APPLICATION NOTE

FT-IR Spectroscopy

Determining the Source Oil of Biodiesel with Infrared Spectroscopy

Introduction

Biodiesel is a renewable fuel produced from a wide range of naturally occurring fats and oils by a transesterification reaction in which the triglycerides are broken down and fatty acid methyl esters (FAMEs) are formed. The fatty acid distribution of the original oil is retained in the biodiesel, thus the physical and chemical properties of the biodiesel have some dependence on the feedstock used.

One property particularly influenced by the feedstock is the cloud point, the temperature at which solid crystals start to form creating a cloudy suspension and potentially blocking fuel filters. For operation in cool climates, a low cloud point is essential. A wide range in cloud points is seen among biodiesel samples from various feedstocks: a sample of palm biodiesel may have a cloud point around 15 °C; biodiesel from rapeseed oil may be closer to -10 °C. The reason for the difference is that the saturated fatty acid chains that predominate in palm oil pack more readily to form crystals.

PerkinElmer®
For the Better

A rapid method for identifying the origin of a biodiesel sample is therefore desirable. Infrared spectroscopy is particularly suitable for the identification of materials, even when the differences between the materials are subtle variations in complex mixtures. In this note we demonstrate that biodiesel from several common feedstocks can be distinguished on the basis of absorption bands arising from double bonds in the fatty acid chains.

Experimental

Samples were obtained of palm, soy, and rapeseed biodiesel. The infrared spectra were measured using a PerkinElmer® Spectrum™ 100 FT-IR spectrometer[1] equipped with a single-bounce diamond UATR accessory.

Results and discussion

The FT-IR spectra are plotted in Figure 1. Clear differences are visible in the intensities of bands related to alkene functional groups. The intensities of these bands increase in the order palm < rapeseed < soy.

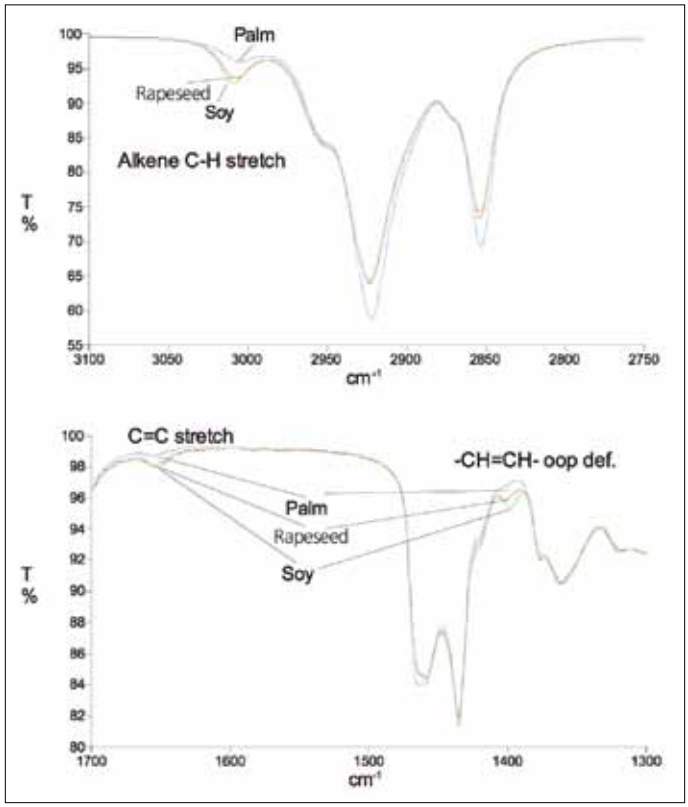

Figure 1. FT-IR spectra of the three biodiesel samples, showing the bands useful for discrimination. These bands are all due to vibrational modes of alkenes and increase in intensity with the average double bond density in the fatty acid chains.

These observations can be explained by considering the distribution of fatty acid chains present in each oil. Table 1 presents some typical distributions for these three oils. Palm oil is composed largely of lauric and myristic acid chains, which are completely saturated; some unsaturation is present as oleic and linoleic acid chains. Rapeseed and soy oil, on the other hand, have high proportions of unsaturated fatty acid chains. Consistent with the FT-IR data, the ratio of double bonds per chain to average chain length (a quantity approximately proportional to the volume density of double bonds) increases in the order palm < rapeseed < soy.

Table 1. **Typical fatty acid distributions for palm, soy, and rapeseed oil (source: www.accustandard.com). The bottom three rows are weighted averages over the distributions for each oil.**

Chain	Length	DB	Palm % chains	Soy % chains	Rapeseed % chains
Caprylate	8	0	7	0	0
Caprate	10	0	5	0	0
Laurate	12	0	48	0	0
Myristate	14	0	15	0	1
Palmitate	16	0	7	6	4
Stearate	18	0	3	3	3
Arachidate	20	0	0	3	3
Behenate	22	0	0	0	3
Lignocerate	24	0	0	0	3
Oleate	18	1	12	35	45
Erucate	22	1	0	0	20
Linoleate	18	2	3	50	15
Linolenate	18	3	0	3	3
Average chain length			**13.28**	**17.94**	**19.04**
Average DBs per chain			**0.18**	**1.44**	**1.04**
DB fraction			**1.4%**	**8.0%**	**5.5%**

Conclusions

The FT-IR spectrum of biodiesel takes only a few seconds to measure with a diamond ATR accessory, and contains readily accessible information about the extent of unsaturation in the fatty acid chains. This information is directly related both to the source oil used and to properties such as the cloud point of the fuel. FT-IR spectroscopy, thus, provides a very simple way to check the provenance of a biodiesel sample.

PerkinElmer, Inc.
940 Winter Street
Waltham, MA 02451 USA
P: (800) 762-4000 or
(+1) 203-925-4602
www.perkinelmer.com

PerkinElmer®

1. Equivalent results can be obtained using the PerkinElmer Frontier FT-IR system.

009163A_01 Printed in United Kingdom