BEYOND MEASURE

SCION INSTRUMENTS

# Analysis of Boiling Point Distributions in Petroleum Fractions using Simulated Distillation (ASTM D2887A).

## Application Note

### INTRODUCTION

In many regions ASTM D2887 may be used for determining the boiling point distribution of petroleum products, feedstocks and fractions that have a final boiling point of 538°C or lower. This provides insight into composition and determining intrinsic product value.

Even though Physical Distillation is still considered the reference method for distillation, and therefore mandatory in many countries for qualifying fuels, Simulated Distillation (SIMDIST) by gas chromatography offers some significant advantages over the physical procedure, making this technique valuable.

Analysis by GC typically has the better precision, more throughput, less hands-on time and lower cost per sample. Lastly, SIMDIST requires considerable less sample and should generally be considered the safer of the two techniques.

In addition to the standard method (procedure A), a second procedure has recently been added into D2887, the accelerated or fast method (procedure B).

This application note demonstrates a solution for D2887 procedure A for analysing Petroleum products covering a boiling point range of 36°C to 545°C. This procedure is not suited for biodiesels. For gasolines, method D7096 should be used.

### EXPERIMENTAL

The SCION SimDist analyser comprises of a SCION 456-GC or 436-GC, configured with a cool on column (COC) injector, a 10m x 0.53mm x 2.65µm SimDist column, and Flame Ionisation Detector (FID). Analytical conditions for the SimDist analysis can be found in Table 1. A qualitative mixture of normal paraffins ($C_5$-$C_{44}$ , 1% wt./wt. each in $CS_2$) was used to determine the relationship of boiling point (BP) versus retention time (RT).
All Samples were diluted prior to injection in $CS_2$ per ASTM D2887-18. Gasoil samples, diluted in $CS_2$ were analysed as a quality control.

**Table 1.** Analytical conditions of the SimDist analyser

| | |
|---|---|
| **Injector** | Cold on Column at 350°C |
| **Column** | 10m x 0.53mm x 2.65µm Scion SimDist Inert Steel (SC37788) |
| **Oven** | -20°C, 10°C/min to 350°C (2min) |
| **Carrier** | Helium at 20mL/min |
| **Detector** | FID at 350°C |
| **Injection Volume** | 1 µl (diluted in CS2) |
| **Software** | Eclipse SIMDIST |

### RESULTS

Figures 1 and 2 show the n-paraffins mixture, and the resulting RT vs BP calibration curve as constructed by the SIMDIS Software

In order to meet the requirements of ASTM D2887, the reference gas oil sample was analysed. The sample was analysed over five consecutive injections as per the ASTM D2887 method.

Figure 3 shows the chromatogram of the reference gas oil sample, with Table 2 showing the total boiling point distribution of the gas sample along with the ASTM D2887 reference values and max deviation criteria.

Differences between Reference BP and Observed BP for each 10% weight slice fraction typically are <2°, with exception of the FBP, which was slightly larger. All these are well within the allowable value of the ASTM D2887 method.

