GLOBAL™ ANALYSER SOLUTIONS

G·A·S

APPLICATION NOTE 205WA1214J

SIMDIST Analysers

*ASTM D3710 D2887 D5307 D5399
D5442 D6352 D7096
D7169 D7213 D7500
*DIN 51435 51581
*EN 15199-1,2&3
*IP 406 480 507 545
*ISO 3924 5442

Simulated distillation (Simdist) is a GC based method for the characterisation of petroleum products, fractions, lube oil and crude oil. Simdist determines the boiling range distribution in a quick, automated and reliable way. This method replaces the labour intensive and dangerous D86/1160 methods. True boiling point (TBP) data is vital information for improving refinery profit margins. Samples are analysed on a non polar column, separating hydrocarbons in boiling point order. Boiling points are correlated with retention time from a range of n-alkanes eluting under exact the same conditions and in the range of the sample. A blank analysis is subtracted from the sample chromatogram in order to correct for column bleeding. It is of great importance that the GC instrument has a very good run to run reproducibility. Results are reported as a correlation between boiling points and percentages of the sample eluted from the column. The results are confirmed by running a well known reference sample. The Simdist data correlates with ASTM D86 or D1160. The determination of boiling point distribution of petroleum products and crudes by conventional GC is a rapid and reliable tool, which is widely used to replace conventional distillation methods. This proven technology is supported by several standardised methods.

The fully automated solution for Simdist enables you to generate TBP data according to international reference methods. The G.A.S Simdist Calculator software is completely integrated in Chromeleon data system, with a clear and user friendly workflow as a result. Figure 1 shows a sample sequence list with samples, calibrations runs, blanks and check standards, while figure 2 displays a typical Simdist chromatogram with baseline substraction.

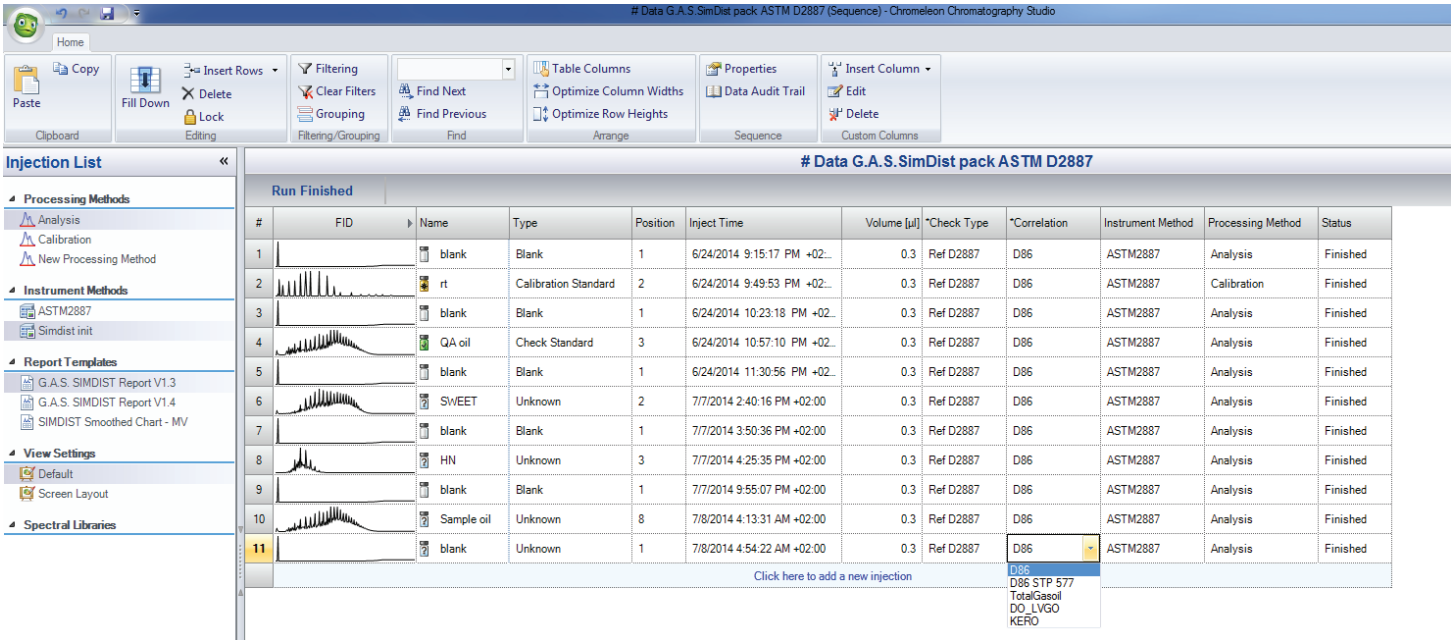


Figure 1: Chromeleon with G.A.S Simdist Calculator software: transparent acquisition list

