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Analysis of *Datura stramonium* Linn. biodiesel by gas chromatography - mass spectrometry (gc-ms) and influence of fatty acid composition on the fuel related characteristics

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Abstract

Biodiesel is a mixture of fatty acid alkyl esters obtained by the reaction of triglycerides of vegetable or animal origin with alcohol in the presence of a catalyst. The fatty acid profile influences the overall properties of the biodiesel. The properties of individual fatty acid depend on the occurrence of double bonds, fatty acid chain length and branching. Better understanding of the fatty acid composition and correlating the fuel properties is of utmost importance in improving the optimal performance. In the present study, *Datura stramonium* biodiesel is analyzed for its fatty composition using Gas chromatography assisted with mass spectrometry. The influence of fatty acids of the fuel related properties is discussed.

Keywords: Biodiesel, *Datura stramonium,* Gas chromatography mass spectrometry

INTRODUCTION

Biodiesel is composed of a combination of fatty acid alkyl esters. The properties of the various fatty esters are in turn determined by the structural features of the fatty acid and the alcohol moieties that comprise a fatty ester. The type and concentration of fatty acids has an outstanding effect on the specific physico-chemical properties of biodiesel (Moser, 2009; Knothe and Steidly, 2005).

Most common biodiesel sources such as vegetable oils possess fatty acid profiles consisting of six common fatty acids i.e. palmitic acid ($C_{16:0}$), stearic acid ($C_{18:0}$), palmitoleic acid ($C_{16:1}$), oleic acid ($C_{18:1}$), linoleic acid ($C_{18:2}$)and linolenic acid ($C_{18:3}$). Moreover, biodiesel from different or even from the same source may have different chemical structures and consequently different properties. Structural features that influence the physical fuel properties of a fatty ester molecule include chain length, degree of unsaturation and branching of the chain (Mittelbach and Remschmidt, 2004). Important fuel properties of biodiesel that are influenced by the fatty acid composition are viscosity, cetane index (ignition quality), heat of combustion, cloud point, oxidative stability, and lubricity (Knothe, 2009). Better perceptive of the fatty acid profile and its related structure help in predicting the influence of fatty acids on various fuel related properties of biodiesel.

There are three main types of fatty acids that are present in a triglyceride: saturated ($C_{n:0}$), monounsaturated ($C_{n:1}$) and polyunsaturated ($C_{n:2,3}$). The percentage of these compounds differs for each vegetable oil. Unsaturation in the fatty acid chain is a significant factor causing lower cetane number (Knothe *et al.*, 2003). The feed stock with relatively low concentration of saturated fatty acids shows lower cloud point (Refaat, 2009; Imahara *et al*., 2006). The more unsaturation is present in the oil, the higher the iodine value (Knothe, 2002) and higher is the tendency of the oil to polymerize. The density of biodiesel varies depending on its feedstock. Longer and straighter chains (saturated fats) tend to have higher density than shorter and unsaturated molecules. Gross heat of combustion (HG) is another fuel property indicating the suitability of fatty compounds as diesel fuel. HG increases with chain length. It therefore appears reasonable to select the oil samples with certain fatty acid esters with desirable properties in the fuel in order to develop quality product.

Muniyappa *et al.,* (1996) reported that density, viscosity and cloud point of two biodiesel samples synthesized from soybean and beef tallow oil are influenced by their fatty acid composition. Lang *et al.,* (2001) tested several oils (rapeseed, sunflower, canola and linseed oil) on the biodiesel production and compared some physical and fuel properties of biodiesel with those of conventional diesel fuel. Dmytryshyn *et al.,* (2004) performed the transesterification of four vegetable oils and compared properties like density, viscosity, cloud point and pour point, and established differences between them. Sarin *et al*., (2007) have studied the physico-chemical properties of some blends of biodiesel from Jatropha and Palm oils, in order to improve the oxidation stability. In the present study, *Datura stramonium* biodiesel is analyzed for its fatty acid composition using GC MS and important fuel related properties such as kinematic viscosity, cetane index (ignition quality), heat of combustion, cloud point and density are studied.

MATERIALS AND METHODS

Biodiesel was prepared from the extracted of seed oil of Datura *stramonium* by two way process comprising of acid catalyzed esterification followed by base catalyzed transesterification.

The fatty acid composition of the biodiesel sample was analyzed by gas chromatography coupled with mass spectrometer.

