Fourier Transform Infrared Spectroscopy – An Ideal Candidate Tool for Instant Quantification and Validation of Bio-Diesel and Bio-Diesel Blends

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Abstract: This experimental quantification research work reports how FTIR spectroscopy technique would be an ideal candidate tool, for researchers and industrial quality control specialist, to judge and analysis Bio-diesel and its blends. Few drops of oil is used for sampling and with interpretation of peaks from absorption spectra, it is directly related to quality of the bio-diesel. These observations well corroborate with ASTM standard quantification of Bio-diesel.

Keywords: FTIR, Bio-diesel, FAME content, quantification tool, spectra

1. Introduction

Bio-diesel, unlike the conventional diesel, is generated from edible and non-edible oil feed stocks like, soy bean oil, jatrobha oil, cotton seed oil, Kranja oil etc..., Bio-diesel is made of Fatty acid Methyl esters(FAME), the conversion takes by trans-esterification reaction, as displayed elsewhere in this journal.

One of the key parameters for determining the quality of bio-diesel and the extent of conversion of trans-esterification reaction is FAME content. FAME Content should be greater than 96% of above. FTIR is an ideal tool to judge the quality of Bio-diesel instantly. FTIR technique is called as finger-print technique by research community, given the high precision nature in terms of validation. This technique is widely used to detect contaminations in food industry (1) and hard disk drive industry (5).Apparently, in this research article, author presents the methods, procedure, and ease of quantification of FTIR technique is well explained.



Figure 1: Trans-esterification of vegetable oil into Biodiesel (FAME) and Glycerin

2. Materials and Methods

1 mole oil + 6 moles MeOH = 3 moles FAME + 1 mole glycerin + 3 moles MeOH

The bio-diesel was produced in-house as per the above mentioned stoichiometry by conventional mixing route. The catalyst (NaOH 0.5 wt%) of the oil was used. The Bio-diesel was subjected to quantification using FTIR spectrophotometer.

3. Equipment and Technique

FTIR stands for Fourier transform infrared, the preferred method of infrared spectroscopy. When IR radiation is passed through a sample, some radiation is absorbed by the sample and some passes through (is transmitted). The resulting signal at the detector is a spectrum representing a molecular 'fingerprint' of the sample. The usefulness of infrared spectroscopy arises because different chemical structures (molecules) produce different spectral fingerprints.



Figure 2: Working principle of FTIR interferometer

The FTIR uses interferometry to record information about a material placed in the IR beam. The Fourier Transform results in spectra that analysts can use to identify or quantify the material.

- An FTIR spectrum arises from interferograms being 'decoded' into recognizable spectra
- Patterns in spectra help identify the sample, since molecules exhibit specific IR fingerprints.

The equipment used for this analysis is PerkinElmer spectrometer 100. The given samples were injected into glass sample slit holder, and FTIR equipment was turned ON

4. Results and Discussion

FTIR Spectra of Bio-diesel B 99 Grade, generated from Palm Oil feed stock

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Figure 3: FTIR Absorption spectra of Bio-diesel(B 99 grade), generated from Palm Oil feedstock

The observed FTIR spectra, of Palm oil Bio-diesel(see fig 3), shows CO stretching bonds of methyl esters at 1743 cm^{-1} , and C-O bands at 1243.86 Cm^{-1} , 1170.58 cm^{-1} . CH stretching vibration of CH₃molecule, at 2855.1 cm⁻¹ and 3005.52 cm⁻¹.



Figure 4: FTIR spectra of palm oil+ mineral diesel Blend(1:1 Ratio)



Figure 5: FTIR Spectra of Mineral diesel

The observed spectra of the palm oil + diesel blend, (1:1), displays the spectral vibrations from bio-diesel and mineral diesel in equal proportions. It is well evident from Ester Carbonyl C=O vibrations (1741.41 cm⁻¹) and ester c-vibrations (1169.62 cm⁻¹) concerned with Bio-diesel and C=C Aromatic(1456 cm⁻¹), stretch medium-weak, Multiple bands, Alkane C-H stretching concerned with Mineral diesel.

5. Conclusion

It is well evident from the experimental observation, FTIR(Fourier Transform infrared spectroscopy) is an ideal tool, to quantify the purity of the Bio-diesel and Bio-diesel Blends. Any Impurity detected in the Bio-diesel can be well detected, in relative terms. For quick identification and judgment the peaks mentioned in the experimental report would be beneficial to research communities.

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