Application Note 20582

Analysis of Petroleum Fractions by ASTM D2887

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Key Words
Simulated distillation, D2887, TRACE TR-SimDist

Abstract
ASTM method D2887 describes a simulated distillation protocol for the separation of petroleum fractions over the boiling points range of 55.5 to 538 °C. The Thermo Scientific™ TRACE™ TR-SimDist GC column has been shown to achieve this separation in less than 20 minutes.

Introduction

ASTM method D2887 describes the gas chromatography (GC) conditions for simulated distillation of petroleum fractions in the boiling point range of 55.5 to 538 °C.[1]

Simulated distillation by GC is used to determine the boiling point range of a petroleum sample. Column heating causes the sequential elution of sample components based on their boiling point. A calibration curve is constructed that relates carbon number and boiling point to retention time and allows for the determination of boiling points for the components in an unknown test sample.

ASTM method D2887 presents a chromatographic challenge as the boiling point range is wide. To resolve hydrocarbons in the C5–C12 range, a particularly thick film is used. To elute heavier hydrocarbons, a high temperature is required.

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Experimental Details

Chemicals and Reagents

1. A commercially available standard containing all components in Table 1 was prepared in carbon disulfide at a concentration of 800 µg/mL. This concentration was found to give the optimum sensitivity and peak shape.

2. A commercially available gas oil reference mix, diluted twenty fold in carbon disulfide, was used to demonstrate the performance of the TRACE TR-SimDist GC column in a real sample.

Peak Number	Compound Name	Boiling Point (°C)	Peak Number	Compound Name	Boiling Point (°C)
1	n-pentane (C5)	36	**10**	n-hexadecane (C16)	287
2	n-hexane (C6)	69	**11**	n-octadecane (C18)	316
3	n-heptane (C7)	98	**12**	n-eicosane (C20)	344
4	n-octane (C8)	126	**13**	n-tetracosane (C24)	391
5	n-nonane (C9)	151	**14**	n-octacosane (C28)	431
6	n-decane (C10)	174	**15**	n-dotriacontane (C32)	466
7	n-undecane (C11)	196	**16**	n-hexatriacontane (C36)	496
8	n-dodecane (C12)	216	**17**	n-tetracontane (C40)	522
9	n-tetradecane (C14)	254	**18**	n-tetratetracontane (C44)	545

Table 1: ASTM D2887 Calibration standard containing C5–C44

Sample Handling Equipment		Part Number
Vials and closures:	9 mm screw cap vial with Blue Silicone/PTFE Closure	60180-599

Separation Conditions		Part Number
Instrumentation:	Thermo Scientific TRACE GC	
Column:	TRACE TR-SimDist 10 m x 0.53 mm x 2.65 µm	260S348P
Septum:	Thermo Scientific BTO Septa, 12.7 mm	31303228
Liner:	Thermo Scientific PTV Silcosteel Liner for PTV simulated on-column injection	45322052
Column ferrules:	Graphite ferrules to fit 0.53 mm ID columns	29053488
Injection syringe:	10 µL fixed needle 80 mm cone tip	36502019
Carrier gas:	Helium	
Column flow:	12 mL/min (constant flow)	
Oven temperature:	40 °C hold 1 minute, 20 °C/min to 370 °C, hold 5 minutes	
Injector type:	Programmable temperature vaporizer (PTV)	
Injector mode:	Simulated on-column	
Injection volume:	1 µL	
Injector temperature:	40 °C, 10 °C/s to 370 °C, hold 20 minutes	
Detector details:	Flame ionization detector (FID), 370 °C	

Data Processing	
Software:	Thermo Scientific Xcalibur™

Results

The lower boiling point components in the C5–C10 region exhibited good retention and resolution (Figure 1) because the 2.65 µm film gave greater retention than a thinner film column would.

