

Product Composition/Monitoring

Test Substance

Category Name: KEROSENE/JET FUELS CATEGORY

Category Chemical :

hydrodesulfurized kerosene, CAS No. 64742-81-0

Test Substance :

hydrodesulfurized kerosene, CAS No. 64742-81-0

Test Substance Purity/Composition and Other Test Substance Comments :

Relative Density, ASTM D40520.8204
 API Gravity @ 60 °C.....41.0
 Boiling Range Distribution, ASTM D2887
 Initial:107.9 °C
 Final:341.0 °C
 Hydrocarbon Types by FIA, ASTM D1319
 Aromatics16.8 Vol %
 Olefins2.9 Vol %
 Saturtes80.4 Vol %
 Aromatic content by SFC, ASTM D5186
 Monoaromatics22.0 Wt %
 Polynuclear Aromatics.....0.8 Wt %
 Total Aromatics22.8 Wt %

CAS definition of hydrodesulfurized kerosene (CAS No. 64742-81-0):
 A complex combination of hydrocarbons obtained from a petroleum stock by treating with hydrogen to convert organic sulfur to hydrogen sulfide which is then removed. It consists of hydrocarbons having carbon numbers predominantly in the range of C9 through C16 and boiling in the range of approximately 150 °C to 290 °C (302 °F to 554 °F).
 Data source: Intertek (Caleb Brett). 2007. Report of analysis, Reference No. US785-0016408. Intertek, Deer Park, TX.

Reference :

ExxonMobil Research and Engineering Co. Company Data. Annandale, NJ, USA.

Description :

The results field provides an attachment containing high resolution two dimensional gas chromatography (2D-GC) with flame ionization detection of a sample of hydrodesulfurized kerosene (CAS No. 64741). This sample was used in aquatic toxicity testing for complete data gaps for biodegradability, fish acute toxicity, invertebrate acute toxicity, invertebrate chronic toxicity, and algal toxicity.

GCxGC Chromatographic Conditions
 The kerosine sample was analyzed directly by GCxGC using the conditions shown below. The saturate fractions were analyzed under similar conditions with the only difference in 1st and 2nd dimensional column length.

Whole sample (including aromatic fraction):
 Instrument: Agilent Technologies 6890 Series GC
 Injector: Split/Splitless in Split Mode
 Initial Temp 60° C
 Ramp 3° C/sec
 Final Temp 240° C
 Column flow at 1 mL/min in constant flow mode
 Split ratio at 1:50
 Sample injection: Agilent ALS- Injection volume 0.2 µL

Modulator: Cryogenic modulator, single jet loop type (ZOEX Corporation)
Modulation time 10 sec
Pulse width 400 ms
N2 Flow rate approx 5L/min, controlled by a flow meter
Detector: Flame-ionization
Temperature at 300° C
Makeup gas He
Makeup flow 20 mL/min
Hydrogen flow 40 mL/min
Air flow 450 mL/min
Column 1: 30 m x 0.25 mm i.d. 5% phenyldimethylpolysiloxane column (BPX-5) with film thickness of 1.0 µm
Column 2: 2m x 0.25 mm i.d. polysilphenylene-siloxane column (BPX-50) with film thickness of 0.25 µm
(One end of 2nd Dim column forms loop modulation, and the other end direct into FID)
Carrier gas: Helium
Oven temperature: 60° C (0 min isothermal) then 3.0° C/min to 240° C
Hot Jet: 180° C offset from Oven: 240° C (0 min temperature isothermal) then 3.0° C/min to 390° C (10 min isothermal)

Saturate fraction only:

Instrument: Agilent Technologies 6890 Series GC
Injector: Split/Splitless in Split Mode
Initial Temp 60° C
Ramp 3° C/sec
Final Temp 240° C
Column flow at 1 mL/min in constant flow mode
Split ratio at 1:50
Sample injection: Agilent ALS- Injection volume 0.2 µL
Modulator: Cryogenic modulator, single jet loop type (ZOEX Corporation)
Modulation time 10 sec
Pulse width 400 ms
N2 Flow rate approx 5L/min, controlled by a flow meter
Detector: Flame-ionization
Temperature at 300° C
Makeup gas He
Makeup flow 20 mL/min
Hydrogen flow 40 mL/min
Air flow 450 mL/min
Column 1: 15 m x 0.25 mm i.d. 5% phenyldimethylpolysiloxane column (BPX-5) with film thickness of 1.0 µm
Column 2: 3m x 0.25 mm i.d. polysilphenylene-siloxane column (BPX-50) with film thickness of 0.25 µm
(One end of 2nd Dim column forms loop modulation, and the other end direct into FID)
Carrier gas: Helium
Oven temperature: 60° C (0 min isothermal) then 3.0° C/min to 240° C
Hot Jet: 180° C offset from Oven: 240° C (0 min temperature isothermal) then 3.0° C/min to 390° C (10 min isothermal)

