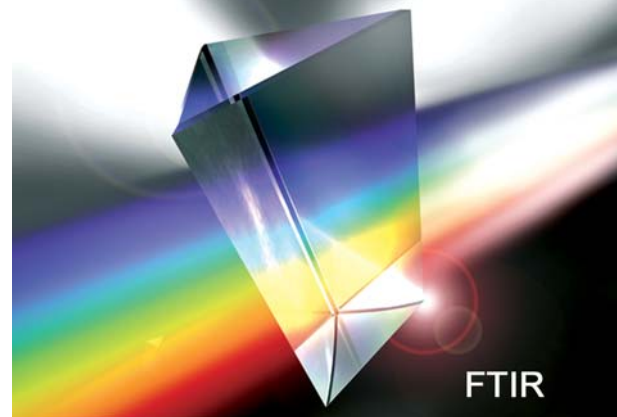


Application Note

Identification of Biodiesel Blends by HATR-FTIR Spectroscopy – Soy bean oil based –



Soy bean diesel is the most promising of several varieties of agriculturally produced alternatives to petroleum fuels. This application note showcases the ability of HATR in combination with FTIR-spectroscopy to identify commercially available biodiesel blends. While FTIR does not possess the detection limits or industry acceptance of GCMS, it does provide the advantages of quick, non-destructive, and inexpensive analysis. Our results indicate that it is an excellent choice as a quality control technique for large batches of biodiesel blends.

Biodiesel is made through a chemical process called transesterification. The process leaves behind ethyl esters, the

chemical name for biodiesel and glycerine. Biodiesel contains no petroleum, but it can be mixed at any level with petroleum diesel to create a biodiesel blend. Fuel-grade biodiesel must be produced to strict industry specifications as ASTM D6751 in order to insure proper performance. All newer diesel powered vehicles can run on this fuel without further modification.

The biodiesel analyzed in this application note was based on soybean diesel. Biodiesel is commonly mixed with ordinary petroleum diesel to make blends such as B5 or B20. B5 is a blend of 5% biodiesel and 95% petroleum diesel. The sample set for this experiment contained biodiesel blends B0 to B100, in 20% increments.

Pure biodiesel petrodiesel by
FTIR 10 bounce horizontal
ATR (ZnSe)



● The spectral fingerprints are very different and that is the key to the blend

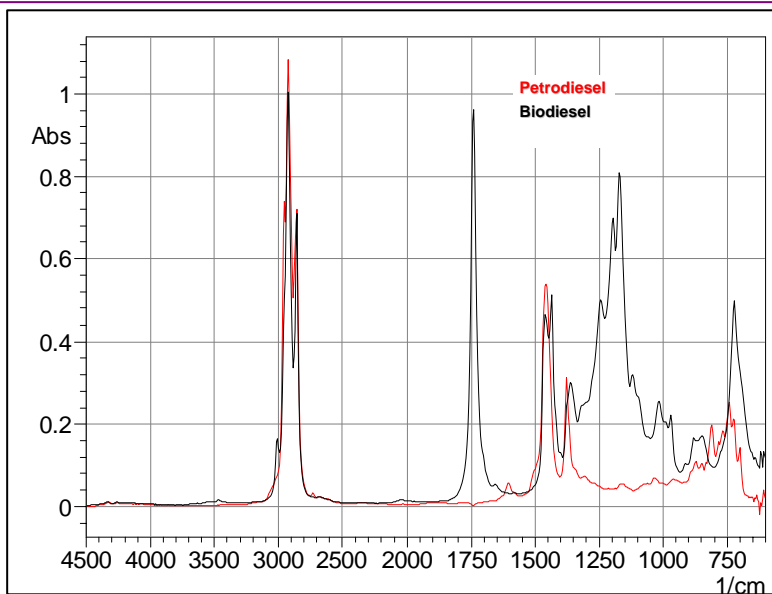


Fig. 1 FTIR spectra showing neat diesel (red) and biodiesel (black) and at left the accessory used for the analysis

The FTIR analysis was performed on a Shimadzu IRPrestige-21 equipped with an HATR accessory. This particular HATR employs a ten bounce crystal which provided an absorbance spectrum with sufficiently intense peaks. The use of a HATR accessory

affords an ease of use not available with other analytical techniques. In order to perform the measurement, a liquid sample can be poured onto crystal surface. After the analysis is complete, the sample can be wiped off the crystal and then rinsed with an

appropriate solvent. Judicious selection of the crystal material ensures the sample will not damage the surface of the crystal and that the desired wavenumber range can be achieved. The technique has been shown to be non-destructive in nature, simple and quick to perform, and does not require consumable goods such as solvent, carrier gases, etc. The summation of these favourable attributes results in an extremely economical quality control technique.

