Application Note

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Simulated Distillation Analysis of Middle Distillates Using the Accelerated ASTM D2887 Method

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Abstract

This Application Note describes the performance of the Agilent 8890 gas chromatograph when running ASTM D2887B using each of the three capillary columns specified by the method. Key performance measures were easily met using each tested configuration.

Introduction

ASTM D2887 is a gas chromatographic method used to determine the boiling point distribution of middle distillates such as kerosene, aviation fuel, diesel, and selected light oils[1]. ASTM developed an accelerated version of D2887 using the same capillary columns as the original D2887 method. For the accelerated D2887, analysis times were reduced from 30 minutes to nine minutes using higher column flows and faster oven temperature programming ramps. ASTM has designated this method as D2887B with the operating conditions incorporated into the existing D2887 document.

Experimental

Instrument configuration and operating conditions

An Agilent 8890 GC was configured according to the ASTM D2887B specifications using each of these three columns:

- **Column 1:**
  HP-1, 10 m × 0.53 mm id, 0.88 mm (p/n 19095Z-021)
- **Column 2:**
  HP-1, 5 m × 0.53 mm id, 2.65 mm (p/n 19095S-100)
- **Column 3:**
  DB-1, 7.5 m × 0.53 mm id, 1.5 mm (p/n 125-1002)

Table 1 shows the hardware configuration for the 8890 GC, and Table 2 shows the specific operation conditions used for each column.

A calibration standard containing normal hydrocarbons from C_5 to C_{44} was prepared by dissolving the Agilent D2887 Calibration Mixture (p/n G3440-85037) in 15 mL of carbon disulfide. This solution was analyzed on each column using the instrument conditions listed in Table 2. After calibration, the system performance was verified by analyzing Reference Gas Oil (RGO) Sample 1, batch 2 (p/n 5060-9086). Three middle distillate samples, representing boiling ranges across the D2887 scope, were then analyzed on each column. Both the RGO sample and three middle distillate samples were injected neat.

Table 1. 8890 configured for ASTM D2887B.

Parameter	Value
Automatic Liquid Sampler	Agilent 7650 ALS
Syringe	Autosampler syringe 5 µL (p/n G4513-80206)
Inlet	Cool-on-column (COC)
Detector	Flame ionization (FID)

Table 2. 8890 Operating conditions for ASTM D2887.

ALS	Column 1	Column 2	Column 3
Sample injection volume	0.1 µL	0.1 µL	0.1 µL
Pre-injection solvent washes	5 × 0.25 µL CS_2	5 × 0.25 µL CS_2	5 × 0.25 µL CS_2
Pre-injection sample washes	none	none	none
Sample pumps	5	5	5
Post injection solvent washes	5 × 0.25 µL CS_2	5 × 0.25 µL CS_2	5 × 0.25 µL CS_2
Viscosity delay	2 seconds	2 seconds	2 seconds
Inlet			
Initial temperature	100 °C	100 °C	100 °C
Initial hold time	0.1 minutes	0.1 minutes	0.5 minutes
Ramp rate	35 °C /min	35 °C /min	35 °C /min
Final temperature	350 °C	350 °C	350 °C
Column			
Flow rate	26 mL/min helium	35 mL/min helium	37 mL/min helium
Initial temperature	60 °C	40 °C	40 °C
Initial hold time	0.1 minutes	0.1 minutes	0.5 minutes
Ramp rate	35 °C /min	35 °C /min	35 °C /min
Final temperature	360 °C	360 °C	360 °C
FID			
Temperature	360 °C	350 °C	350 °C
Hydrogen flow	40 mL/min	40 mL/min	40 mL/min
Air flow	400 mL/min	400 mL/min	400 mL/min
Make-up flow	N_2 at 15 mL/min	N_2 at 15 mL/min	N_2 at 15 mL/min

Results and discussion

Figure 1 shows the calibration standard runs from all three columns. Each column showed good separation of the C_5 to C_8 normal alkanes with average peak skewness of 1.1 for all peaks from C_6 to C_{44}. Additionally, the chromatographic resolution for *n*-C_{16} and *n*-C_{18} was greater than 4 on each column. Figure 2 shows a typical boiling point calibration report for column 1 obtained using the Agilent SimDis software. Similar reports were obtained for the calibration data from columns 2 and 3 (not shown).

