

**Detection and Measurement of Methyl Tert-Butyl Ether (MTBE)
Contamination in Ground Water using
UV-Vis and FTIR**

by

Mohammad Ilham Bin Mat Hussin

Dissertation submitted in partial fulfilment of
The requirement for the
Bachelor of Engineering (Hons)
(Chemical Engineering)

SEPTEMBER 2012

Universiti Teknologi PETRONAS
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CERTIFICATION OF APPROVAL

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Approved by,

(Ir. Dr. Abdul Halim Shah bin Maulud)

UNIVERSITI TEKNOLOGI PETRONAS
TRONOH, PERAK
SEPTEMBER 2012

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

MOHAMMAD ILHAM BIN MAT HUSSIN

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Finally, I would like to appear my hope that I can apply what I learnt when finished my study soon.

ABSTRACT

Methyl tert-butyl ether (MTBE) is a volatile oxygenate commonly used in fuels, is a frequent contaminant of the ground water. The contamination mostly in the Europe and United States has become widespread due to the mandated use of automobile gasoline oxygenated with MTBE.

Because of this issue, a lot of technology has been developed in order to detect the contamination and overcome this problem. For example, the current technology exist using gas chromatography such as EPA method 8021B by using photo ionization detection (PID). However, it has its own limitation and weakness to employ the detection. Therefore, efficient analytical technique is necessary to quantify MTBE in ground water.

This research is to determine the lowest concentration of MTBE contamination that can be detected by using the UV-Vis or FTIR. In addition, it is also to establish appropriate correlation between UV-Vis and FTIR. The advantage of using these methods is that it will provide with faster measurement.

The outcome from this research shows that the UV-Vis equipment does not accurate enough to detect the MTBE contamination in water. It shows inconsistence reading through the graphs and data taken. While for FTIR equipment is more reliable and can detect the MTBE contamination in water better compared to UV-Vis equipment. Correlation for FTIR can be observed on the Results and Discussions section.

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CHAPTER 1

INTRODUCTION

1.1 PROJECT BACKGROUND

Nowadays, the technology of fuels has become increasingly modern. Many research and study has been done in order to get the best fuels consumption. One of the technology is the development of oxygenates.

The development of oxygenates such as MTBE are widely used in the USA and other European countries as the additive in the fuel and gasoline. The United States is the largest producer among the 38 nations producing MTBE. In each year during 1994-98, U.S. MTBE production was more than four times that of the second largest MTBE- producing nation, Saudi Arabia; it was also more than the combine annual production of the next eight leading producer nations ^[1].

It is come into problem when the storage of MTBE in the underground gasoline tanks has leakage and caused the ground water contamination ^[2]. It is mainly affected the countries that used this fuel technology. Because of that, some of the standards and regulation has been gazette to overcome this issue. It can cause the bad effects in term of environment and health. Prior to that, we have to know the allowable limits of the MTBE contamination in the ground water so that we can control this problem.

1.2 PROBLEM STATEMENT

In recent years, MTBE has been detected extensively in groundwater supplies and other water reservoirs at different sites, especially in USA and other Europe countries. MTBE is one of the most frequently detected volatile organic compounds in groundwater and, thus, has become a priority groundwater pollutant over the previous decade. The most concern about MTBE has come from its contamination of ground water.

Therefore, researches on several analytical techniques are carried out in order to measure the contamination.

1.3 OBJECTIVES AND SCOPE OF STUDY

The objectives of this study are:-

- 1) To measure the lowest detectable limit of MTBE contamination in water using UV-Vis and FTIR.
- 2) To establish the correlation between spectrums of UV-Vis and FTIR with MTBE concentration in water.

The scope of the study will be based on the information and study case that happen around the world especially at the USA and Europe. This is due to the most production and consumption that comes from there. Several experiments will be conducted by using distilled water and mineral water to achieve the above objectives.

CHAPTER 2

LITERATURE REVIEW

2.1 WHAT IS MTBE?

In the past, oxygenates, such as methyl tert-butyl ether (MTBE) were developed in the 1970's. The purpose of oxygenates were as octane enhancers to replace toxic additives, such as lead, which were being phased out of gasoline. The presence of oxygenates in gasoline promotes cleaner fuel combustion within the engine, boosts fuel-octane values and reduces air emissions from vehicles ^[3]. Two types of oxygenates are commonly used in gasoline: ethers and alcohols. MTBE is by far the most commonly used ether oxygenates, due to its high-octane properties, cost effectiveness and supply flexibility.

2.2 ALTERNATIVES BESIDES MTBE

Besides that, there are other alternative fuel oxygenates include several alcohols and other dialkyl ethers. However, only methanol (in blends with gasoline) in Brazil, ethanol (mainly in US Mid-west), tert-amyl methyl ether (TAME) in Finland, and ethyl tert-butyl ether (ETBE) in France, Spain, Italy are of economic importance today. Tert-butyl alcohol (TBA) is of considerable interest mainly because it is the key intermediate in the degradation of MTBE and ETBE ^[4].

2.3 CASE STUDY FOR MTBE CONTAMINATION

The use of the fuel oxygenate MTBE in gasoline has led to intense discussion about its environmental benefits and impacts in the USA and Europe. However, the situation in Europe and USA differs substantially with respect to the use and emission of MTBE ^[4]. In recent years, MTBE has been detected extensively in ground water supplies and other water reservoirs at different sites, especially in the USA ^[2]. The ground water problems have given a huge quantity of scientific studies, media coverage, and reports. The bad effects on human health and the environment area a growing cause for concern. It is because the MTBE contamination of ground water has come from leaking underground gasoline tanks. In the USA, the 1990 Amendments to the Clean Air Act still require a minimum oxygen content of 2.7%

(w/w) for oxyfuels and 2.0% (w/w) for reformulated gasoline in CO and Ozone non-attainment areas, respectively. In the European Union, there is no least requirement but the addition of up to 15% (v/v) is allowed ^[4].

2.4 PROPERTIES OF MTBE

Compared with classical fuel-related contaminants, such as benzene and other aromatics, alcohol and ethers have higher water solubility, lower Henry's Law constant and lower sorption constants. These properties make them more difficult to determine at trace levels ($\mu\text{g/L}$ range and below) in aqueous sample ^[4]. In ground water, MTBE is more resistant to degradation than other fuel constituents of environmental concern, in particular under anaerobic conditions ^[4].

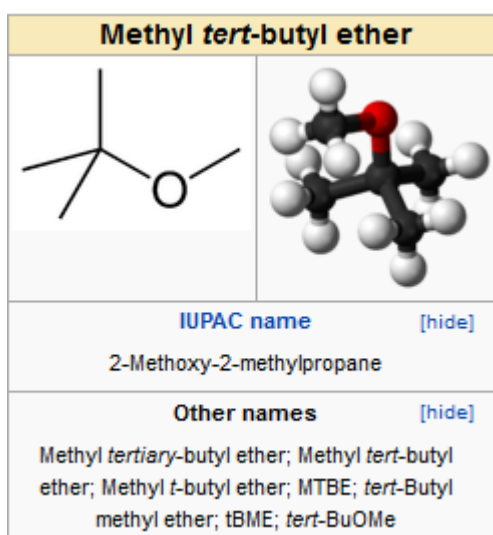


Figure 1: MTBE graphic structure ^[6]

Properties	
Molecular formula	C ₅ H ₁₂ O
Molar mass	88.15 g mol ⁻¹
Density	0.7404 g/cm ³
Melting point	-109 °C, 164 K, -164 °F
Boiling point	55.2 °C, 328 K, 131 °F
Solubility in water	26 g/L (20 °C) ^[1]

Figure 2: MTBE properties ^[6]

2.5 ALLOWABLE LIMIT STANDARDS

Efficient analytical techniques are necessary for quantifying MTBE in water at least as low as 20-40 $\mu\text{g/L}$ which is the limit level of concern for odor and taste (Environmental Protection Agency (EPA), 2002) ^[5]. Based on current MTBE toxicology data with emphasis on carcinogenic potential and reproductive and development effects, a maximum drinking water level of 100 μg MTBE/L is suggested.

