The Relative Abundance of Volatile Organic Compounds in the Water Soluble Fraction of B20 Biodiesel

MATERIALS AND METHODS

Water Soluble Fraction Extraction. Five milliliters (mL) of B20 Biodiesel and 5 mL of deionized (DI) water were placed into a 40 mL glass vial. The mixture was vortexed for 3 minutes, then was allowed to equilibrate for approximately 4 hours. The product layer was then removed and the aqueous layer was transferred to a 4 mL glass vial. A tenfold dilution was performed on an aliquot of the aqueous layer prior to analysis.

Water Soluble Fraction Analysis. The aqueous layer was analyzed for volatile organic compounds (VOCs) using an Agilent 6890N gas chromatograph (GC) fitted with a 5975B mass selective detector (MSD) and a Tekmar ATOMX Purge and Trap autosampler. The VOC analysis included analytes calibrated against known standards as well as compounds tentatively identified using a mass spectral library. Only compounds with a qualifier value greater than 85 and a relative concentration of 0.1% or higher of the total dissolved VOC burden were included in this evaluation.

RESULTS

The non-hydrocarbon and hydrocarbon VOCs identified in the water soluble fraction of B20 biodiesel are provided in Tables 1 and 2, respectively. The boiling point range of this analysis was between -0.5°C and 256°C. Approximately 42% of the total dissolved VOC burden was not identified in this analysis.

TABLE 1. Water Soluble Non-Hydrocarbon VOCs

Compound	Percent of VOC Burden
Butanoic acid, methyl ester	5.7
Ethanol	1.8
Propanoic acid, methyl ester	1.4
Pentanoic acid, methyl ester	1.1
Hexanoic acid, methyl ester	0.66
Acetone	0.42

TABLE 2. Water Soluble Hydrocarbon VOCs

Compound	Percent of VOC Burden
Indane	5.0
1,2,4-Trimethylbenzene	4.3
Benzene, 2-ethenyl-1,4-dimethyl-	4.1
Benzene, 1-ethyl-3-methyl	4.0
m,p-Xylene	3.3
Toluene	3.0
Naphthalene, 1,2,3,4-tetrahydro-	2.7
Benzene, 1-ethenyl-4-ethyl-	2.3
o-Xylene	2.2
Naphthalene, 1,2,3,4-tetrahydro-6-methyl-	1.9
Naphthalene	1.5
1,3,5-Trimethylbenzene	1.3
Benzene, 1-ethyl-2-methyl-	1.3
1,3-Cyclopentadiene, 1,2,3,4-tetramethyl-5-methylene-	1.3
1H-Indene, 2,3-dihydro-1,2- dimethyl-	1.1
p-Cymene	1.0
Ethylbenzene	1.0
n-Propylbenzene	1.0
Naphthalene, 1,2,3,4-tetrahydro-8-methyl-	0.89
Benzene, 2-ethyl-1,4-dimethyl	0.86
Benzene, (3-methyl-2-butenyl)-	0.79
1H-Indene, 2,3-dihydro-1,3-dimethyl-	0.69
Benzene	0.68
n-Butylbenzene	0.44
Butane, 2-methyl-	0.30
Isopropylbenzene	0.24
4-Isopropyltoluene	0.15

DISCUSSION

A suite of non-hydrocarbon VOCs was identified in the water soluble fraction of B20 biodiesel. This suite included ethanol and fatty acid methyl esters (FAME). Although the major FAME peaks typically found in biodiesel include hexadecanoic acid methyl ester and isomers of octadecanoic acid methyl ester, lower molecular weight FAME compounds such as propanoic acid methyl ester, butanoic acid methyl ester, pentanoic acid methyl ester, and hexanoic acid methyl ester were also identified in this analysis.

FAME is typically manufactured by the transesterification of vegetable/seed oils or animal fats. Alcohols such as methanol or ethanol can be used as reactants in the transesterification process. The presence of ethanol in the water soluble fraction may be attributed to these reactants being present or could be related to contamination occurring during transport/storage of the fuel in a system where oxygenated gasoline is also handled.

A suite of hydrocarbon VOCs was also identified in the water soluble fraction of B20 biodiesel. This hydrocarbon suite had a boiling range of approximately 80°C to 230°C. The dominant hydrocarbons identified were indane, 1,2,4-trimethylbenzene, 2-ethenyl-1,4-dimethyl-benzene, 1-ethyl-3-methyl-benzene, *m,p*-xylene, and toluene.

FOR FURTHER READING

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