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The Effect of Biodiesel Feedstocks on Infrared Blend Measurements

What is the effect of biodiesel feedstocks on measurement accuracy?

This common question coming from individuals measuring the percent biodiesel in diesel leads to several other questions before the answer is complete.

1. How does infrared measure biodiesel content?

Fortunately for manufacturers of infrared instrumentation, biodiesel has a unique signature from diesel in the infrared range of the spectrum. This means that at a wavelength specific to biodiesel, which is the carbonyl band at 5.73 micrometers (1745cm^{-1}), the intensity of the absorbance increases as the concentration of biodiesel increases (see Figure 1). The change in absorbance is correlated to a percent biodiesel value.

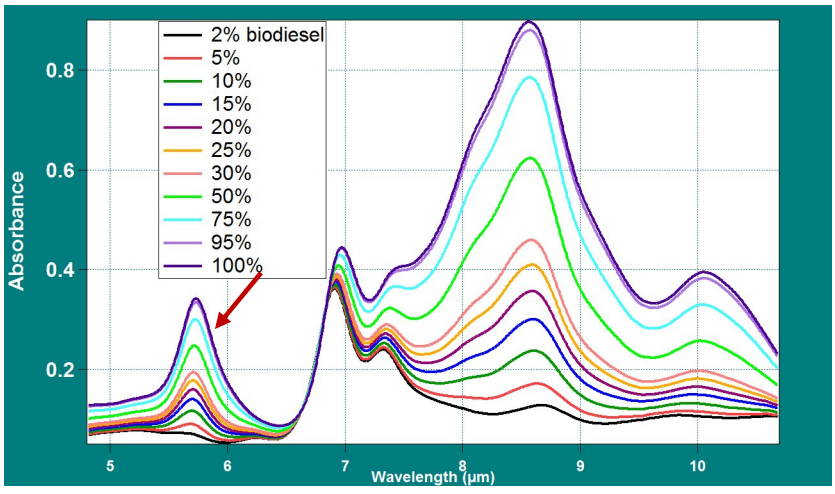

Figure 1: IR Spectra from a Wilks InfraSpec VFA-IR Spectrometer of Different Biodiesel Concentrations

Details of infrared analysis:

Carbonyl infrared absorbance is due to the stretching vibration of the carbon-oxygen double bond (C=O) and this absorption directly correlates with the biodiesel concentration result. In general, the wavelength and intensity of a carbonyl absorption will be affected by the mass and nature of the atoms attached to the C=O group.

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2. How does the feedstock make biodiesel different?

The primary difference between the fatty acid esters in oils from various feedstocks is the length of the hydrocarbon chains and the number and position of the C=C bonds. Most feedstocks such as soy, canola and yellow grease (or waste vegetable oil-WVO) have chain lengths between C16 and C22 with C18 predominating.

3. How do the differences in feedstock affect infrared measurements?

As mentioned in the previous "details of infrared analysis" side bar, the wavelength and intensity of a carbonyl absorption will generally be affected by the mass and nature of the atoms attached to the C=O group. The table below shows that the average molecular weight (mass) for five different feedstocks are very similar for all but one (more about the difference later).

More details of infrared analysis:

Different chain length means that the chains have different masses. However these aliphatic chains are quite flexible so that a few carbon atoms more or less at the end far removed from the carbonyl will have no significant affect on the infrared absorption. When carbon-carbon double bonds are present (unsaturated oils) these are found near the center of the chain i.e. far removed from the carbonyl group, so these too have little effect on the carbonyl absorption.

4. How does this translate to the primary concern of whether your biodiesel blend measurements will be accurate?

This table shows the results from a B20 blend with five different feedstocks measured with a Wilks InfraCal Biodiesel Blend Analyzer. As indicated in the B20 column, most of the feedstocks perform quite nicely for infrared analysis with the exception of coconut oil.

Feedstock	B20	Average Molecular Weight
Soybean	20.1	249
Yellow Grease	19.8	Unknown
Rapeseed [2]	20.6	281
Palm	20.2	239
Coconut	26.1	180

Table 1: Biodiesel feedstock comparison[1]

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For the math minded folks:

(240÷180) x 20 = 26.7%
(Average molecular weight of the methyl esters from the other feedstocks divided by the average molecular weight of the methyl esters from coconut oil times the biodiesel concentration.)

Note that each type of oil will yield a mixture of esters so there is no single molecular weight for the product from coconut oil.

The third column of the table shows the average molecular weight of the FAME (fatty acid methyl ester). Notice that the coconut oil is significantly different from the other oils with a molecular weight of 180. According to the molecular weight the coconut-based FAME should give a response of about 26.7% (see sidebar). Any infrared analyzer can be calibrated specifically for a coconut oil so the concentration measurement will be correct in spite of the molecular weight difference. Conveniently, the biodiesel made from coconut oil does not perform well in cold or temperate climates so its use is restricted to more tropical parts of the world.

Infrared measurements typically see little effect from a majority of the biodiesel feedstocks, making infrared analysis a simple and reliable analytical technique for checking biodiesel blend.

Infrared instruments, such as the InfraCal Biodiesel Blend Analyzer and InfraSpec VFA-IR Spectrometer, enable petroleum terminals, fuel distributors, fleet operators and regulatory agencies to make quick, on-site measurements with little or no technical training.



1 "Chemistry of Organic Compounds, 3rd Edition",Carl R. Noller, W. B. Saunders, Philadelphia (1965)
2 http://www.welch-holme-clark.com/products2.htm

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