2.6 CURRENT TECHNOLOGY FOR DETECTION

There are many analytical techniques that may be used to quantify MTBE in water with gas chromatography, such as EPA method 8021B by using photo ionization detection (PID), EPA method 8260B with mass selective detection (MS), and ASTM method D4815 using flame ionization detection (FID). These methods are successfully applied with method detection limits for MTBE in purified water of 0.2, 0.2-1.0, and 1.1 $\mu\text{g/L}$ for each of the methods respectively. For MTBE, injection techniques such as direct aqueous injection, purge and trap, and headspace methods are employed. SPME is a recently developed technique to concentrate analytes prior to thermal desorption in a GC injection port. The wide variety of SPME extraction materials available provides a technique amenable for concentrating polar and non-polar compounds from water. SPME has been successfully used for MTBE analysis with method detection limits as low as 1 $\mu\text{g/L}$ ^[2]. Besides that, other methods for decomposing VOCs in contaminated water are air stripping, adsorption to granular activated carbon, biodegradation processes, and advanced oxidation processes (AOPs).^[6]

2.7 UV-VIS

Ultraviolet–visible spectroscopy or ultraviolet-visible spectrophotometry (UV-Vis) refers to absorption spectroscopy or reflectance spectroscopy in the ultraviolet-visible spectral region. This means it uses light in the visible and adjacent (near-UV and near-infrared (NIR)) ranges. The absorption or reflectance in the visible range directly affects the perceived color of the chemicals involved. In this region of the electromagnetic spectrum, molecules undergo electronic transitions. This technique is complementary to fluorescence spectroscopy, in that fluorescence deals with transitions from the excited state to the ground state, while absorption measures transitions from the ground state to the excited state.^[8]



Figure 3: Beckman DU640 UV-Vis Spectrophotometer^[9]

Molecules containing π -electrons or non-bonding electrons (n-electrons) can absorb the energy in the form of ultraviolet or visible light to excite these electrons to higher anti-bonding molecular orbital. The more easily excited the electrons, the longer the wavelength of light it can absorb.

UV/Vis spectroscopy is commonly used in analytical chemistry for the quantitative determination of different analytes. Spectroscopic analysis is commonly carried out in solutions but solids and gases may also be studied.

Solutions of transition metal ions can be colored because d electrons within the metal atoms can be excited from one electronic state to another. The color of metal ion solutions is strongly affected by the presence of other species, such as certain anions or ligands.

Besides that, every compound has its own degree of absorption. Organic compounds, especially those with a high degree of conjugation, also absorb light in the UV or visible regions of the electromagnetic spectrum.

The Beer-Lambert law states that the absorbance of a solution is directly proportional to the concentration of the absorbent in the solution and the path length. For a fixed path length, UV/Vis spectroscopy can be used to determine the concentration of the absorber in a solution.

The presence of an analyte gives a response assumed to be proportional to the concentration. For accurate results, the instrument's response to the analyte in the unknown should be compared with the response to a standard. The wavelengths of absorption peaks can be correlated with the types of bonds in a given molecule and are valuable in determining the functional groups within a molecule.

The method is most often used in a quantitative way to determine concentrations of an absorbing species in solution, using the Beer-Lambert law:

$$A = \log_{10}(I_0/I) = \epsilon \cdot c \cdot L,$$

where A is the measured absorbance, I_0 is the intensity of the incident light at a given wavelength, I is the transmitted intensity, L the path length through the sample, and c the concentration of the absorbing species. For each species and wavelength, ϵ is a constant known as the molar absorptivity or extinction coefficient. This constant is a fundamental molecular property in a given solvent, at a particular temperature and pressure, and has units of $1/M \cdot cm$ or often $AU/M \cdot cm$.

The absorbance and extinction ϵ are sometimes defined in terms of the natural logarithm instead of the base-10 logarithm.

Below are the basic steps-to steps procedure to run the UV-Vis instrument:-

- 1) Connect the power supply to the instrument
- 2) Switch on Instrument and PC.
- 3) Click on the UVProbe software. Once the software open, clicks CONNECT. A series of test will be automatically conducted which takes about five minutes. Make sure all checklists are green.
- 4) Before perform the analysis, set the method according to you requirement. To do so, Click button M.
- 5) Then save the method. Click FILE menu. Create your own folder.
- 6) Calibration must be performed using BaSO₄ as the standard. Place the BaSO₄ sample cell at sample holder. Then click BASELINE. Wait until the calibration finish, and then click AUTOZERO.
- 7) Prepare your own sample into the sample cell. Press the sample to make sure no powder will come off when it is inserted into the instrument. Typical thickness for the sample is 3mm.
- 8) Place your sample at the sample holder and click button START. Measurement will start. Wait until you are instructed to save the file. Click OK.
- 9) Click on OPERATION menu, choose manipulate button. Select equation type according to your requirement. Then, Save all.
- 10) To save the graph, move your cursor on the graph and right click on your mouse, select Copy. Then open Paint, paste in the new file and save.
- 11) You can also copy raw data to construct the graph using Microsoft Excel. To do so, click on OPERATION menu, go to Data Print. Raw data table will be displayed on the right of the monitor. Select and copy all the data, paste into a new text document then save.

- 12) Once you have finish with your current sample, click FILE menu, select Properties and delete the current sample file. The new page will be displayed.
- 13) Now you can start to analyze the next sample by repeating step 5 until step 10.
- 14) After completing all analysis, click button DISCONNECT.
- 15) Make sure the software is already disconnected with the instrument.
- 16) Switch OFF Instrument and PC.

2.8 FTIR

Fourier transform infrared spectroscopy (FTIR), ^[10] is a technique which is used to obtain an infrared spectrum of absorption and emission of a solid, liquid or gas. An FTIR spectrometer simultaneously collects spectral data in a wide spectral range. This confers a significant advantage over a dispersive spectrometer which measures intensity over a narrow range of wavelengths at a time. The term *Fourier transform infrared spectroscopy* originates from the fact that a Fourier transform (a mathematical algorithm) is required to convert the raw data into the actual spectrum. The goal of any absorption spectroscopy is to measure how well a sample absorbs light at each wavelength. By using this technique, rather than shining a monochromatic beam of light at the sample, it shines a beam containing many different frequencies of light at one shot, and measures how much of that beam is absorbed by the sample. Next, the beam is modified to contain a different parameter combination of frequencies, giving a second data point. This process is repeated many times. Afterwards, a computer takes all these data and works backwards to infer what the absorption is at each wavelength.

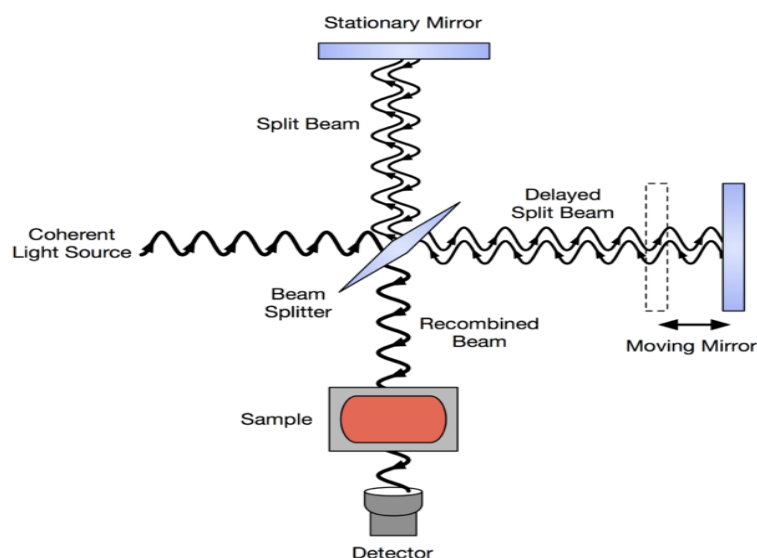


Figure 4: Schematic diagram of a Michelson Interferometer, configured for FTIR^[11]

Below are steps-by-steps on how Michelson Interferometer configured for FTIR works:-

- 1) One beam reflects off a flat mirror which is fixed in place. Another beam reflects off a flat mirror which travels a very short distance (typically a few millimeters) away from the beam splitter.
- 2) The two beams reflect off of their respective mirrors and are recombined when they meet together at the beam splitter. The re-combined signal results from the *interfering with each other*.
- 3) The resulting signal is called interferogram, which has every infrared frequency encoded into it.
- 4) When the interferogram signal is transmitted through or reflected off of the sample surface, specific frequency of energy are absorbed by the sample due to the excited vibration of functional groups in molecules.
- 5) The infrared signal after the interaction with the sample is uniquely characteristic of the sample.
- 6) The beam finally arrives at the detector and is measured by the detector.

- 7) The detected interferogram cannot be directly interpreted. It has to be “decoded” with well-known mathematical technique called *Fourier Transform*.
- 8) The computer performs the Fourier transformation calculation and presents an infrared spectrum – plot absorbance (or transmittance) vs. wave number.

