k
   else
      yy_even(:,k)=data(cur_ind-points-4:cur_ind+points-4);
y=data(cur_ind+c/6-2:cur_ind+c*10/6-2);
      [max_val, max_ind]=max(y);
cur_ind=cur_ind+c/6+max_ind;
k
   end
end

y_odd_ave=sum(yy_odd,2)/(scans/2);
y_even=sum(yy_even,2)/(scans/2);
y_even_ave=fliplr(y_even);

%Triangular Apodization
for p=1:points*2+1
   tri(p)=1-abs(p-(points+1))/points;
end
tri_rot=rot90(tri);
y_tri=tri_rot.*y_odd_ave;
y_final=[zeros(3000,1);y_tri;zeros(3000,1)];
x=[-points*2:points*2];
 ffty=fft(y_final);
ffty(1)=[];
n=length(ffty);
spec_odd=sqrt(real(ffty(1:n/2)).^2+imag(ffty(1:n/2)).^2);

nyquist=1/(632.8*10^-7/4*2);
freq=(1:n/2)/(n/2)*nyquist;
plot(freq,spec)

for p=1:points*2+1
   tri(p)=1-abs(p-(points+1))/points;
end
tri_rot=rot90(tri);
y_tri=tri_rot.*y_even_ave;

y_final=[zeros(3000,1);y_tri;zeros(3000,1)];
x=[-points*2:points*2];
fft0=fft(y_final);
fft0(1)=[];
n=length(fft0);
spec_even=sqrt(real(fft0(1:n/2)).^2+imag(fft0(1:n/2)).^2);

nyquist=1/(632.8*10^-7/4*2);
freq=(1:n/2)/(n/2)*nyquist;

spec=(spec_odd+spec_even)/2;

Program 2: Evaluating Spectrum Based on Spectral-Domain Averaging

function [freq, spec]=spectra(data);
scans=input('Number of scans?
');
points=2000;
h=632.8*10^-7/8;
c=6000;

[max_val, max_ind]=max(data(c/6:c+c*10/6));
cur_ind=max_ind+c/6;

for k=1:scans
    yy(:,k)=data(cur_ind-points:cur_ind+points);
y=data(cur_ind+c/6:cur_ind+c*10/6);
    [max_val, max_ind]=max(y);
cur_ind=cur_ind+c/6+max_ind;
    k

    %Triangular Apodization
    for p=1:points*2+1
        tri(p)=1-abs(p-(points+1))/points;
    end
    tri_rot=rot90(tri);
    y_tri=tri_rot.*yy(:,k);
    y_final=[zeros(3000,1);y_tri;zeros(3000,1)];
    fft0=fft(y_final);
    fft0(1)=[];
n=length(fft0);
spec_temp(:,k)=sqrt(real(fft0(1:n/2)).^2+imag(fft0(1:n/2)).^2);
nyquist=1/(632.8*10^-7/4*2);
freq=(1:n/2)/(n/2)*nyquist;
end
spec=sum(spec_temp,2)/scans;
plot(freq,spec)
Program 3: Fourier Filtering with a Gaussian-Shaped Filter

function [spec_final,gaus]=fourier_filter(data)
data=data(912:970);
x=[1:1:59];
x=flipud(rot90(x));
sigma=1.25;
mu=5;
gaus=1/(sigma*sqrt(2*pi))*exp(-((x-mu).^2/(2*sigma^2)));
gaus=1/max(gaus1).*gaus1;

ftdata=fft(data);
filt_data=ftdata.*gaus;
inv_data=ifft(filt_data);
spec_final=real(inv_data(1:59))+imag(inv_data(1:59));

Program 4: Evaluating SNR About a Third-Order Polynomial Fit

function [y,snr]=curve_fit(data)

degree=input('Degree of polynomials?\n');
x1=input('frequencies to observe?');
x=[1:1:length(x1)];
x=rot90(rot90(rot90(x)));
p=polyfit(x,data(x1),degree);

for i=1:length(x1)
    y(i)=p*[i^3;i^2;i;1];
end

rms=sqrt((1/length(x1))*sum((data(x1)-flipud(rot90(y))).^2));

snr=1/rms;

abs_data=data(x1);
y=flipud(rot90(y));
peak=abs_data-y;
**APPENDIX 8: Circuit for Motion Control Feedback Signal**

Schmitt Trigger

![Circuit Diagram]

\[
\text{High Treshold} = \left( \frac{12}{R_1} + \frac{5}{R_3} \right) \frac{R_1 R_2 R_3}{R_1 R_2 + R_1 R_3 + R_2 R_3}
\]

\[
\text{Low Treshold} = \frac{12 R_2 R_3}{R_1 R_2 + R_1 R_3 + R_2 R_3}
\]