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The gas chromatographic analysis was made using Agilent 7890A series chromatograph equipped with a Mass Spectometer Detector (Make No. 5975). A capillary column 30m x 250µm x 0.25µm dimension packed with non-polar HP-5 column was used. The sample was diluted in hexane and 1µl of this solution was injected into the column. The injection was performed in split mode with a split ratio of 50:1. The column temperature was programmed initially at 100ºC (held for 20 mins), and then increased to 180 ºC at the rate of 10 ºC/min, held for 10 mins and then increased to 290 ºC. The inlet temperature was set at 300 ºC. Helium was used as the carrier gas at a flow rate of 0.8ml/m. The mass spectrometry detector was operated in the positive electron impact mode with ionization energy of 70eV of accelerating voltage in the ion source. The identification of peaks was done by comparison of their retention time and mass spectra with Mass Spectral Library (Fu *et al.,* 2008).

RESULTS AND DISCUSSION

Biodiesel produced from different feedstock have distinct fatty acid composition which influence the fuel related properties (Moser, 2009). The physical characteristics of the fatty acids are determined by the length of the carbon chain and the number of double bonds (Mittelbach and Remschmidt, 2004). Cetane number, heat of combustion, melting point, and viscosity of neat fatty compounds increase with increasing chain length and decrease with increasing unsaturation (Knothe, 2005). Hence, it appears reasonable to select the feedstock with certain fatty esters with desirable properties in the fuel. Fatty acid alkyl esters with long chain fatty or saturated acids show higher cetane number, better oxidative stability, increased heat of combustion and poor cloud point. Esters prepared with unsaturated fatty acids show lower cetane number, better cold flow properties and suffer oxidative stability (Knothe *et al.,* 2003).

The fatty acid chromatogram showing the different components present in *Datura stramonium* methyl ester is shown in Fig.1. The major fatty acid component present was Oleic acid 22.76 % followed by Elaidic acid 21.87 %.

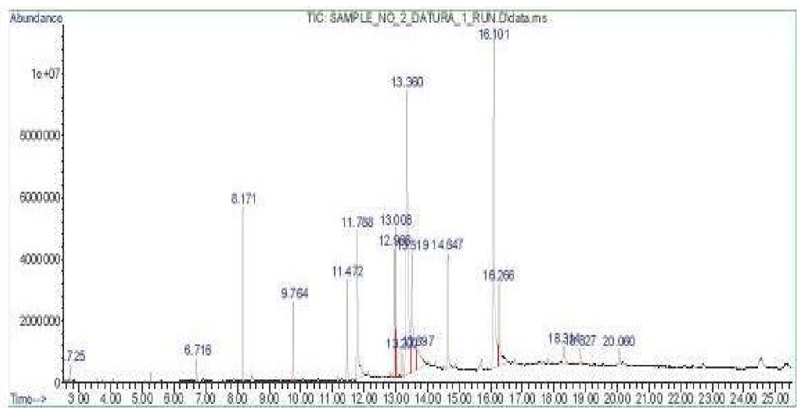

Fig1.GC-MS chromatogram of fatty acid methyl ester of *Datura stramonium*

Table 1. Fatty Acid Profile of *Datura stramonium* FAME using Gas Chromatography- Mass Spectrometry

S.No.	Retention time	Fatty acid	%
1	2.725	Caprylic acid methyl ester	0.378
2	6.716	Capric acid methyl ester	0.548
3	8.171	Lauric acid methyl ester	4.274
4	9.764	Myristic acid methyl ester	2.242
5	11.472	Palmitic acid methyl ester	2.960
6	11.788	Palmitoleic acid methyl ester	8.559
7	12.966	Linoleic acid methyl ester	4.096
8	13.008	Vaccenic acid methyl ester	5.177
9	3.200	Stearic methyl ester	0.805
10	13.360	Oleic acid methyl ester	22.760
11	13.519	α Linolenic acid methyl ester	10.321
12	13.697	γ Linolenic acid methyl ester	3.304
13	14.647	Arachidic acid methyl ester	4.300
14	16.101	Elaidic acid methyl ester	21.866
15	16.226	Gondoic acid methyl ester	5.767
16	18.314	Erucic acid methyl ester	1.461
17	18.827	Behenic acid methyl ester	0.551
18	20.060	Lignoceric acid methyl ester	0.630