Below are the basic steps-to steps procedure to run the FTIR instrument:-

- 1) The sample is prepared by grinding 1 to 3 mg of unknown sample into fine powder using agate mortar.
- 2) Approximately 250 to 300 mg of standard sample is weighted using small scoop.
- 3) The unknown sample and standard sample is grinded together using agate mortar.
- 4) The mixture of unknown sample and standard sample is transferred into the die.
- 5) The die is placed into the hydraulic pressure. Vacuum is applied for 1 minute before the pressure is gradually increased to 10 tons for 1 minute.
- 6) The pressure and vacuum are released. The disc of unknown sample and standard sample is formed.
- 7) The unknown sample – standard sample mixture disc is removed and transferred to the sample holder. All the steel parts are cleaned from any previous residue sample prior to transferring to sample holder.
- 8) The name of the sample is keyed in.
- 9) The sample holder with the sample is placed into the Spectrum One.
- 10) The spectrum of the sample is scanned.
- 11) The spectrum of the sample is analyzed for its concentration.

CHAPTER 3

PROJECT WORK / METHODOLOGY

Methodology and project work of this research has been constructed in order to overview the flow and forecast the results so that the objectives of this research can be determine whether it is achievable or not.

3.1 PROJECT WORKS

The project works flow is as the figure below:-

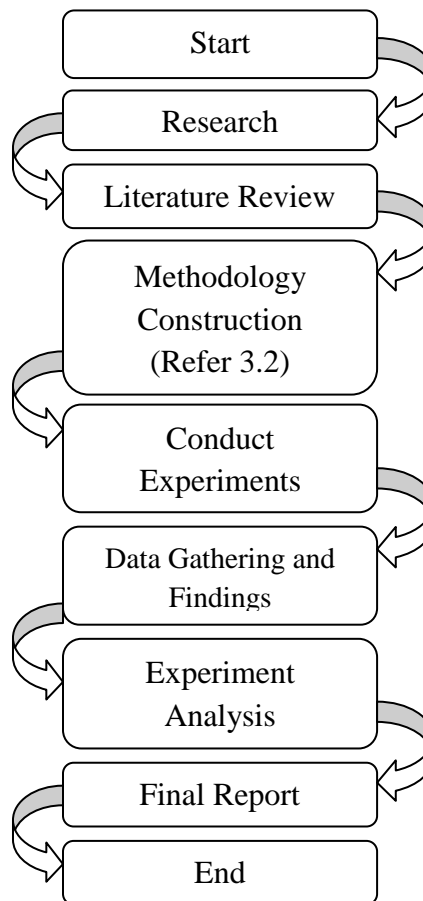


Figure 5: Project Activities Flow

This project is an experiment base project. Specifically, it is a study to measure the lowest detectable limit of MTBE contamination in water using UV-Vis and FTIR. First and for most, the project will begin with the research on MTBE and all the things which are related to it. With the collective information, the project will proceed with the literature review on MTBE effects to the environment, its properties, allowable limits according to the authority standards, and other current technology to measure the MTBE concentration. All of this information is coming from the several journals and websites. After completing the literature review, the further studies will move on to the drafting and finalization of methodology on how to conduct experiment and research.

Lastly, all the studies and discussion will be compiled in the final report. Apart from that, the findings and analysis will be further explain and justifies. The operational and safety requirements also can be developed from the study.

3.2 RESEARCH METHODOLOGY

Research is a method taken in order to gain information regarding the major scope of the project. The sources of the research cover the e-journal, e-thesis, handbook, and several trusted link. Reference used must be related to the MTBE.

The steps of methodology:

1. Preparation of sample.
 - Several trials of experiments will be done with different concentration of MTBE. For examples, by using 50%, 40%, 30%, 20%, and 10% of MTBE concentration for the samples and test them with the UV-Vis and FTIR.
2. Identify the characteristics of UV-Vis and FTIR.
 - Spectrum generation using UV-Vis and FTIR.
3. Specific research and on the experiments.
 - Perform spectrum analysis.

3.3 EXPERIMENT METHODOLOGY

- 1) Weigh 1 ml of MTBE.
- 2) Purge 1 ml of MTBE into volumetric flask and filled it with distilled water for dilution.
- 3) Proceed the dilution process for several times until it achieves the desired concentrations.
- 4) After achieved the desired concentration, take the samples and test them with UV-Vis equipment.
- 5) Collect and analyze the results interpretation from the UV-Vis equipment.

3.4 ACTIVITIES/GANTT CHART AND MILESTONES

Below are the activities gantt chart and the milestones of this research for the first phase:-

No	Detail/Week	1	2	3	4	5	6	Mid-Semester Break	7	8	9	10	11	12	13	14	
1	Selection of Project Topic: Development of Reliability Model for System with Rare Failure Analysis	■	■														
2	Preliminary Research Work: Research on literatures related to the topic		■	■	■												
3	Submission of Draft Project Proposal					●											
4	Submission of Project Proposal						●										
5	Project Work: Study on the research scope and method								■	■							
6	Submission of Progress Report										●						
7	Project work continues: Further investigation on the project and do modification if necessary								■	■	■	■	■	■	■		
8	Submission of Interim Report Final Draft															●	
9	Oral Presentation								During Study Week								

Table 1: Gantt chart and Key Milestone (First Semester)

Below are the activities gantt chart and the milestones of this research for the second phase:-

No	Detail/Week	1	2	3	4	5	6	Mid-Semester Break	7	8	9	10	11	12	13	14	
1	Weekly consultation with supervisor			■	■	■	■		■	■	■	■	■	■	■		
2	Project work continues: Further investigation on the project	■	■	■	■	■	■		■	■	■	■	■	■	■		
3	Submission of Progress Report									●							
4	Submission of Final Report Draft												●				
5	Project Final Presentation														●	●	

Table 2: Gantt chart and Key Milestone (Second Semester)

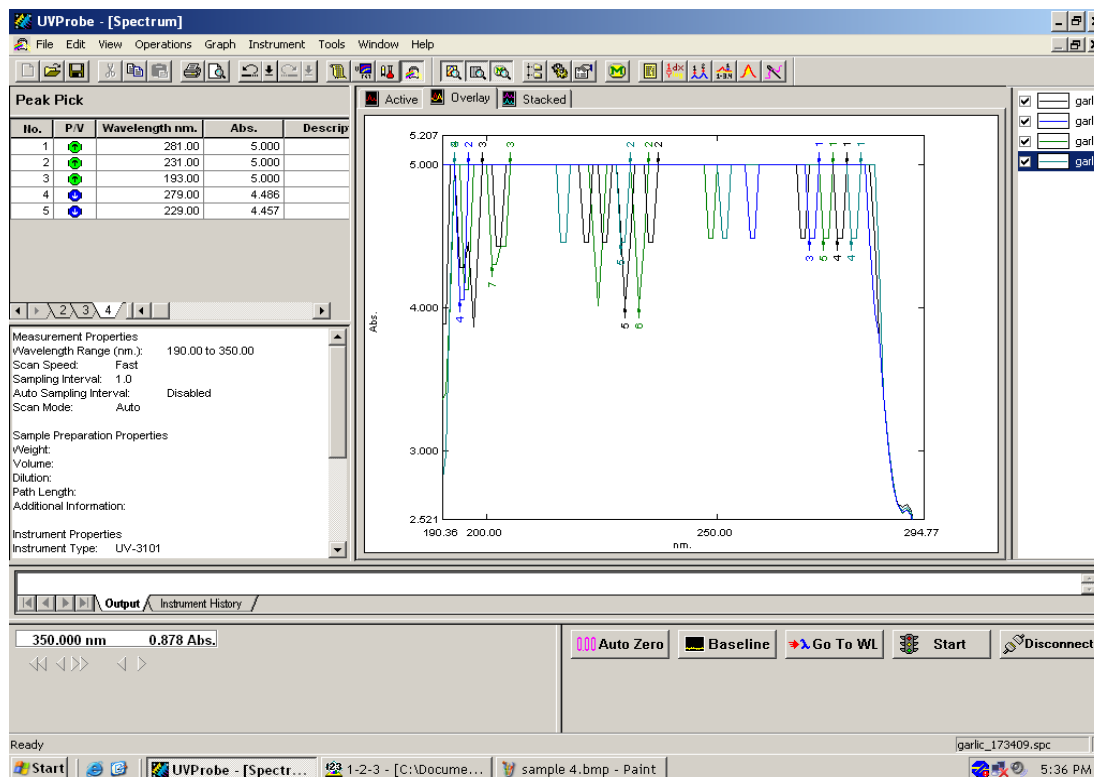
CHAPTER 4

RESULTS AND DISCUSSIONS

Samples have been tested using UV-Vis and FTIR equipment. From there, data and graphs have been taken so that we can justify and analyze from the findings. Samples that we tested were 7.6×10^{-3} mol/L, 7.6×10^{-6} mol/L, 0.45×10^{-6} mol/L, and 0.23×10^{-6} mol/L. Below were the results taken from the UV-Vis equipment:-

