

FOURIER TRANSFORM INFRARED SPECTROPHOTOMETRIC ANALYSIS OF FUNCTIONAL GROUPS IN BIODIESEL PRODUCED FROM OILS OF *RICINUS COMMUNIS*, *HEVEA BRASILIENSIS* AND *JATROPHA CURCAS* SEEDS

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Abstract: Fourier transform infrared spectrometry (FTIR) was used to evaluate the possible functional groups present in biodiesel. It is an easy way to identify the presence of functional groups in the sample and its structure based on the energies associated with the molecular vibration when irradiated. In these work three samples; *ricinus communis*, *Hevea brasiliensis* and *Jatropha curcas* oils were run through FTIR, the bonds as well as functional groups present are found to respond differently to the incoming radiation, due to variation in their molecular vibration of stretching and bending. The response of the functional groups are characterized by observing the transmission of infrared radiations and comparing it with known standards in order to identify the type and the nature of functional groups present in the samples. The presence and the nature of functional groups among other factors provide information on the stability of the biodiesel fuel. This paper is thus designed to evaluate the functional groups and structure in order to establish the reactivity of these fuels as a function of possible degradation.

Keywords: Biodiesel, degradation, functional groups, infrared, radiation.

Introduction

Biodiesel is an emerging renewable fuel proved to be environmentally friendly, biodegradable with low emission properties, and capable of substituting the fossil diesel. This fuel is receiving much attention world over as a means of preventing global climate change. It is produced from vegetable oils or animal fats through catalytic transesterification process using methanol and sodium hydroxide or potassium hydroxide. The finished biodiesel can only be used in ignition engine when the quality of the product is guaranteed. This is to safe our environment from obnoxious emissions due to low quality fuel.

There are various methods for measuring the quality of finished biodiesel, the commonest one is the use of Gas chromatography based on ASTM and EN standards, but the main

shortcoming of Gas chromatographic method is that it consumes time in sample preparation which involve the derivatization of fuel sample prior to GC analysis (Zagonel *et al*, 2004).

The FTIR spectroscopy has an excellent potential in providing qualitative and quantitative data for fuels including biodiesel without much rigor in sample preparation; it is used extensively as a quantitative analytical procedure for assessing edible oil quality parameter (Ma *et al*, 1997). Similarly, it was also developed for determining the acidity and moisture content in lubricants (Van de Voort *et al*, 2006), as well as providing information about the functional groups in molecules and the structure of the molecules based on energies associated with molecular vibration. There are two types of vibration motion.

- Stretching vibration is the vibration motion in which internuclear distance between the bonded atom increase and decreases along the bond axis.
- Bending vibration is the type of vibrational motion in which position of the bonded molecule change with respect to the bonded atom; the interatomic distance remain unchanged (Younis *et al.*, 2009)..

Materials

Biodiesel used in this study is produced from oils of *ricinus communis* (castor seeds), *hevea brasiliensis* (rubber seeds) and *jatropha curcas* seeds.

Methods

The major component of the FTIR system are; the radiation source, the interferometer, the slit, beam splitter and the detector. The radiation source generates a radiation in form of light which was directed to the sample through the interferometer. The interferometer separates the source radiation into its different wavelength, and the slit selects the collection of wavelength that passes through the sample at any given time. The beam splitter separates the incident beam into two; half of the incident beam goes to the fuel sample and the other half to the reference standard. The sample absorbs light according to its chemical properties. A detector collects the radiation that passes through the fuel sample and compares its energy to that going through the reference, and then put the electric signer which is normally sent directly to a recorder linked back to the interferometer so as to allow the interpretation of energy as a function of frequency or wavelength translated into a finger print which appear in a computer monitor attached directly to the detector, and printed out as hard copy. The functional groups are identified by comparing the peaks generated by the fuel sample with that of the reference standard.

Results

The FT-IR analysis of functional groups of castor biodiesel is presented in Table 1. It is observed from the table that =C-H groups were the most abundant in castor biodiesel, and they all possess bending type of vibrations appearing at low peak of the spectrum and are all double bonded. Though the remaining functional group is quite different in terms of structure, wave number and vibration, they all possess single bonds as a unifying factor.

Table 1: FTIR functional group frequencies of Castor Biodiesel

Wave Number cm^{-1}	Types of Vibration	Functional groups
723.33±0.3	Bending	=C-H
856.42±1.2	Bending	=C-H
923.93±2.5	Bending	=C-H
1031.95±0.8	Stretch	C-O
1112.96±1.0	Stretch	C-O
1199.78±0.0	Stretch	C-N
1464.02±2.3	Stretch	C-C
1743.71±4.8	Stretch	C-O
2929.97±9.0	Stretch	C-H
3354.32±0.5	Stretch	O-H

Table 2. Show the result of functional group analysis for rubber biodiesel. the most abundant chemical group is O-H with stretch mode of vibration that show a peak at different band wave number 2854.74cm^{-1} , 2926.11cm^{-1} , and 3416.05cm^{-1} respectively. The only carbonyl group present occurs at band wave number 1743.71cm^{-1} .