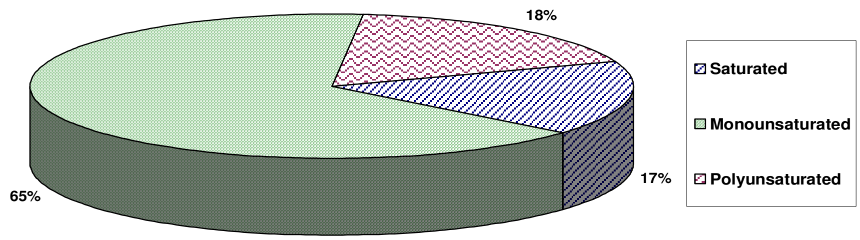

Fig 2. Percentage of saturated, monounsaturated and polyunsaturated fatty acids of *Datura stramonium* FAME

The saturated fatty acids (16.69 %) in the sample included Caprylic acid , Capric acid, Lauric acid, Myristic acid, Palmitic acid, Stearic acid , Arachidic acid , Behenic acid and Lignoceric acid. The monounsaturated fatty acids identified were Palmitoleic acid 8.56 %, Oleic acid isomers 49.6 %, Gonodoic acid 5.77 % and Erucic acid 1.46 %, whereas polyunsaturated fatty acids identified in the *Datura stramonium* biodiesel included Linoleic acid 4.10 % and Linolenic acid 13.62 % (Table 1). 83.3 % of unsaturated fatty acids have been identified of which 65.59 % was monounsaturated and 17.72 % was polyunsaturated (Fig. 2).

The unsaturated fatty acids were found higher in *Datura stramonium* methyl ester and specifically monounsaturated (65.59 %). Knothe (2008) has reported that methyl oleate can be the desirable fatty acid among the other common fatty acids that can enrich the fuel properties of biodiesel produced. It is considered that the quality of the fuel is reflected by the composition of these fatty acids. The presence of low levels of saturated and poly unsaturated fatty acids, the occurrence of high levels of mono nsaturated fatty acids in a biodiesel sample exhibit properties of high quality biodiesel (Knothe, 2009).

Higher composition of saturated fatty acid in feedstock increases the oxidation stability but lowers the cloud point and pour point of biodiesel, whereas, higher composition of unsaturated fatty acids enhances cloud point but possess a poor oxidative stability. Hence, a balance has to be maintained between the ratio of saturates and unsaturates for an oil to be used as a feedstock for biodiesel production (Sharma *et al.,* 2008).

Various studies have shown that the physical and chemical properties of biodiesel are mainly influenced by the fatty acids in the feedstock. The results obtained by Srivastava and Prasad (2001), with methyl esters from soybean and mustard seed oils reported that high viscosity at lower temperatures could be a result of micro-crystal formation and would cause serious problems in fuel lines and in engine filters. Biodiesel fuels derived from used frying oils tend to possess higher viscosity than those from most vegetable oils, owing to their higher content of trans FA and saturated, and less unsaturated FA (Knothe, 2006).

A high value of CN was observed in saturated FAME such as palmitate and stearate, i.e. greater than 80 (Knothe *et al.,* 2003) while the CN is in the medium range (55-58) in mono-unsaturated FAME. Bangboye and Hansen (2008) observed that a feedstock that is high in saturated fatty esters has a high CN, while feedstock predominant in unsaturated fatty acid have lower CN values (20-40). In the present study, the cetane index values of the *Datura stramonium* biodiesel tested were found to be 56, in the medium range, reflecting the dominance of monounsaturated fatty acids.

Biodiesel made from feedstock containing higher concentrations of high melting point saturated long-chain fatty acids tends to have relatively poor cold flow properties (Dunn, 2005). The length of the FA chain was shown to have a marked influence on the crystallization temperature of the produced biodiesel (Rodrigues *et al*., 2006). Due to its content of saturated compounds, tallow methyl ester has CP 17°C and palm oil methyl ester posses CP 13°C. On contrary, feedstock with relatively low concentrations of saturated long-chain fatty acids generally yields biodiesel with much lower cloud point. Thus, feedstock such as linseed, olive, rapeseed, and safflower oils tend to yield biodiesel with CP<0°C. In *Datura stramonium* methyl ester cloud point was determined in the range 6°C which showed the occurrence of more of unsaturated fatty acid than saturated.

CONCLUSION

The study reveals that biodiesel samples with high monounsaturates mainly methyl oleate can exhibit better fuel properties in terms of ignition quality, cloud point and heating value. Engineering the fatty acid composition may offer a quality biodiesel which is yet to be explored.

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