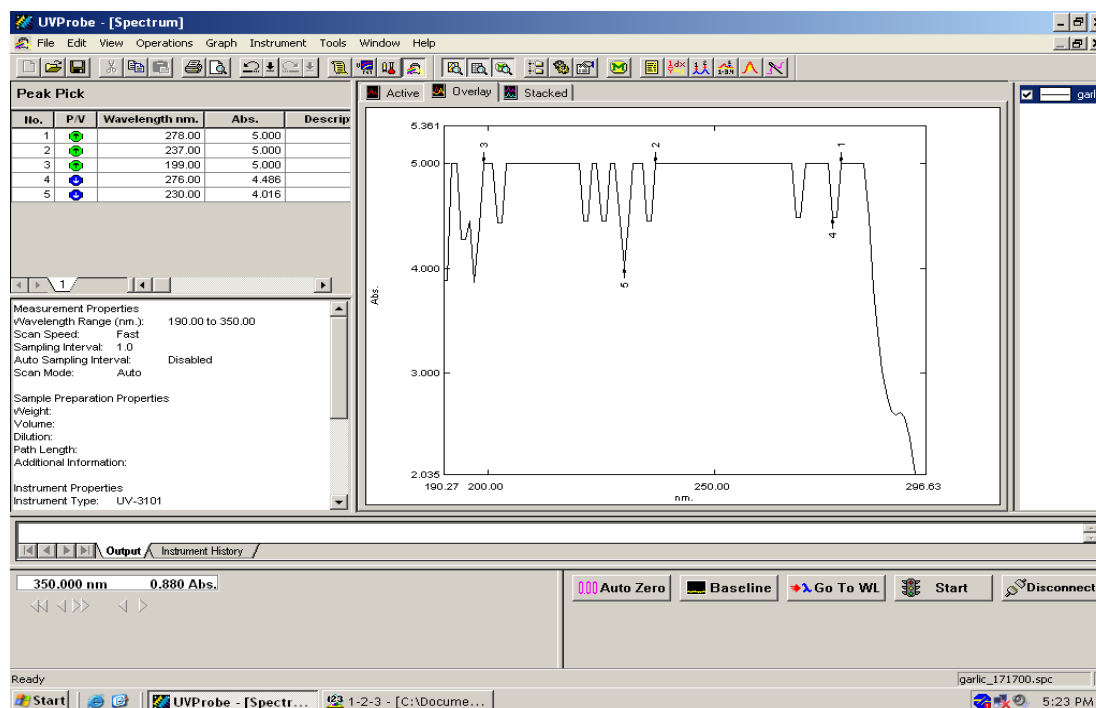
4.1 RESULTS OF UV-VIS EQUIPMENT

4.1.1 Combine Graphs of different concentrations



The combine graphs above showed the peak values of different concentrations of MTBE. We can observe some inconsistency of readings between the graphs of different concentrations according to the respective region of after 250 nm and before 250nm of wavelength.

4.1.2 Sample of 7.6×10^{-3} mol/L

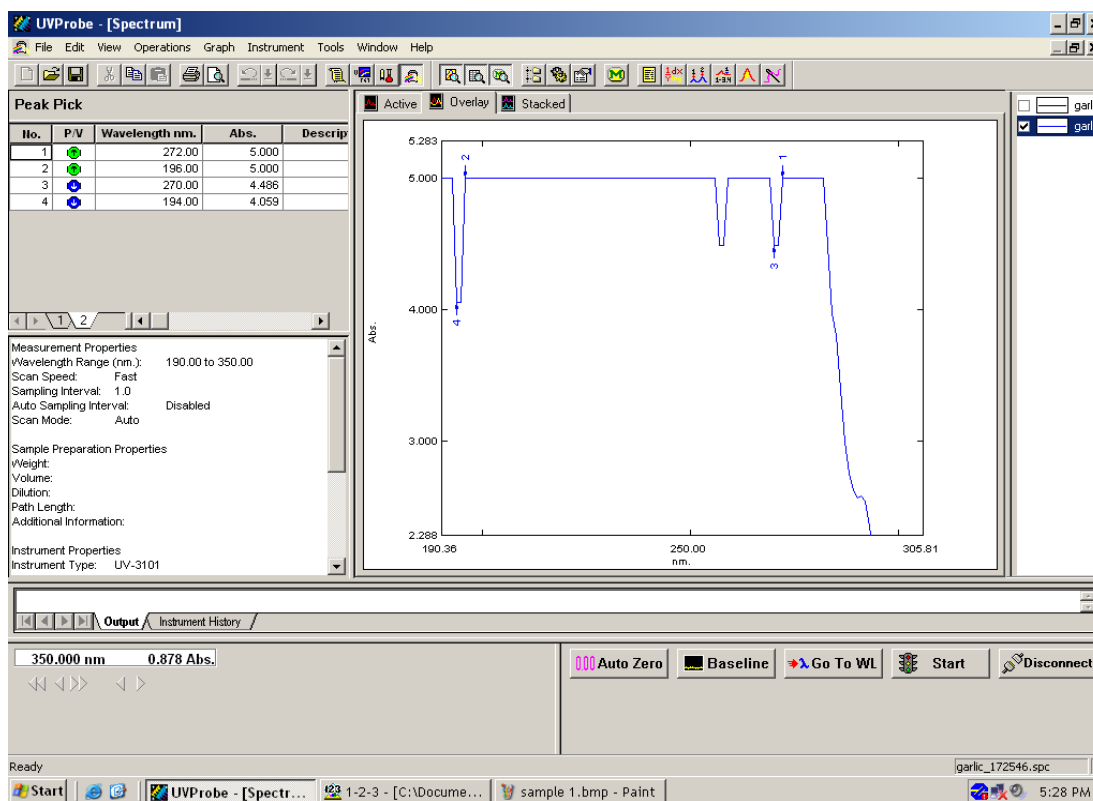


The graph above shows the peak value reading for 7.6×10^{-3} mol/L concentration of MTBE in water. Chosen peak values have been recorded at the table below.

No.	P/V	Wavelength nm.	Abs.
1	Crest	278	5
2	Crest	237	5
3	Crest	199	5
4	Trough	276	4.486
5	Trough	230	4.016