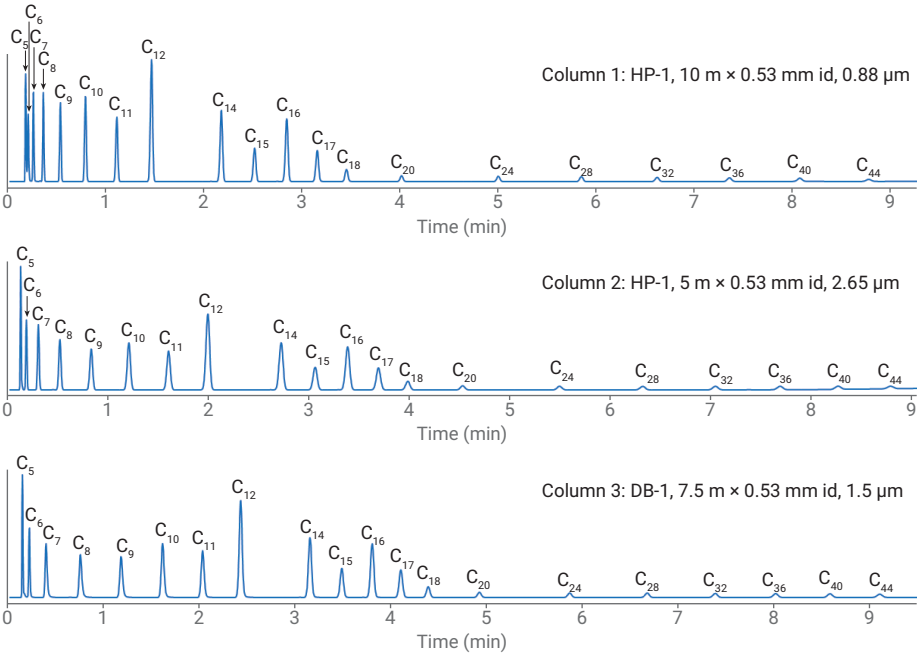

Figure 1. Calibration standards run on each column specified in ASTM D2887B.