Figure 2 overlays multiple spectra which are blends of the two pure diesel seen in Fig. 1. It is readily apparent that the two pure compounds possess distinct spectral signatures. The strong carbonyl peak at 1750 cm^{-1} in the biodiesel spectrum is representative of ester functionality which is absent in the petrodiesel. The additional ester bands in the finger print range at 1200 to 1000 cm^{-1} in the biodiesel spectra provide an additional region to distinguish between the two components of interest. The overlays spectra for the blends B0 to B100 illustrates that both the carbonyl and ester bands can be used to quickly and easily differentiate between the blends.

One very popular tool to use these differences and also the visibility of quantitative aspects is to perform qualitative identifications by building spectral libraries and searching unknown compounds against them.

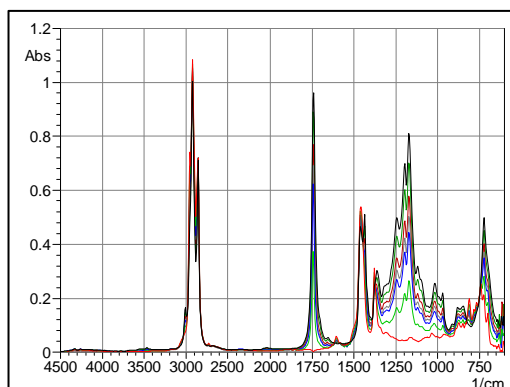


Fig. 2a: IR spectra from petrodiesel and blends of biodiesel

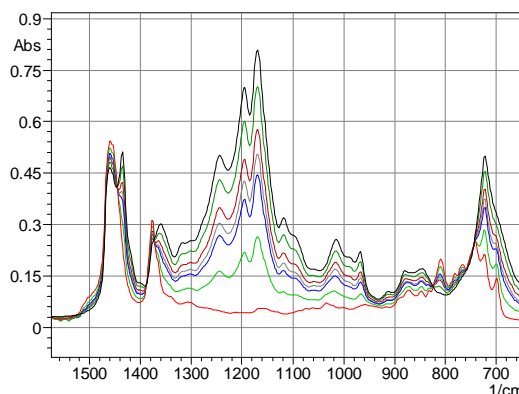
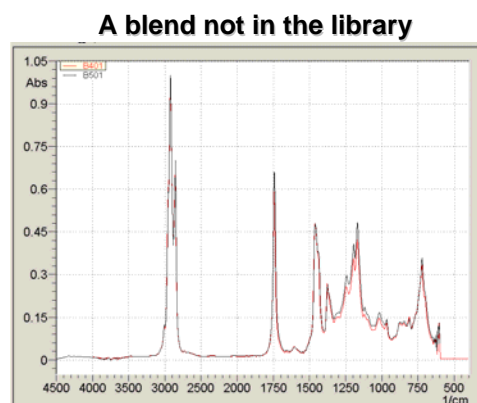


Fig. 2b: zoom of the infrared region with most impact of FAME



	Score	Library	
1	983	4 - Biodiesel Blends	B401; DE
2	980	5 - Biodiesel Blends	B601; DE
3	945	6 - Biodiesel Blends	B801; DE
4	943	3 - Biodiesel Blends	B201; DE
5	913	1 - Biodiesel Blends	B1002; C
6	889	2 - Biodiesel Blends	B01; DE

Fig. 3: IR spectrum of unknown and the result using a search in spectral library which is based on biodiesel blends

This application note has shown that FTIR analysis with HATR accessory can be used as a quick and selective quality control method for biodiesel blends.

Instrumentation:

Shimadzu IRPrestige-21 FTIR
IRsolution software and search Library-
Biodiesel Blends
HATR 10-bounce with ZnSe crystal

Many thanks to Shimadzu Scientific Instruments, North America
Based on NA-00105-A2 December 2005

The given specifications serve purely as technical information for the user.
No guarantee is given on technical specification of the described product and/or procedures.