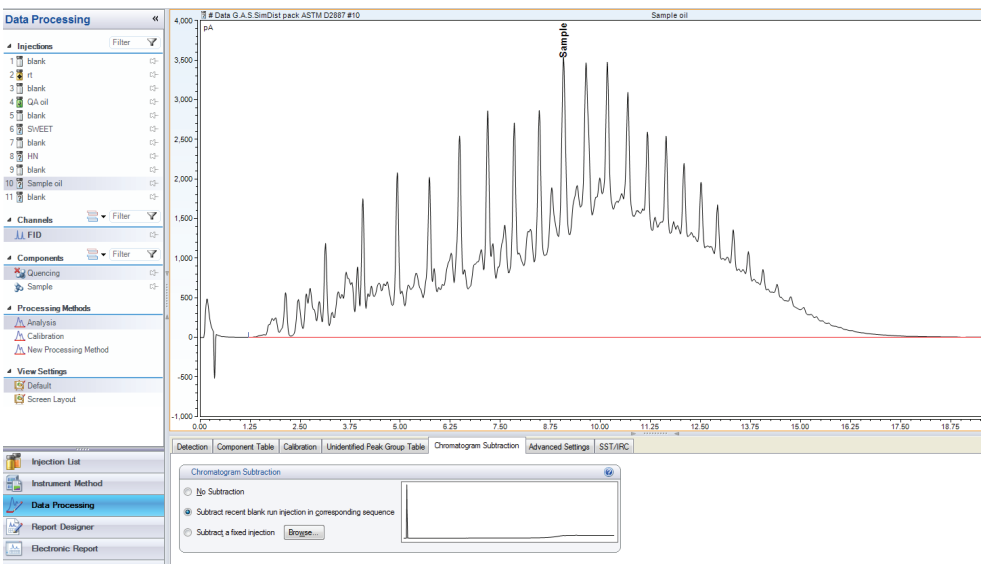


Figure 2: Simdist D2887 chromatogram with baseline substraction

Figure 3: GC Trace 1310 with RSH autosampler

Reporting and hardware solutions

Simdist Calculator software provides:

- ASTM D86 and D1160: correlation for atmospheric and vacuum distillation
- Custom correlation models can be added by the user
- DIN 51.581 (NOACK): evaporative loss in mass% of lubricants at 250°C
- ASTM D6417 (MOV): evaporation loss in mass% of lubricants at 371°C
- Flashpoint correlations according to ASTM D56, D93 and D3828
- Cut point tables
- Simdist/DHA MERGE of ASTM D7169/ IP545 data according to ASTM D7900

Besides the boiling point distribution report (figure 4), a quality control report is available as well (figure 5). This report shows the conformity with reference samples, and is therefore very important for the overall reliability of the method.

Available hardware solutions:

- Thermo Trace 1300/1310 GC with InstantConnect injector and detector modules
- On-Column injector module for true quantitative analytical results
- PTV including Backflush, for light-end Simdist of heavy oil and crude oil
- Triplus RSH or AI/AS 1310 autosamplers

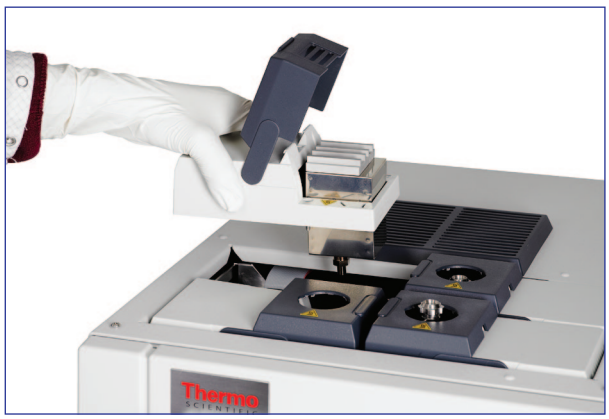


Figure 6: easy InstantConnect injector/detector exchange

Simdist application package including:

- Set of standards, Polywax (500, 655 or 1000) or hydrocarbon mix according to the required method to set the Boiling point distribution versus retention time
- External reference sample, for quantification and performance verification
- Analytical column, MXT-1 2887, or MXT-1HT for high temperature Simdist up to FBP 750 °C
- System performance check