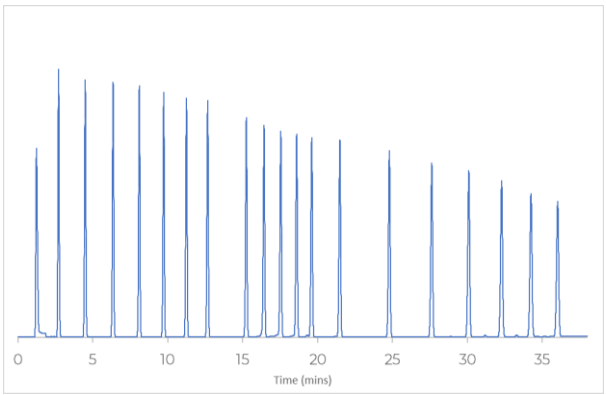


**Fig 1**. C5-C44 n-Paraffins Calibration Mix, 1% in $CS_2$

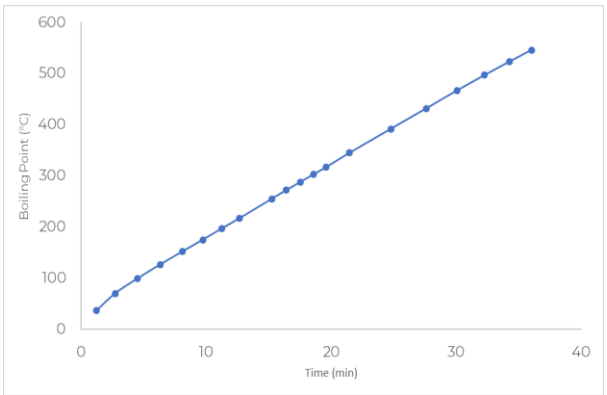


**Fig 2**. C5-C44 n-Paraffins RT vs Boiling Point Calibration

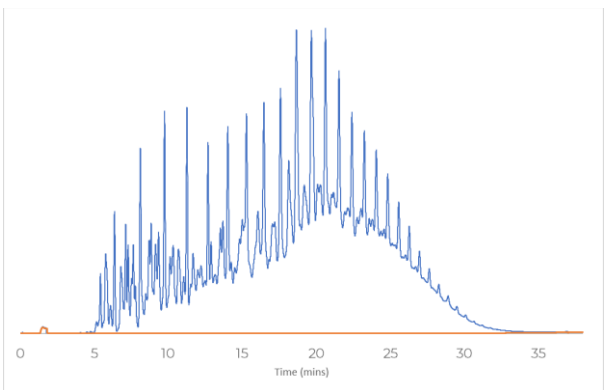


Fig 3. Overlay of Reference Gas Oil Sample with $CS_2$ Blank

**Table 2.** Observed Values and ASTM Consensus values for Reference Gas Oil 1, Lot # 2 Sample (n=5)

| OFF% | Observed BP °C | ASTM Ref BP°C | Allowable Difference (°C) | Observed Difference (°C) |
|---|---|---|---|---|
| IBP | 115.5 | 115 | 7.6 | 0.5 |
| 5 | 150.0 | 151 | 3.8 | 1.0 |
| 10 | 174.4 | 176 | 4.1 | 1.6 |
| 20 | 222.5 | 224 | 4.9 | 1.5 |
| 30 | 258.0 | 259 | 4.7 | 1.0 |
| 40 | 288.1 | 289 | 4.3 | 0.9 |
| 50 | 311.3 | 312 | 4.3 | 0.7 |
| 60 | 330.8 | 332 | 4.3 | 2.2 |
| 70 | 352.8 | 354 | 4.3 | 1.2 |
| 80 | 377.3 | 378 | 4.3 | 0.7 |
| 90 | 406.8 | 407 | 4.3 | 0.2 |
| 95 | 430.0 | 428 | 5.0 | 2.0 |
| FBP | 482.5 | 475 | 11.8 | 7.5 |

## CONCLUSION

It is demonstrated that Scion SIMDIS solution passes criteria as described in ASTM D2887, procedure A. Differences between observed values and consensus value for the reference gasoil used were generally small, typically 2° or lower, with exception of the FBP.

Please note that:
- Boiling range distributions obtained by this test method are essentially equivalent to those obtained by true boiling point (TBP) distillation (see Test Method D2892).
- They are not equivalent to results from low efficiency distillations such as those obtained with Test Method D86 or D1160.
- The gas chromatographic simulation of this determination can be used to replace conventional distillation methods for control of refining operations.
- This test method can be used for product specification testing with the mutual agreement of interested parties [1].

## References

[1] ASTM D2887 – 18. Standard Test Method for Boiling Range Distribution of Petroleum Fractions by Gas Chromatography. https://www.astm.org/Standards/D2887.htm

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