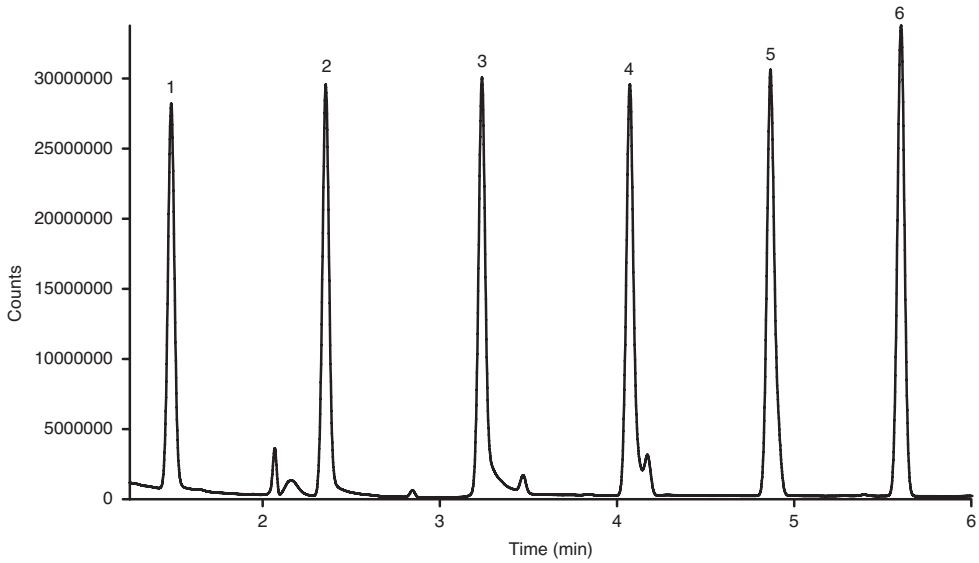

Figure 1: Compounds C5–C10

The resolution between the C16 and C18 peaks (10 and 11) was calculated to be 6.12, exceeding the minimum specification of 3 as set out in the ASTM method (Figure 2).

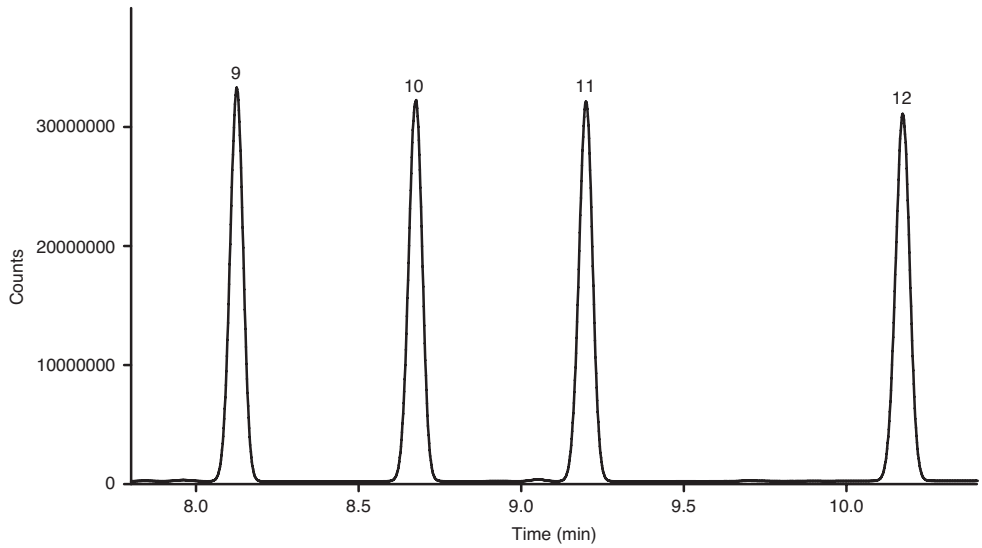

Figure 2: Resolution between the C16 and C18 (peaks 10 and 11)

Peak shapes across the boiling point range were symmetrical and showed no evidence of overload at a concentration of 800 µg/mL. This allowed a calibration curve to be constructed of retention time against boiling point (boiling point data taken from ASTM method) showing a linearity of greater than 0.99 (Figure 3).