SimDist calculation pack V1.4

SimDist Analysis Report

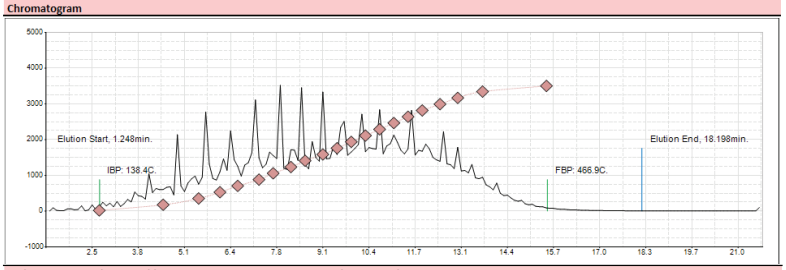
Injection Name:	SWEET	Run Time (min):	23.25	
Vial Number:	2	Injection Volume:	0.30	
Injection Type:	Unknown	Sample Weight:	0	gram
Sequence:	# Data G.A.S.SimDist pack ASTM D2887	Solvent Weight:	0	gram
Instrument Method:	ASTM2887	Quenced Area	n.a.	
Processing Method:	Analysis	Sample Area	16046.501	
Injection Date/Time:	07/Jul/14 14:40	Total Area	16046.501	

Used data files

Blank:	1: blank (24-6-2014 23:30:56)
RT Calibration:	2: rt (24-6-2014 21:49:53)
QA / RF Standard:	3: QA oil (24-6-2014 22:57:10)

General Results			Integration		
Total Chromatogram Area	16046.4		Integration Start:	1.248	min
Total Corrected Sample Area:	16026.9		Integration End:	21.597	min
Recovery	100.0	%			
Initial Boiling Point:	138.4	°C	Initial Elution Time:	1.248	min
Final Boiling Point (@ 99.5%)	466.9	°C	Final Elution Time:	18.198	min

Chromatogram



Boiling Point Distribution Table

%OFF	BP (°C)
0.5	138.4
5.0	185.1
10.0	208.7
15.0	226.6
20.0	238.9
25.0	253.4
30.0	265.5
35.0	277.5
40.0	288.3
45.0	301.2
50.0	311.8
55.0	321.8
60.0	332.3
65.0	343.9
70.0	354.6
75.0	365.2
80.0	376.1
85.0	388.3
90.0	401.6
95.0	420.0
99.5	466.9

Correlation Results

Model:	D86
%OFF	BP (°C)
IBP	192.9
5.0	219.8
10.0	231.6
20.0	252.0
30.0	272.2
40.0	
50.0	307.1
60.0	
70.0	341.3
80.0	357.0
90.0	377.2
95.0	393.4
FBP	404.9
%vol @ 350°C	75.5

Flash point (°C):

D56 (Jet Fuel)	79.3
D93 (Diesel)	78.9
D3828 (Jet Fuel)	82.8

Cut Points

BP (°C)	%OFF
150.0	1.0
200.0	8.1
250.0	23.4
300.0	44.2

	mass %
DIN 51581 (Noack)	Not valid
	mass %
ASTM D6417(MOV)	77.5

Figure 4: sample report

SimDist calculation pack V1.4

QA System Check Report

Injection Name:	QA oil
Vial Number:	3
Injection Type:	Check Standard
Sequence:	# Data G.A.S.SimDist pack ASTM D2887
Instrument Method:	ASTM2887
Processing Method:	Analysis
Injection Date/Time:	41814.95637
Injection Name:	QA oil

Used data files

Blank:	1: blank (24-6-2014 22:23:18)
RT Calibration:	2: rt (24-6-2014 21:49:53)
QA / RF Standard:	3: QA oil (24-6-2014 22:57:10)

General Results

Reference Check PASSED

Boiling Point Table:

Reference material: Ref D2887

%OFF	Expected BP	Allowable Diff	Boiling Point	Difference	Pass/Fail
0.5	115	7.6	114.8	0.2	Pass
5	151	3.8	151.1	0.1	Pass
10	176	4.1	178.1	2.1	Pass
15	201	4.5	204.2	3.2	Pass
20	224	4.9	227.7	3.7	Pass
25	243	4.9	246.7	3.7	Pass
30	259	4.7	262.7	3.7	Pass
35	275	4.7	278.1	3.1	Pass
40	289	4.3	291.8	2.8	Pass
45	302	4.3	302.3	0.3	Pass
50	312	4.3	313.2	1.2	Pass
55	321	4.3	322.1	1.1	Pass
60	332	4.3	331.3	0.7	Pass
65	343	4.3	342.8	0.2	Pass
70	354	4.3	353.6	0.4	Pass
75	365	4.3	365.7	0.7	Pass
80	378	4.3	378.5	0.5	Pass
85	391	4.3	391.8	0.8	Pass
90	407	4.3	409.1	2.1	Pass
95	428	5	432.1	4.1	Pass
99.5	475	11.8	484.9	9.9	Pass

Figure 5: Quality Control Report

SPECIFICATIONS

Configuration: 1 or 2 channel instrument based on Thermo GC Trace 1300, with InstantConnect SSL , PTV or Cold-On-Column injector module and InstantConnect FID detector module,
Triplus RSH or AS/AI-1310 liquid autosamplers,

Optional: Cryogenic oven cooling (liquid N_2 or liquid CO_2)

Application: Custom configured analyser for light hydrocarbon products up to crude oil, lube oil and residual samples
Simdist analyser tuned for applications according to the standardised methods.