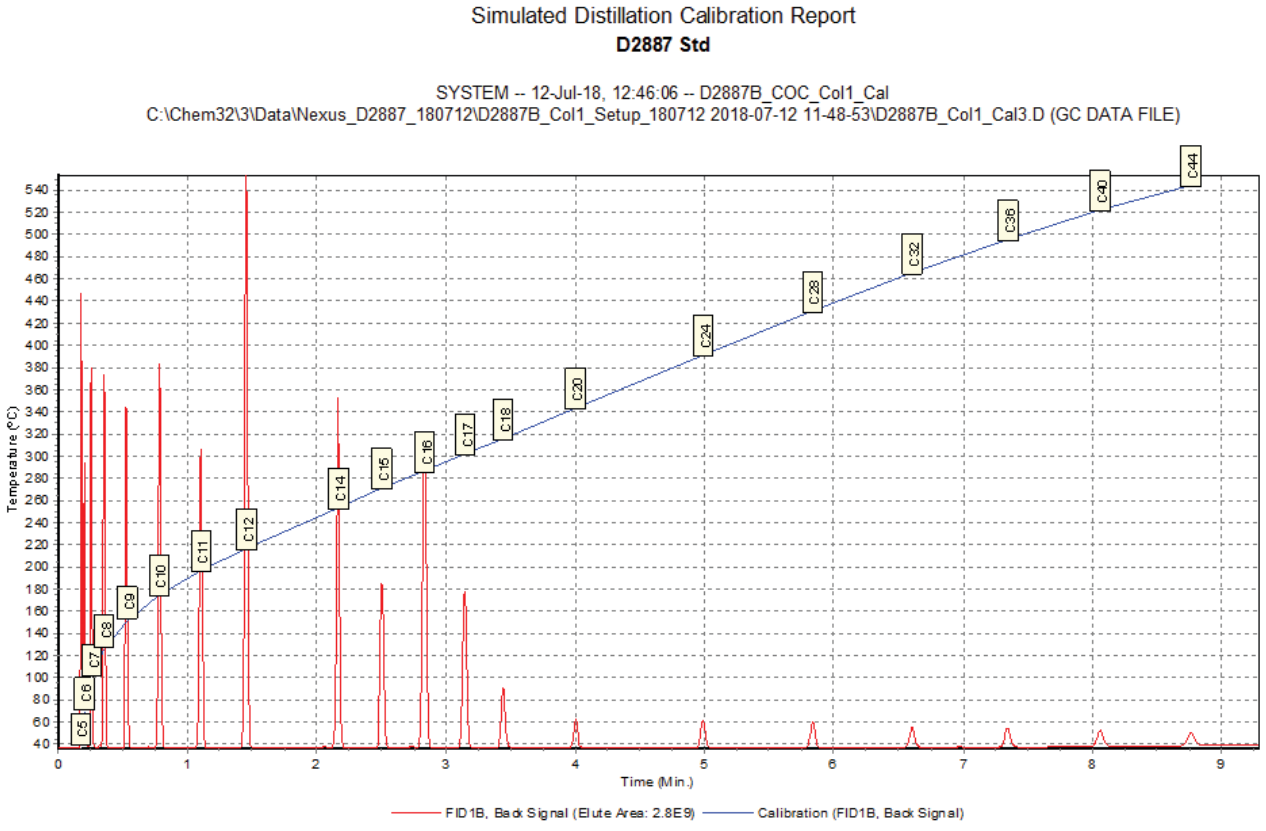

Figure 2. SimDis boiling point calibration curve for column 1.

Before running samples, the system performance was verified by analyzing an RGO sample, and comparing the experimental cut point temperatures to the published reference values. Figure 2 shows an engineering report containing the boiling point yield curve and RGO results obtained with column 1. Table 3 lists the experimental RGO performance results compared to the reference values. For each column, the experimental cut point temperatures fall well within the ranges allowed by ASTM.

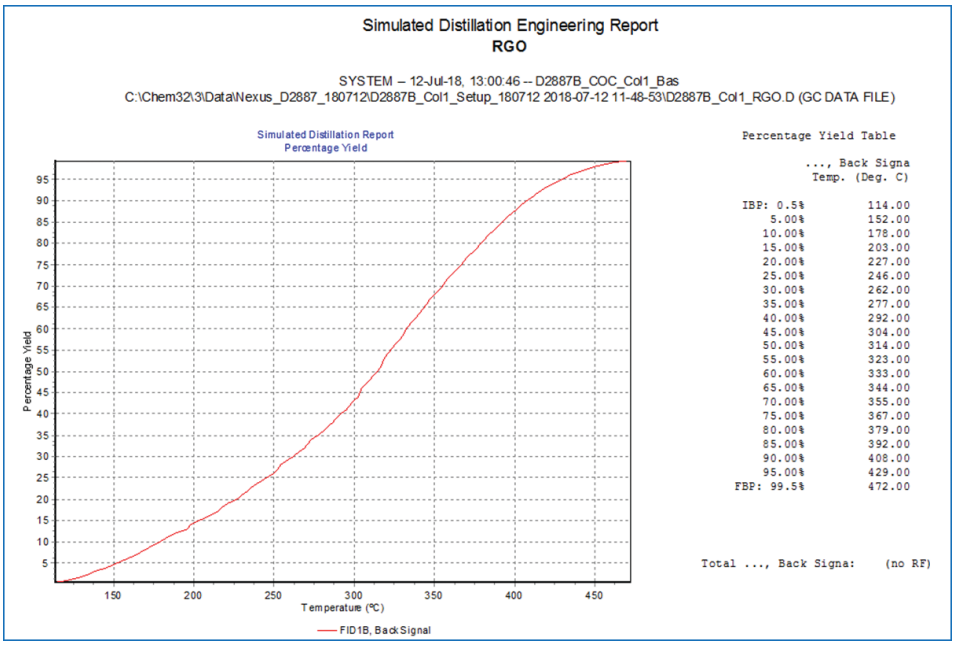

Figure 3. Agilent SimDis Engineering Report showing the boiling point yield curve and results for the RGO analysis on column 1.

Table 3. RGO Performance results for each D2887B column.