Table 3: Sample of 7.6×10^{-3} mol/L

4.1.3 Sample of 7.6×10^{-6} mol/L

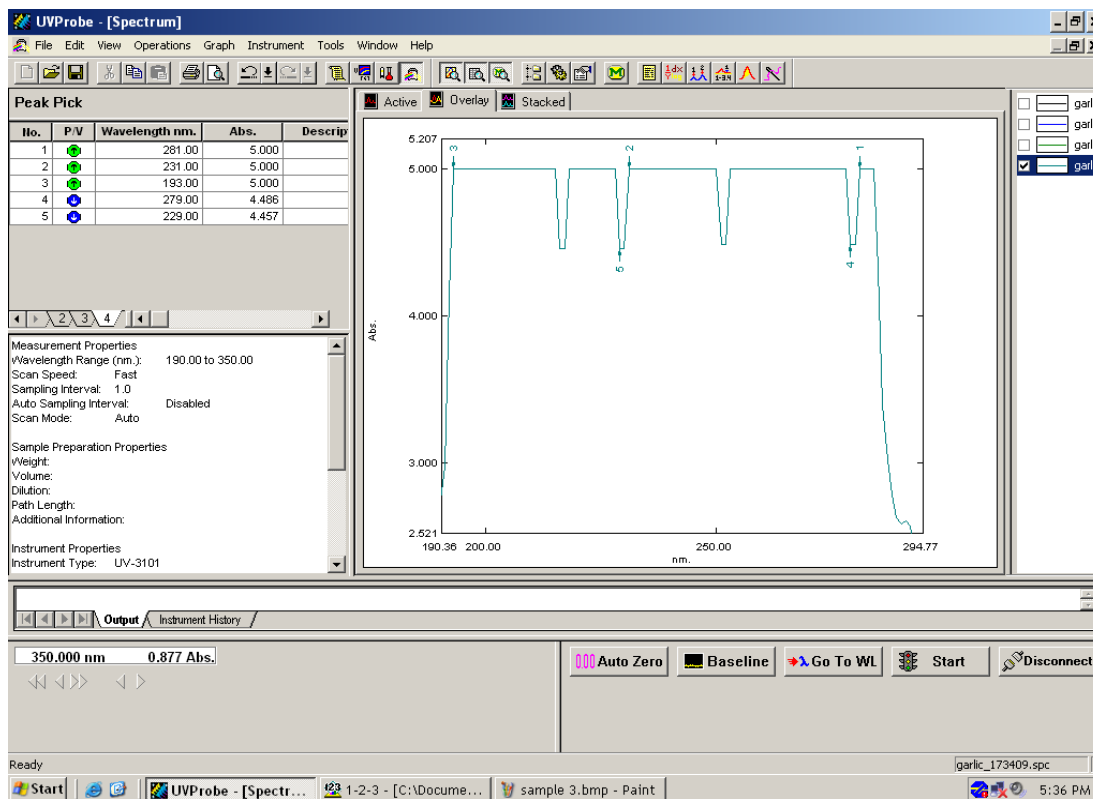


The graph above shows the peak value reading for 7.6×10^{-6} mol/L concentration of MTBE in water. Chosen peak values have been recorded at the table below.

No.	P/V	Wavelength nm.	Abs.
1	Crest	272	5
2	Crest	196	5
3	Trough	270	4.486
4	Trough	194	4.059

Table 4: Sample of 7.6×10^{-6} mol/L

4.1.4 Sample of 0.45×10^{-6} mol/L

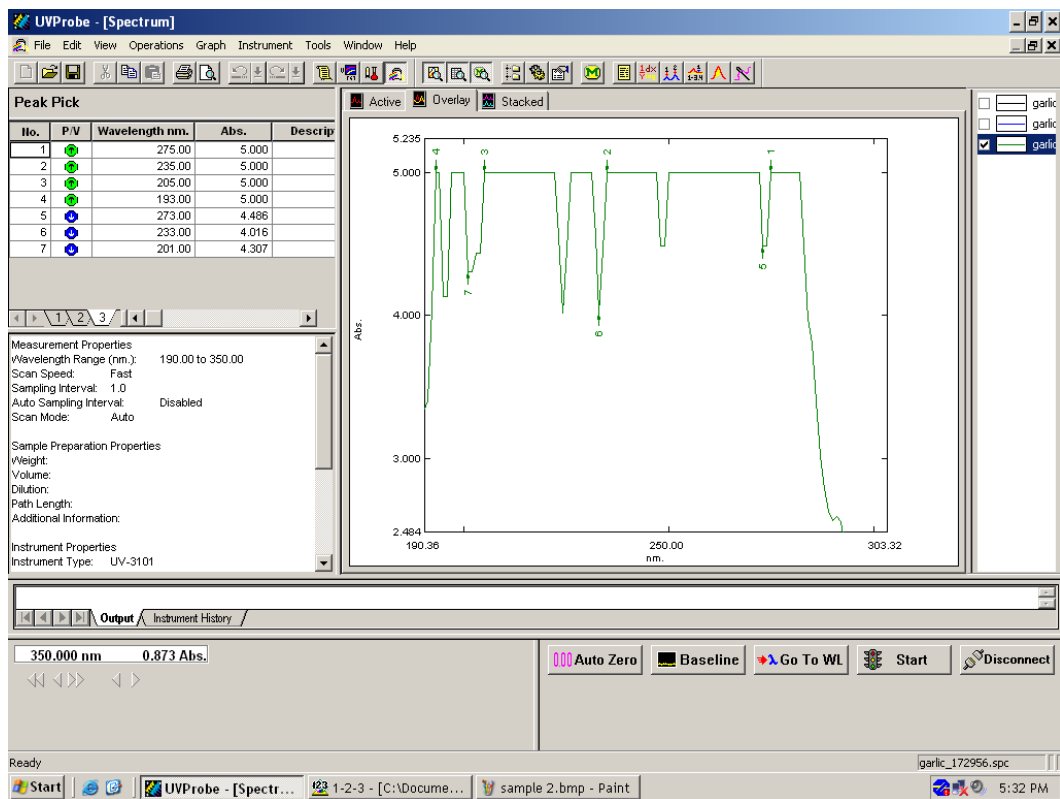


The graph above shows the peak value reading for 0.45×10^{-6} mol/L concentration of MTBE in water. Chosen peak values have been recorded at the table below.

No.	P/V	Wavelength nm.	Absorbance
1	Crest	281	5
2	Crest	231	5
3	Crest	193	5
4	Trough	279	4.486
5	Trough	229	4.457

Table 5: Sample of 0.45×10^{-6} mol/L

4.1.5 Sample of 0.23×10^{-6} mol/L



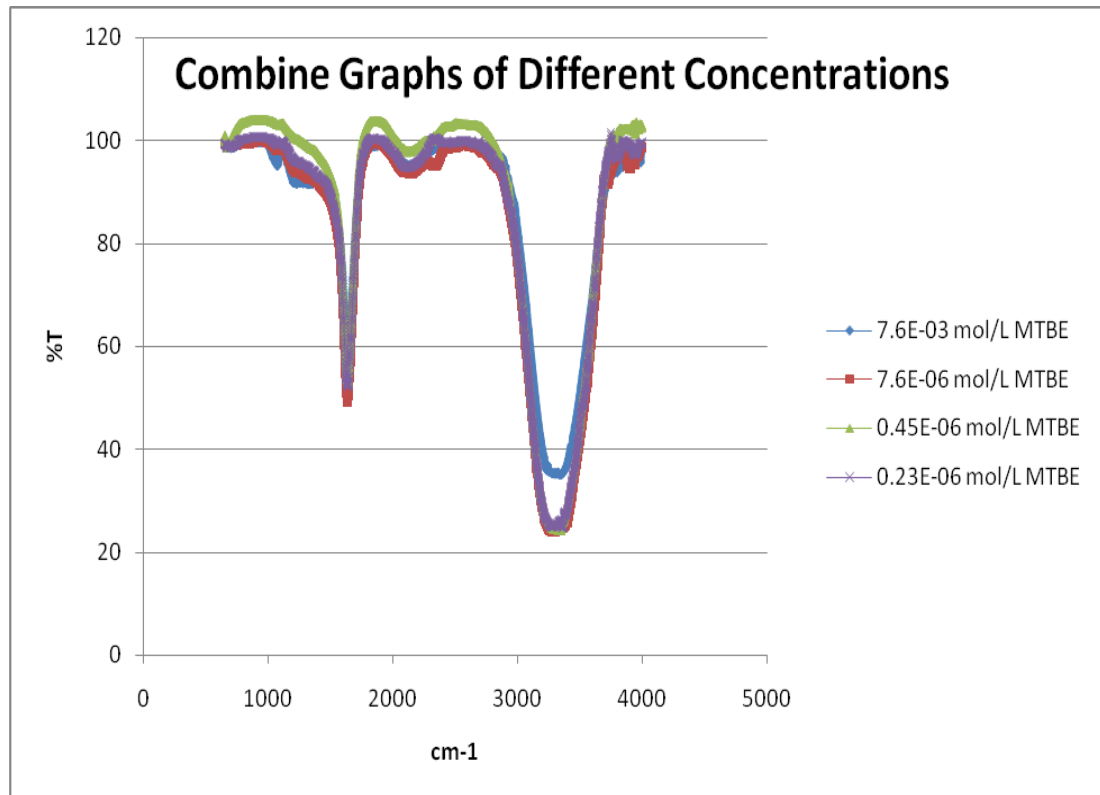
The graph above shows the peak value reading for 0.23×10^{-6} mol/L concentration of MTBE in water. Chosen peak values have been recorded at the table below.

