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Estimation of Wavelength for Measuring Blood Urea using Near Infrared Spectroscopy

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Abstract—*This paper details about the estimation of the proper wavelength for urea using near infrared spectroscopy (NIRS). Theoretical analysis is carried out in order to find out the wavelength of peak absorption. These results are correlated with the experimental data obtained with FTIR spectrometer. It is found that the second overtone falling at 995nm of N-H stretch vibration is more optimal solution for analyzing the Urea sample with minimal cost.*

Keywords: *Near-infrared Spectroscopy;Second overtone; Urea.*

1. INTRODUCTION

Blood ureais the most commonly used blood test to screen for and monitor renal disease.Urea is the waste product of breakdown of protein. The level of these substances rises in the blood as kidney function worsens.It also increases the risk of heart stroke and other heart diseases [1]. More frequent monitoring of concentration of urea in blood is required for identifying acute renal failure. Currently used equipment for the self-monitoring of blood urea is invasive and usually requires pricking of finger tip which is painful. It also involves risk of spreading infectious diseases.

In order to overcome the disadvantages of the invasive methods some non invasive methods have been proposed. However they have the disadvantages require heavy, delicate and expensive instruments like Raman spectroscopy [2], and polarimetric method [3]. For the non-invasive measurement of the blood urea most of the research is done based on Photoplethsymography(PPG) in the mid infrared (2µm-2.5µm) and first overtone regions (1.53µm-1.82µm) [4-6] as the fundamental frequencies and first overtones fall under these regions. The absorbance of the urea bonds (N-H, C=O) is strong in this region [7-8]. The major disadvantage in these regions is due to three reasons. Firstly the drastic rise in the price of components and secondly the strong absorption due to other components like water and lastly the scattering in fatty tissue [9]. This makes the mid and first overtone regionseconomically not viable for developing a noninvasive methodology for estimating the blood urea concentration. This paper details about the identification of the proper spectrum in the nearinfra-red part of the spectrum. Here the cost of the components is less but urea has weaker absorption and it requires the electronic noise in the analog front end to be suppressed much below the signal from the sensor output. Here we have done theoretical analysis based on the molecular structure of the urea and in the next step carried out the experiments on aqueous urea using FTIR spectrometer. After which an LED and a photodiode comprising of optode pair is used to justify whether the wavelength of monitoring identified correlates with the theoretical analysis.

2. THEORETICAL ANALYSIS

2.1 Vibrational modes based on Molecular composition

When a photon is incident on a molecule, there will be bond deformations or bond vibrations at different energy levels related to different bonds, depending on the energy of incident photon [10]. So, only the photon with energy that corresponds to the difference between two of its energy levels can be absorbed. The frequency of the vibration is given by the

$$\vartheta = \frac{1}{2\pi}\sqrt{\frac{k}{m}} \quad (1)$$

Where ‘k’ is the bond strength and ‘m’ is the reduced mass.

For a urea molecule, the molecular structure is as shown in Fig1. Table 1 shows the frequencies corresponding to different bond vibrations in urea molecule [8].

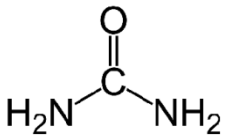

Fig. 1: Molecular structure urea molecule.

Table 1. Absorption bands of urea molecule

Wavelength(nm)	Bond
1160	C=O fourth overtone
1460	Symmetric N-H stretch first overtone
1520	N-H stretch first overtone
1990	N-H stretch/N-H bend combination

2030	C==O stretch second overtone
2070	N-H deformation overtone

At a deeper level absorption of light can be seen as dependent on the probability ofabsorbance of a photon by the molecule. For nth overtone final energy is (n+1)*E, where E is the fundamental energy. As n increases, probability of absorbance decrease rapidly and hence intensities of absorbance decrease as overtones increase. The absorption at fundamental frequency is calculated and from that the absorption at second overtone is calculated relatively [11].

3. WAVELENGTH SELECTION BASED ON PEAK ABSORPTION

The absorption spectrum of the urea has been studied in order to choose the wavelengths for LEDs. For this purpose a IR absorption spectrum of 0.1M aqueous urea solution has been collected and analyzed in second overtone region of the near-infra red spectra using the Bruker tensor 27 FTIR spectrometer. Fig.2 shows the absorption spectrum of the urea over the second overtone region. From the spectra obtained the optimal wavelength where the absorption is considered suitable for urea extraction. We can observe that the absorption peaks in this region are very narrow typically of the order of the 2nm to 5nm but the LED emits the light over a range of wavelengths. The wavelengths are chosen such that the weighted average of the absorption over the spectral bandwidth of the LED is high. While calculating this weighted average the intensity of light emitted by the LED acts as weight for the absorption at that particular wavelength.

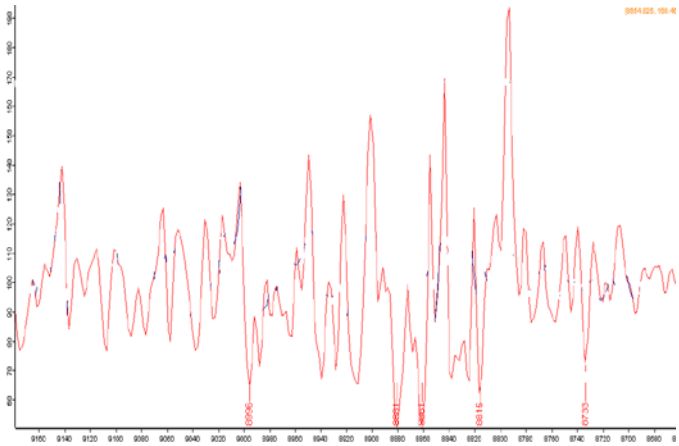

Fig. 2: Spectrum showing the transmitance of glucose

In order to verify whether the theoretical results obtained based on the molecular composition of urea are matching with the experimental results. We have conducted the experiments with FTIR spectrometer to get the IR spectrum of the aqueous urea and analyzed the spectrum to get the wavelength in the range of 750 to 1100nm and it is found that 995nm is an appropriate wavelength for studying the characteristics of urea.