	Ref	Allowed	Column 1		Column 2		Column 3	
% Off	Temp °C	Diff °C	Temp °C	Diff °C	Temp °C	Diff °C	Temp °C	Diff °C
IBP (0.5)	115	7.6	114	1.0	115	0.0	115	0.0
5	151	3.8	152	1.0	151	0.0	151	0.0
10	176	4.1	178	2.0	175	1.0	177	1.0
15	201	4.5	203	2.0	201	0.0	202	1.0
20	224	4.9	227	3.0	224	0.0	225	1.0
25	243		246	3.0	243	0.0	244	1.0
30	259	4.7	262	3.0	259	0.0	259	0.0
35	275		277	2.0	275	0.0	275	0.0
40	289	4.3	292	3.0	289	0.0	289	0.0
45	302		304	2.0	302	0.0	303	1.0
50	312	4.3	314	2.0	312	0.0	312	0.0
55	321	4.3	323	2.0	321	0.0	321	0.0
60	332	4.3	333	1.0	331	1.0	332	0.0
65	343	4.3	344	1.0	342	1.0	342	1.0
70	354	4.3	355	1.0	353	1.0	353	1.0
75	365	4.3	367	2.0	365	0.0	365	0.0
80	378	4.3	379	1.0	378	0.0	378	0.0
85	391	4.3	392	1.0	391	0.0	391	0.0
90	407	4.3	408	1.0	407	0.0	407	0.0
95	428	5	429	1.0	428	0.0	428	0.0
FBP (99.5)	475	11.8	472	3.0	474	1.0	473	2.0

Figures 4, 5, and 6 show the three middle distillate samples and RGO chromatograms obtained with the three columns. The sample chromatograms are remarkably similar, with small differences in profile and retention times due to differences in column dimensions and operating conditions (see Table 2). The data from the sample runs were processed with the SimDis software using the calibration runs from each respective column (Figures 1 and 2). Table 4 compares the results obtained for the three middle distillate samples. The temperatures obtained at each cut point were nearly identical on all three columns.

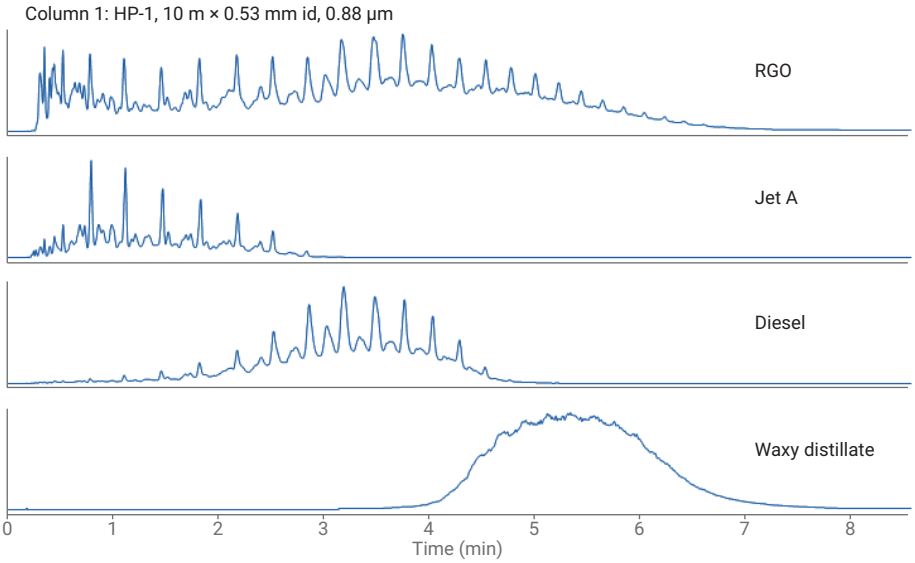

Figure 4. RGO and three middle distillate samples run on column 1.