No.	P/V	Wavelength nm.	Absorbance
1	Crest	275	5
2	Crest	235	5
3	Crest	205	5
4	Crest	193	5
5	Trough	273	4.486
6	Trough	233	4.016
7	Trough	201	4.307

Table 6: Sample of 0.23×10^{-6} mol/L

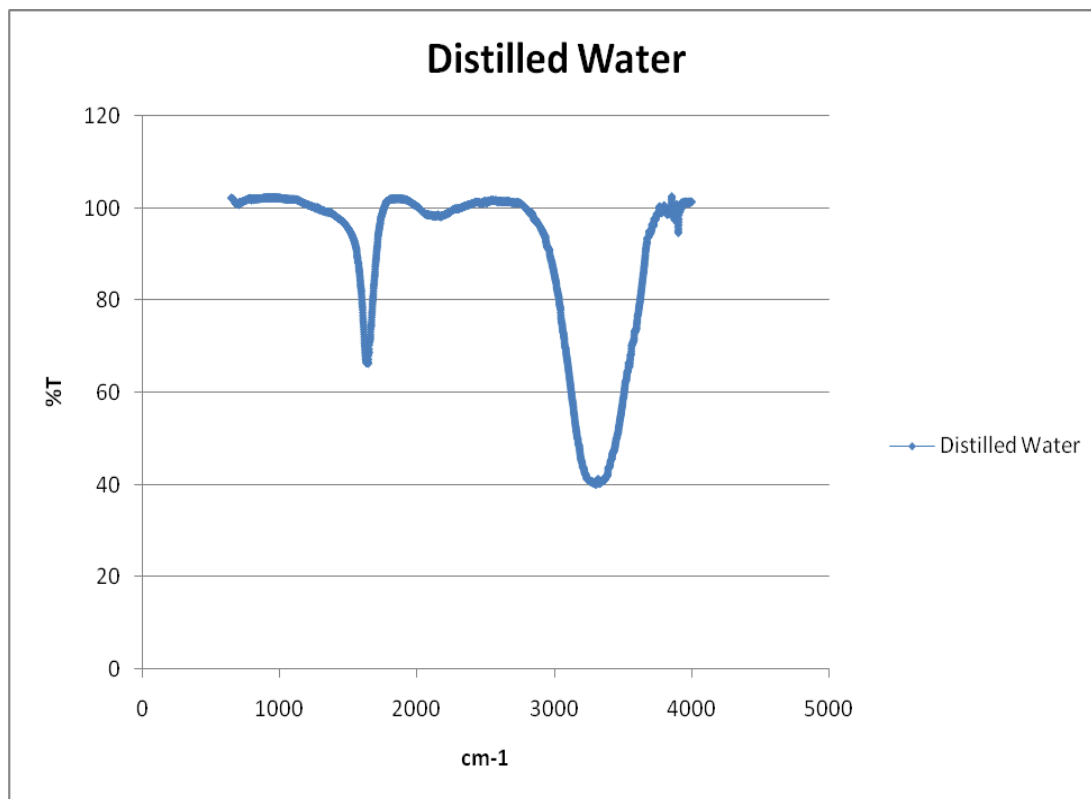
4.2 RESULTS OF FTIR EQUIPMENT

4.2.1 Combine graphs of different concentrations



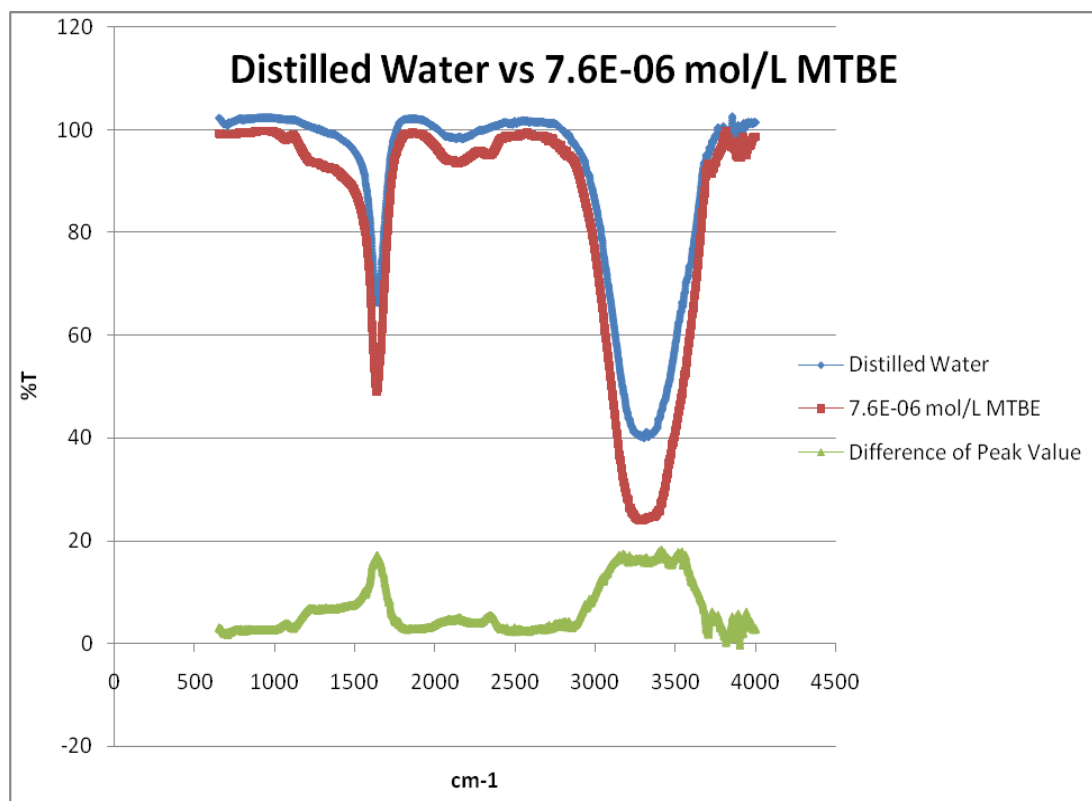
The combine graphs above showed the peak values percentage of transmittance of different concentrations of MTBE. We will compare these values with the percentage of transmittance of distilled water where we can observe the changes that could happen.

4.2.2 Sample of distilled water



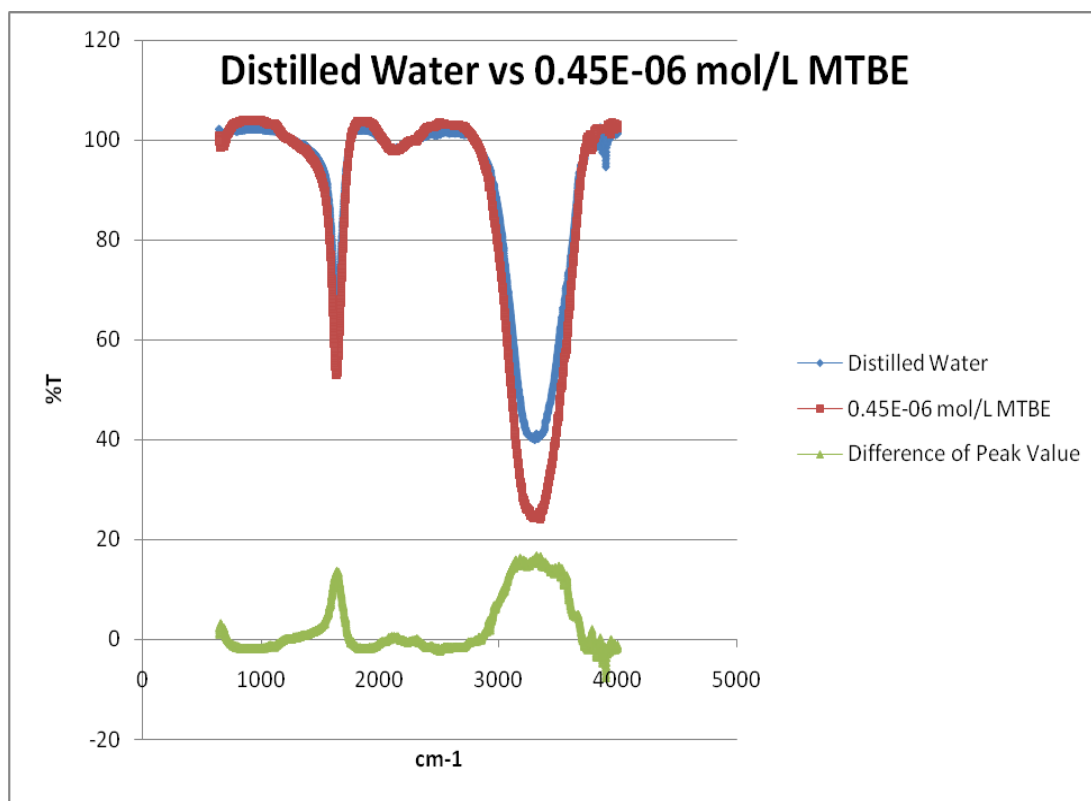
The graph above showed the peak values percentage of transmittance of distilled water. These values will be used to observe the difference of distilled water transmittance with the other concentrations of MTBE in water transmittances.