In order to justify the results obtained an experiment is carried out with optical components like LED and photodiode comprising an optode pair which is discussed in the below section.

4. EXPERIMENTAL SETUP

4.1 Photoplethysmography (PPG)using optode pair

Photoplethysmography is an optical technique widely used to measure the pulse rate, arterial blood oxygen saturation and blood volume changes. It uses a clip which contains a light source and a detector on the opposite sides to detect the cardio vascular pulse wave that propagates through the body. The PPG waves can be described as containing a DC component due to venous blood and an AC component due to blood volume changes in the arteries.

According to Beer-lambert's law the absorbance of light by a liquid is related to the concentration of the material by

$$A = \in Cl \quad (3)$$

Where $\in$ the molar absorptivity of solute at a particular wavelength, C is is the concentration of the solute and l is the path length.

From this we can say that if the intensity (Peak to peak value) of the PPG is high then the absorbance of the chromophore is high in that region, which is in turn directly proportional to the concentration of the chromophore. Fig3. Shows the basic PPG waveform with different components.

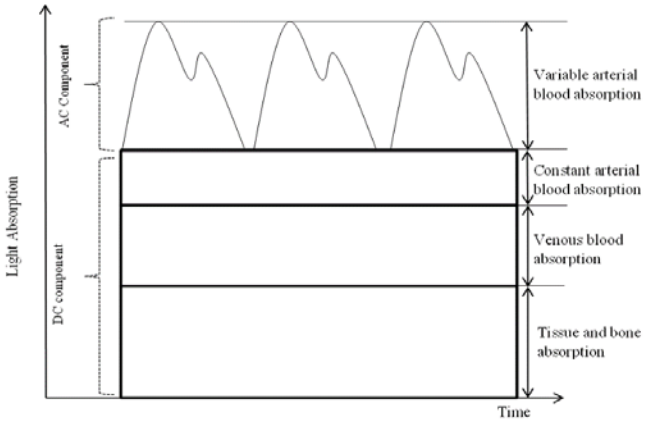

Fig. 3: PPG waveform showing the Basic components

4.2 Testing using optode pair

As discussed in the previous section, the wavelength of peak absorption for urea has been chosen to 995nm.The block diagram of the experimental set up for getting PPG is shown in the Fig.3.

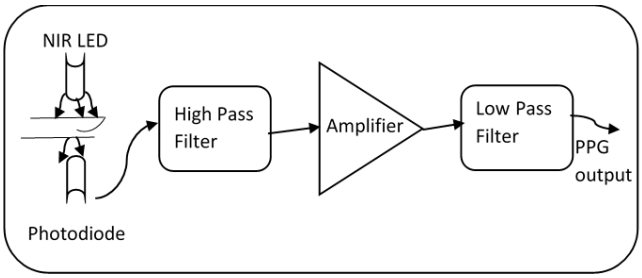

Fig. 4: Experimental setup to obtain PPG

It consists of the finger clip with LED acting as a light sensor and the photodiode as the detector to detect the small changes in the incident light as it passes through the finger. This light is converted in to an equivalent current by the detector and is high pass filtered with a cut off frequency of 0.8Hz. Then it is given to the trans-impedance amplifier for amplification of the signal. After this the signal is low-pass filtered to get the required PPG which is mainly because of the urea. The cut off frequency for low pass filter is 10Hz. Fig. 6 shows the PPG waveform.

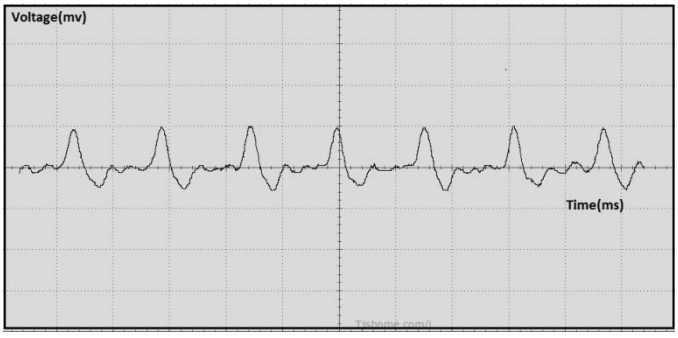

Fig. 5: PPG waveform obtained using urea specific optode pair

From the above figure we can infer that the PPG signal with good intensity signifies that the wavelength identified for estimation of urea in blood is appropriate.

5. CONCLUSION

In the current work, we have attempted to identify a wavelength which falls in the near-infra red part of the region. Theoretical analysis has been carried out based on the vibrational modes of the different bonds present in the urea molecule. The resulting wavelength from theoretical analysis has been first counter checked with the experiment with FTIR spectrometer with aqueous urea solution. Finally it is justified by conducting an experiment with optoelectronics, where the output with high intensity signifies the correlation between the results. The wavelength identified is about 995nm which falls in the near infrared region.

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