Sample requirements: Neat or dissolved in CS_2.
(safety issue: CS_2 is extremely flammable and toxic).

Analysis time: Depending on method

Software G·A·S Simdist Calculator for Chromeleon/ EZChrom/ OpenLab
Simdist/DHA MERGE of ASTM D7169/ IP545 data according to ASTM D7900

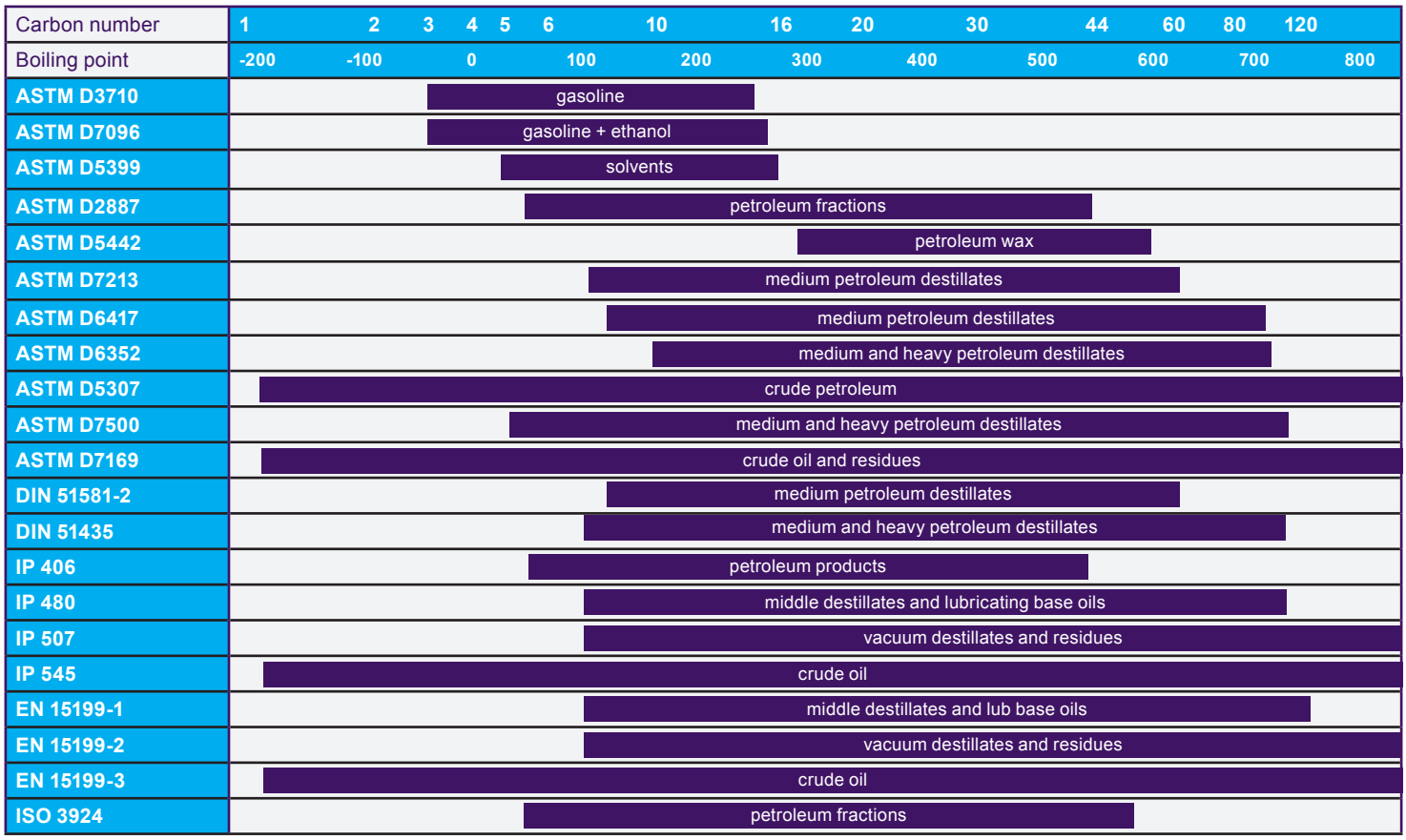


Figure 7: Available standardised methods with boiling point and application range

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