4.2.3 Sample of 7.6×10^{-6} mol/L



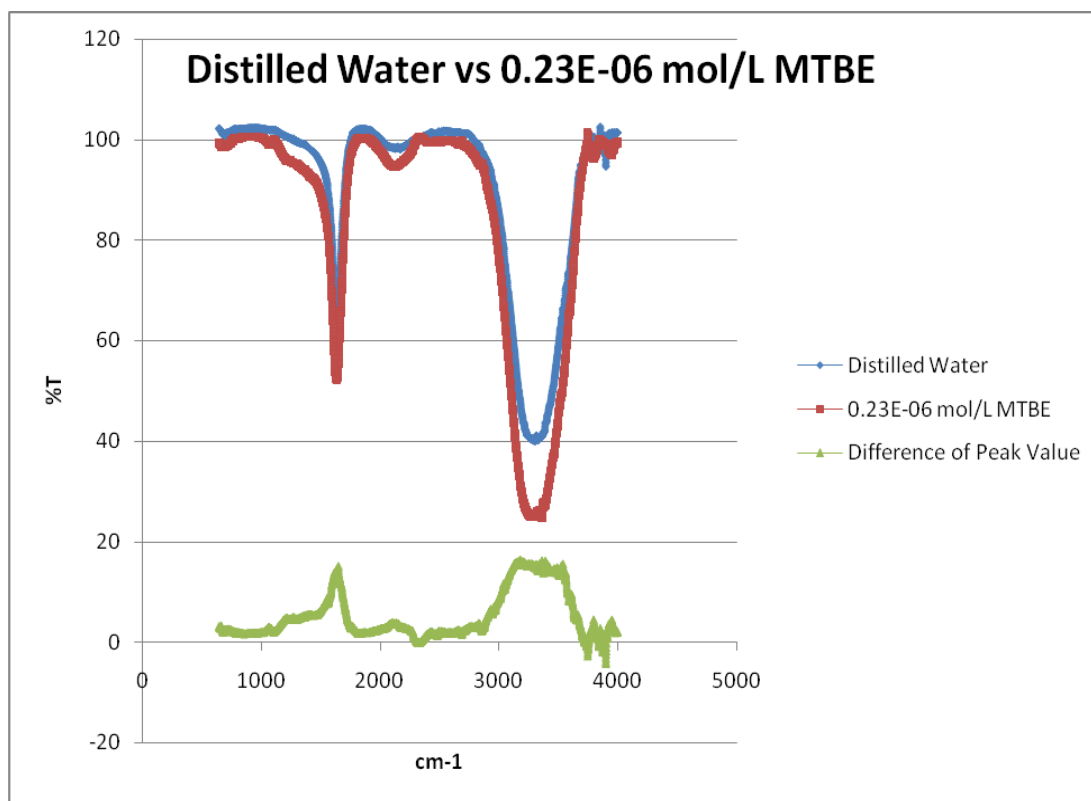
The graphs above showed the peak values percentage of transmittance of distilled water with 7.6×10^{-6} mol/L of MTBE in water. We can observe at certain region of wavelength where it has shows significant difference of changes. The significant changes were at regions of wavelengths between 1500 cm^{-1} and 2000 cm^{-1} and also from region 3000 cm^{-1} until 4000 cm^{-1} .

4.2.4 Sample of 0.45×10^{-6} mol/L



The graphs above showed the peak values percentage of transmittance of distilled water with 0.45×10^{-6} mol/L of MTBE in water. We can observe at certain region of wavelength where it has shows significant difference of changes. The significant changes were at regions of wavelengths between 1500 cm^{-1} and 2000 cm^{-1} and also from region 3000 cm^{-1} until 4000 cm^{-1} .

4.2.5 Sample of 0.23×10^{-6} mol/L



The graphs above showed the peak values percentage of transmittance of distilled water with 0.23×10^{-6} mol/L of MTBE in water. We can observe at certain region of wavelength where it has shows significant difference of changes. The significant changes were at regions of wavelengths between 1500 cm^{-1} and 2000 cm^{-1} and also from region 3000 cm^{-1} until 4000 cm^{-1} .

4.3 DISCUSSIONS

4.3.1 Discussions on UV-Vis results

According to the results and graphs taken, the comparisons between the graphs show that there are no major differences and parameters that we can observe. The graphs are inconsistent and hard to distinguish the differences between the samples. Because of that, it is hard to establish the correlation between spectrums of UV-Vis. One of the reasons is because of the concentration which is very low and affects the UV-Vis equipment detection. Therefore, the detection ability of UV-Vis equipment is not accurate enough to detect the samples concentration.

4.3.2 Discussions on FTIR results

According to the results and graphs taken, we can observe some comparisons and changes between different samples. From the combined graphs of different concentrations, we can observe that the percentage of transmittance (%T) is decreasing as the concentration is decreasing. When we compare each of the concentration samples with distilled water, the obvious changes can be detected at region wavelength of 1500 cm^{-1} until 2000 cm^{-1} and also from region wavelength of 3000 cm^{-1} until 4000 cm^{-1} .

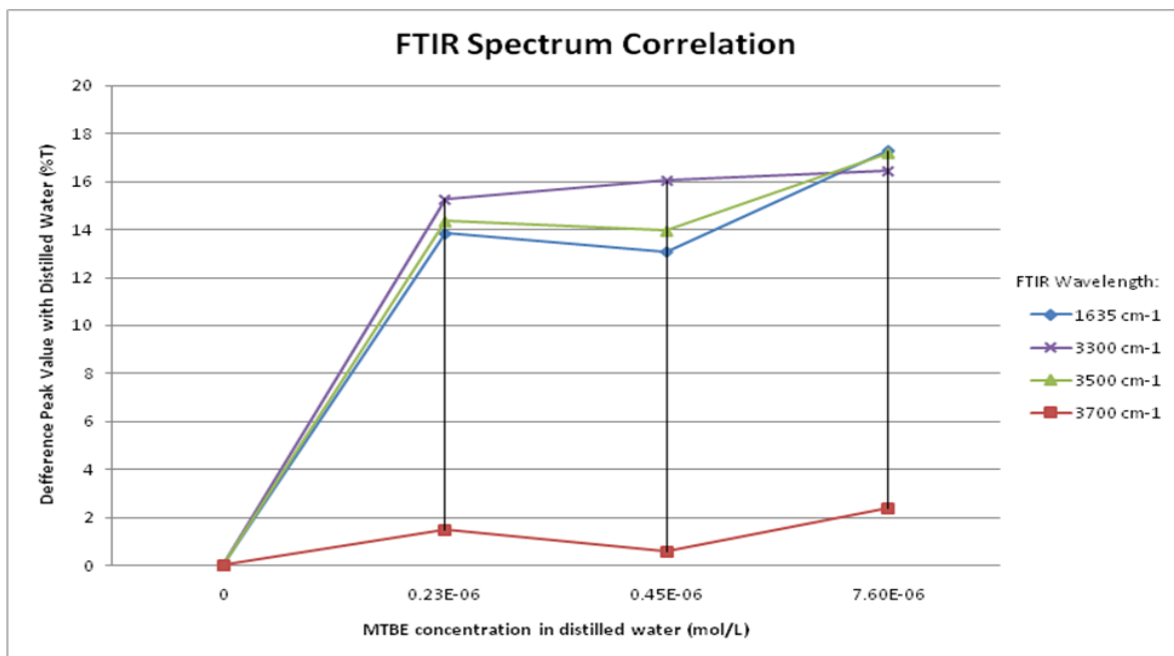


Figure 6: Difference of %T with Distilled Water

The graphs above showed the correlation of FTIR spectrum. Certain values of wavelength have been recorded with their values of difference peak values with distilled water of respective concentration of MTBE. It shows that the difference peak values are gradually decreasing with decreasing concentration of MTBE concentration. The detection of MTBE concentration is also decreasing with increasing value of wavelength as we can observe the difference of peak values are decreasing.

Concentration	W/V	Highest Difference of %T with Distilled Water
7.6E-06	3413	18.360711
0.45E-06	3319	16.801476
0.23E-06	3185	16.447501

Table 7: Highest Difference of %T

Table above showed the highest difference of percentage transmittance (% T) of different concentration with distilled water at their respective wavelength. As we can see, the difference become higher and gradually decreasing as the concentration is decreasing. Their respective wavelength is also increasing and become slowly decreasing as the concentration is decreasing.