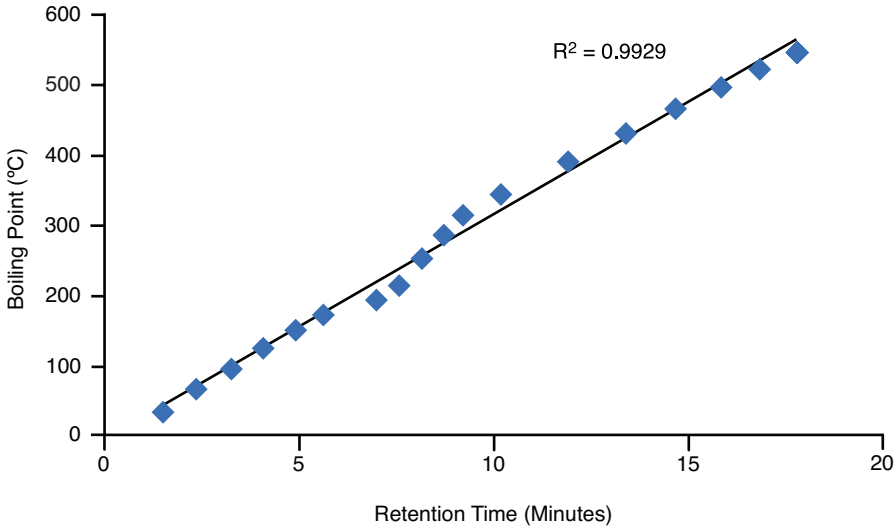

Figure 3: Boiling point calibration curve

The calibration curve was used to determine the boiling point range of a reference gas oil sample. This sample was found to contain compounds with boiling points between 36 and 475 °C (Figure 4).

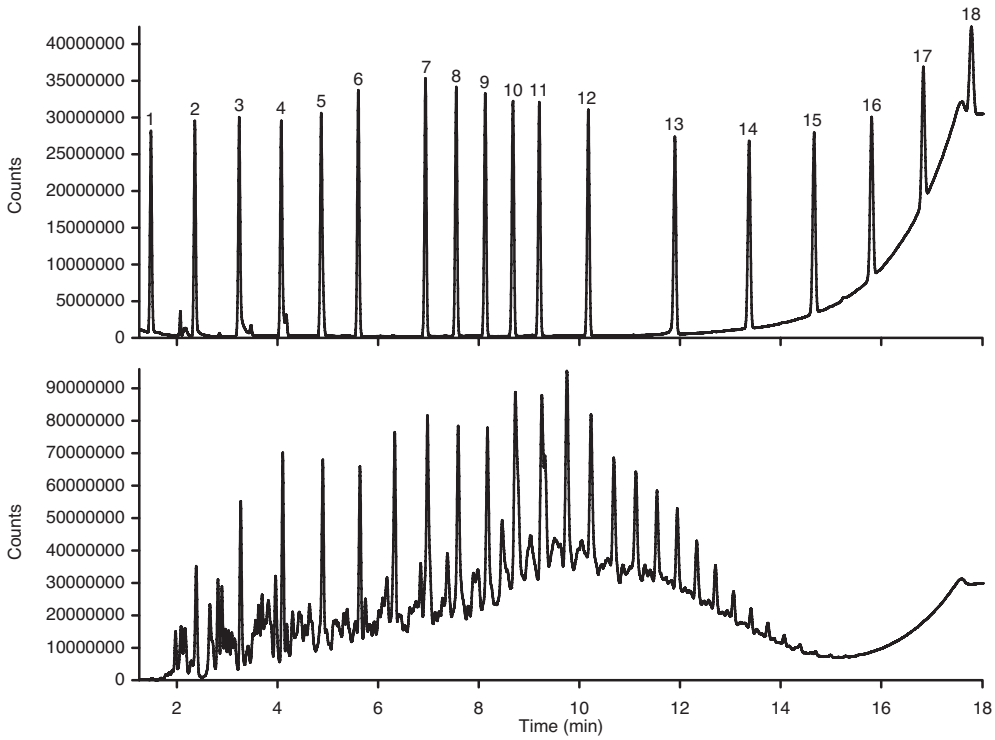

Figure 4: Calibration standard at 800 µg/mL (top chromatogram) overlaid with reference gas oil sample diluted 20 times in CS_2 (bottom chromatogram)

Conclusion

- The TRACE TR-SimDist GC column meets the criteria for the analysis of hydrocarbons with boiling points between 55.5 and 538 °C as required by ASTM D2887.
- A combination of thick film and high temperature allows the separation of these n-alkanes with a broad boiling point range with good peak shape.

References

1. ASTM Standard D2887-08, 2008, "Standard Test Method for Boiling Range Distribution of Petroleum Fractions by Gas Chromatography," ASTM International, West Conshohocken, PA, 2008, DOI: 10.1520/D2887-08, www.astm.org.

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