Table 2: FTIR functional group frequencies of Rubber biodiesel

Wave Number cm^{-1}	Types of Vibration	Functional groups
723.33±1.0	Bending	=C-H
1020.38±5.0	Stretch	C-O
1246.06±2.0	Stretch	C-O
1363.72±1.3	Bending	-C-H
1464.02±3.2	Stretch	-C=C

1743.71±9.5	Stretch	C=O
2854.74±3.0	Stretch	O-H
2926.11±2.0	Stretch	O-H
3416.05±2.5	Stretch	O-H

The result of the FTIR analysis of *Jatropha curcas* biodiesel is presented in

Table 3. From the table, the type of bond found most abundantly and the nature of their vibration are = C-H (bending), C-H (stretch, bending respectively), C = C (stretch) and O-H (stretch). The results suggest the prevalence of properties such as pour and cloud points due to saturated nature of these chemical groups which may affect the free flow of the fuel particularly during cold weather operations.

Table 3: FTIR functional group frequencies of *Jatropha* Biodiesel

Wave Number cm^{-1}	Types of Vibration	Functional groups
723.33±10.2	Bending	=C-H
877.64±0.5	Bending	=C-H
1016.52±1.2	Stretch	C-O
1168.9±3.2	Stretch	-C-H
1369.5±5.2	Bending	-C-H
1462±11.0	Stretch	C=C
1730.21±2.0	Stretch	C=C
2852.81±2.7	Stretch	O-H
2931.9±3.5	Stretch	O-H

Discussion

Table 1 shows the result of FT-IR analysis for castor biodiesel. It is observed from the table that = C-H were the most abundant in castor biodiesel and they all possess bending type of vibrations appearing at low peak wave number 723.33cm^{-1} , 856.42cm^{-1} and 923.93cm^{-1} respectively. They are unsaturated functional groups. Other saturated functional groups detected are C-O, C-H, O-H and C-N groups all of which have stretch mode of vibration at much higher peak except O-H that have both stretch vibration and hydrogen bonding, the hydrogen bonding indicates the presence of undesirable water molecule.

The result of functional group identified for rubber biodiesel is presented in Table 2. It is observed that the nature of the bonds detected and their abundance are quite different from those of *Jatropha* biodiesel. The C-N group (cyanide group detected with stretch mode of vibration and which appeared at 1170.83cm^{-1} may indicate presence of undesirable contaminant at the point of purifying biodiesel. It is also a clear indication that FTIR is not only suitable for the measurement of several important fuel parameters, but also for critical impurities at very low percentage levels in biodiesel. It is also observed that the most abundant chemical group is O-H with stretch mode of vibration that show a peak at different band wave number of 2854.74cm^{-1} , 2926.11cm^{-1} , and 3416.05cm^{-1} respectively are all single bonded. Similarly, other groups such as C-O, -C-H are also detected and are also single bonded functional groups; there is therefore the tendency of the rubber biodiesel to exhibit pour cold flow properties during cold weather operations. The carbonyl group C=O and C=C functional group detected at a peak band wave number 1743.71cm^{-1} and 1464.02cm^{-1} with stretch mode of vibration are double bonded but may not have significant effect in keeping the rubber biodiesel in liquid state. There is therefore the need for injecting cold flow improver into the rubber biodiesel for better performance.

The result of the FTIR analysis of *Jatropha curcas* biodiesel is presented in Table 3. The type of bonds found most abundantly were = C-H (bending), C-H (stretch, bending respectively), C = C (stretch) and O-H (stretch). The presence C-H and indicates prevalence of properties such as pour and cloud points that affect the performance of biodiesel during cold weather engine operation (Younis *et al.*, 2009). However the presence of groups with carbon to carbon double bonds (C = C, = C-C) which are the most abundant can cause the fuel to remain in liquid state but may be liable to possible oxidation during storage.

Conclusion

The increasing emphasis on the use of quality biodiesel in automobiles and electricity generating plants required a rapid and reliable analysis, so as to reveal some properties that are so insensitive to manual analysis. However with modern instrumentation such as the FTIR spectrometry as an emerging technique for analysis of biodiesel even at low concentrations was used for evaluating functional groups which indicate biodiesel reactivity and stability. All the absorption corresponding to C-O stretches reveal that the molecule contains ester functional groups.

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