It shows that as the concentrations decreasing, the difference of transmittance is increasing and the presence of MTBE in distilled water become lower. The fraction of incident rays is increasing because the concentration of MTBE is decreasing. The light can travel with a full intensity because the concentration of MTBE is decreasing. Therefore, we can detect and measure the MTBE concentration in water better by using FTIR equipment compared to UV-Vis equipment which is inconsistency.

CHAPTER 5

CONCLUSION

From the results taken, it can be concluded that UV-Vis equipment cannot detect low concentration of MTBE in water very well. Therefore, analysis and correlations of the spectrums cannot be constructed due to the small changes of results and inconsistency of the readings and graphs. When using FTIR equipment, it shows better results which we can observe from the graphs and data taken. The changes and comparisons are detectable so that we can observe and correlate the changes to give the justifications. The correlation of MTBE concentrations with water according to their transmittance has been constructed and it shows significant observation according to the changes.

Therefore, FTIR equipment gives better measurement compare to the UV-Vis equipment. Correlation of FTIR has been constructed while UV-Vis correlation cannot be constructed as the changes are inconsistence. However, we cannot manage to measure the lowest detectable limit of MTBE contamination in water using UV-Vis and FTIR due to lack of time and other obstacles.

CHAPTER 6

RECOMMENDATION

There are some recommendations that can be made in order to have better research results and findings. First of all, we can exchange the sample from using distilled water with the real ground water. With that, the findings will become more specific and relevant. Besides that, we also can have the experience by visiting and doing field trip to the subjected site according to the project background and problem statements. With all of these recommendations, it will surely give a good result and findings in pursuing this research.

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APPENDIX

Transmittance of distilled water from wavelength 4000 cm^{-1} until 3500 cm^{-1}

Wavelength	Transmittance (%T)
4000	101.424253
3999	101.412071
3998	101.398518
3997	101.392046
3996	101.38507
3995	101.366967
3994	101.33868
3993	101.316896
3992	101.321248
3991	101.358675
3990	101.416703
3989	101.466037
3988	101.475807
3987	101.433249
3986	101.349554
3985	101.253302
3984	101.177402
3983	101.144525
3982	101.157652
3981	101.196298
3980	101.227702
3979	101.228754
3978	101.200876
3977	101.173368
3976	101.182958
3975	101.244363
3974	101.340779
3973	101.430776
3972	101.47393
3971	101.457497
3970	101.400633
3969	101.336383
3968	101.28492

3967	101.245032
3966	101.209482
3965	101.180238
3964	101.166153
3963	101.16889
3962	101.176004
3961	101.171975
3960	101.157058
3959	101.15347
3958	101.18869
3957	101.271554
3956	101.379091
3955	101.465659
3954	101.494719
3953	101.457749
3952	101.369897
3951	101.264349
3950	101.183825
3949	101.160563
3948	101.195903
3947	101.258071
3946	101.305662
3945	101.317008
3944	101.296449
3943	101.272567
3942	101.2829
3941	101.331998
3940	101.371508
3939	101.343066
3938	101.234476
3937	101.09492
3936	100.991581
3935	100.932555
3934	100.847937
3933	100.66457
3932	100.405367
3931	100.190752
3930	100.121174
3929	100.210106
3928	100.423551

3927	100.725379
3926	101.05929
3925	101.279788
3924	101.213607
3923	100.877315
3922	100.513521
3921	100.359322
3920	100.465832
3919	100.684646
3918	100.766901
3917	100.541323
3916	100.053456
3915	99.527226
3914	99.206604
3913	99.226629
3912	99.581414
3911	100.086981
3910	100.389499
3909	100.189652
3908	99.489094
3907	98.551223
3906	97.679966
3905	96.998724
3904	96.330689
3903	95.505393
3902	94.79622
3901	94.649704
3900	95.155876
3899	95.982582
3898	96.726205
3897	97.284082
3896	97.772292
3895	98.299727
3894	98.927378
3893	99.660946
3892	100.374125
3891	100.816184
3890	100.889694
3889	100.717763
3888	100.345393

3887	99.769298
3886	99.2013
3885	98.998355
3884	99.298054
3883	99.848392
3882	100.258066
3881	100.309553
3880	99.982029
3879	99.440274
3878	98.974153
3877	98.678558
3876	98.389994
3875	98.005423
3874	97.64377
3873	97.509227
3872	97.713304
3871	98.185558
3870	98.691097
3869	98.980296
3868	99.010022
3867	98.899712
3866	98.742277
3865	98.63177
3864	98.698832
3863	98.959706
3862	99.265844
3861	99.493739
3860	99.650787
3859	99.813123
3858	100.088445
3857	100.592377
3856	101.358723
3855	102.184554
3854	102.619473
3853	102.390996
3852	101.81044
3851	101.229453
3850	100.642945
3849	100.10596
3848	99.812963

3847	99.843358
3846	100.068516
3845	100.234883
3844	100.125761
3843	99.716785
3842	99.200341
3841	98.832636
3840	98.760184
3839	98.970654
3838	99.350422
3837	99.753116
3836	100.03646
3835	100.091504
3834	99.879106
3833	99.470789
3832	99.056935
3831	98.84832
3830	98.931396
3829	99.212185
3828	99.474035
3827	99.534643
3826	99.38627
3825	99.153371
3824	98.932574
3823	98.744031
3822	98.623521
3821	98.67223
3820	98.918384
3819	99.240465
3818	99.504632
3817	99.651717
3816	99.723327
3815	99.817078
3814	99.94345
3813	100.01726
3812	99.986367
3811	99.8849
3810	99.772493
3809	99.684833
3808	99.64939

3807	99.708064
3806	99.879994
3805	100.101373
3804	100.244785
3803	100.223012
3802	100.08825
3801	100.046559
3800	100.234067
3799	100.52225
3798	100.674945
3797	100.572214
3796	100.263381
3795	99.910199
3794	99.658507
3793	99.547058
3792	99.534614
3791	99.570043
3790	99.622587
3789	99.690563
3788	99.798319
3787	99.961477
3786	100.134714
3785	100.202627
3784	100.06703
3783	99.750692
3782	99.371388
3781	99.066207
3780	98.947974
3779	99.039529
3778	99.240378
3777	99.42517
3776	99.555498
3775	99.647385
3774	99.707744
3773	99.713515
3772	99.64553
3771	99.553987
3770	99.55948
3769	99.732713
3768	100.00036

3767	100.227364
3766	100.355248
3765	100.409317
3764	100.399553
3763	100.272516
3762	99.974702
3761	99.553187
3760	99.182361
3759	99.019339
3758	99.039177
3757	99.088525
3756	99.069409
3755	98.979744
3754	98.842604
3753	98.679635
3752	98.544316
3751	98.507715
3750	98.543038
3749	98.563528
3748	98.587101
3747	98.671302
3746	98.796303
3745	98.824408
3744	98.64298
3743	98.396825
3742	98.280069
3741	98.246918
3740	98.190748
3739	98.077329
3738	97.895454
3737	97.66971
3736	97.51793
3735	97.54728
3734	97.682647
3733	97.750865
3732	97.716793
3731	97.673669
3730	97.694635
3729	97.763861
3728	97.81228

3727	97.755931
3726	97.530344
3725	97.161864
3724	96.779653
3723	96.505628
3722	96.356666
3721	96.264252
3720	96.167663
3719	96.075879
3718	96.04006
3717	96.08682
3716	96.193773
3715	96.313291
3714	96.410416
3713	96.485949
3712	96.557099
3711	96.564114
3710	96.377259
3709	95.998088
3708	95.582073
3707	95.278565
3706	95.13501
3705	95.109111
3704	95.111279
3703	95.047981
3702	94.879688
3701	94.666693
3700	94.533198
3699	94.564293
3698	94.737912
3697	94.952941
3696	95.096332
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3694	95.009679
3693	94.90869
3692	94.930181
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3646	85.607213
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3607	76.806096
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3605	76.456223
3604	76.15268
3603	75.819284
3602	75.52405
3601	75.270152
3600	74.990137
3599	74.644384
3598	74.280875
3597	73.980398
3596	73.794102
3595	73.737302
3594	73.772326
3593	73.796351
3592	73.707833
3591	73.496239
3590	73.257239
3589	73.147457
3588	73.25763
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3585	73.403531
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3506	59.582572
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3500	58.65304