Data Analysis

	<p>GCxGC data processed and visualized with in- house developed software.</p> <p>Having acquired the raw GCxGC data on the sample, the profile was examined and templates constructed to group individual components into the appropriate carbon number (C5 to C30) and chemical functionalities shown below:</p> <ul style="list-style-type: none">• n-paraffins• iso-paraffins• n-alkane substituted cyclohexane and cyclopentane• mono-naphthenics• di-naphthenics• mono-aromatics• naphthenic mono-aromatics• di-aromatics
<p><u>Results:</u></p>	<p>The peak area for each component or component group identified was directly integrated with the assumption of a universal unit response factor to all hydrocarbons by the flame ionization detector</p> <p>The components found in the kerosine sample has been determined and tabulated in compound classes and carbon number order, as shown in the table. Corresponding GCxGC chromatogram of the whole sample is attached for reference purpose.</p>

2D-GC Analysis Results for Hydrodesulfurized Kerosene, CAS No. 64742-81-0

C no.	n-P	iso-P	n-CC5/6	iso-N	DiN	mono-Ar	N mono Ar	Di Ar	N Di Ar	Tri Ar	N Tri Ar	
6	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	
7	0.02	0.00	0.09	0.00	0.00	0.06	0.00	0.00	0.00	0.00	0.00	
8	0.16	0.19	0.19	0.11	0.00	0.35	0.00	0.00	0.00	0.00	0.00	
9	0.55	0.60	0.38	0.48	0.47	0.69	0.90	0.00	0.00	0.00	0.00	
10	2.63	1.63	1.44	4.26	1.69	3.30	0.61	0.00	0.00	0.00	0.00	
11	5.32	6.35	0.93	6.36	2.64	3.45	1.55	0.00	0.00	0.00	0.00	
12	2.38	4.45	0.76	4.32	3.07	2.22	2.11	0.00	0.00	0.00	0.00	
13	1.45	2.87	0.42	2.39	2.94	1.41	1.58	0.00	0.00	0.00	0.00	
14	0.91	1.71	0.28	1.63	1.69	0.92	1.14	0.00	0.00	0.00	0.00	
15	0.53	1.12	0.19	0.97	1.01	0.67	0.75	0.00	0.00	0.00	0.00	
16	0.32	0.59	0.09	0.60	0.58	0.30	0.42	0.00	0.00	0.00	0.00	
17	0.24	0.43	0.05	0.36	0.33	0.21	0.25	0.00	0.00	0.00	0.00	
18	0.14	0.21	0.03	0.22	0.18	0.12	0.15	0.00	0.00	0.00	0.00	
19	0.06	0.14	0.01	0.10	0.11	0.07	0.09	0.00	0.00	0.00	0.00	
20	0.03	0.06	0.01	0.04	0.06	0.00	0.00	0.00	0.00	0.00	0.00	
21	0.01	0.04	0.00	0.02	0.02	0.00	0.00	0.00	0.00	0.00	0.00	
22	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
Total	14.75	20.40	4.87	21.86	14.78	13.80	9.55	0.00	0.00	0.00	0.00	100.00

Heading Codes:

C-num = number of carbon atoms in group; nP = normal paraffins; isoP = iso-paraffins; n-CC5/6 = n-alkane substituted cyclopentane and cyclohexane; iso-N = iso-naphthenes; diN = di-naphthenes; mono-A = monoaromatics; N-mono-A = naphthenic-mono-aromatics; Di-A = di-aromatics; N-Di-A = naphthenic-di-aromatics; tri-A = tri-aromatics; N-tri-A = naphthenic-tri-aromatics.

2d-GC chromatogram of hydrodesulfurized kerosene, CAS No. 64742-81-0