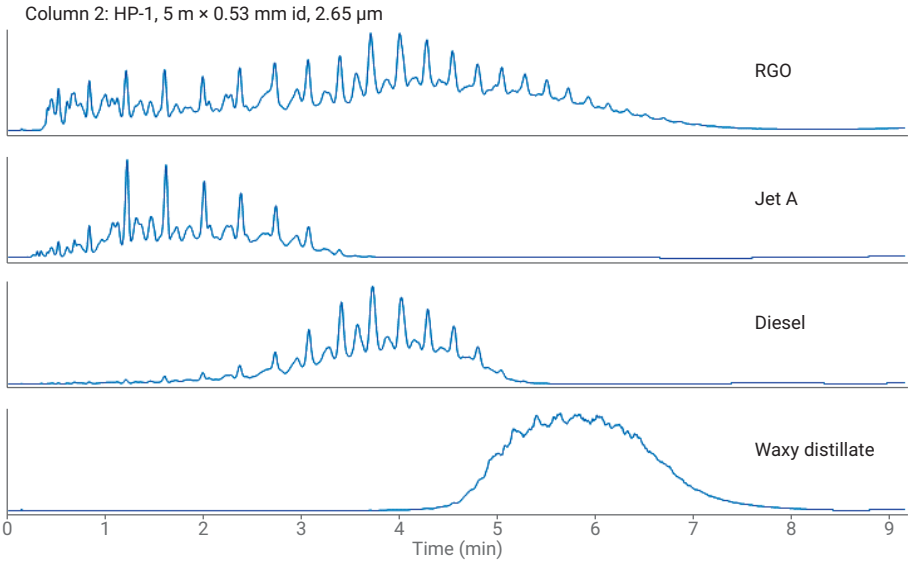

Figure 5. RGO and three middle distillate samples run on column 2.

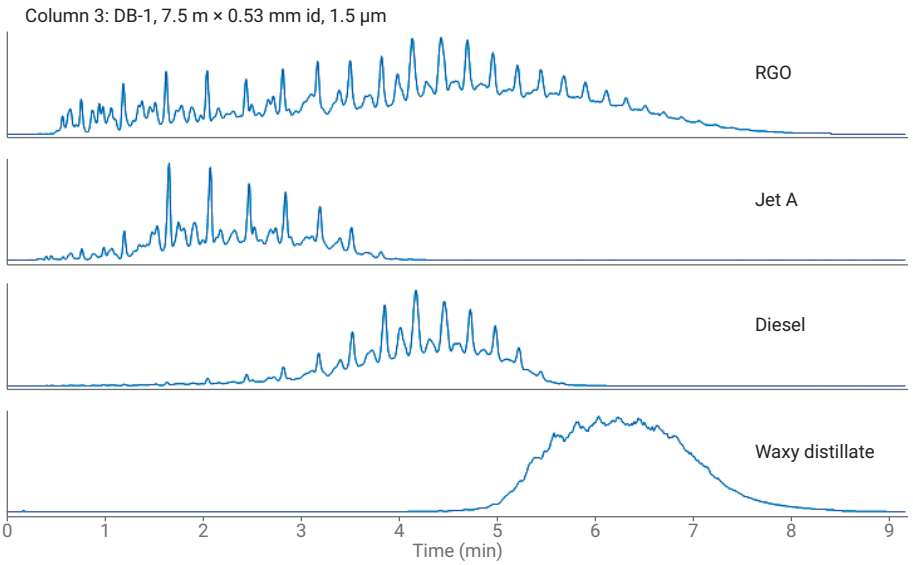

Figure 6. RGO and three middle distillate samples run on column 3.

Table 4. Comparison of results of three samples run on three D2887B columns.

	Jet A			Diesel			Waxy distillate		
% Off	Column 1	Column 2	Column 3	Column 1	Column 2	Column 3	Column 1	Column 2	Column 3
IBP (0.5)	103	104	103	156	152	157	333	336	336
5	145	145	146	230	229	231	363	361	362
10	162	162	163	253	252	254	371	369	370
15	169	169	170	267	266	267	377	375	376
20	175	175	176	274	273	275	382	380	382
25	180	180	181	283	282	283	387	385	387
30	186	186	188	288	288	289	392	390	392
35	193	193	194	295	294	295	396	395	397
40	197	197	198	299	299	300	401	399	401
45	202	202	203	304	303	305	405	404	406
50	209	209	210	307	306	308	409	408	410
55	216	216	217	313	312	314	414	413	415
60	219	219	221	318	317	319	418	417	419
65	227	227	228	321	320	322	423	421	424
70	233	233	235	327	326	328	428	426	428
75	237	237	238	332	331	333	433	431	433
80	246	246	247	337	337	339	438	437	439
85	253	253	254	344	344	345	444	443	445
90	261	260	262	350	350	351	452	451	452
95	271	271	272	358	358	359	465	464	465
FBP (99.5)	292	291	293	379	379	379	503	503	502

Conclusions

The 8890 GC was shown to successfully run a simulated distillation analysis according to the accelerated ASTM D2887B method using any one of the three specified capillary columns. Performance measures for peak symmetry, resolution, and RGO verification were easily met for each configuration. The 8890 GC system provided consistent cut point temperatures for three samples representing boiling ranges across the ASTM D2887 scope.

Reference

1. ASTM D2887-16a, Standard Test Method for Boiling Range Distribution of Petroleum Fractions by Gas Chromatography, ASTM International, West Conshohocken, PA, **2016**, www.astm.org.

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